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**DOCUMENTING GROUND-WATER MODELING  
AT SITES CONTAMINATED  
WITH RADIOACTIVE SUBSTANCES**

A Cooperative Effort By

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## FOREWORD

This report is the product of the Interagency Environmental Pathway Modeling Working Group. The working group includes representatives of the U.S. Environmental Protection Agency's Office of Radiation and Indoor Air and Office of Solid Waste and Emergency Response, the U.S. Department of Energy's Office of Environmental Restoration, and the U.S. Nuclear Regulatory Commission's Office of Nuclear Material Safety and Safeguards. The purpose of the Working Group is to promote the appropriate and consistent use of mathematical models in the remediation and restoration process at sites containing—or contaminated with—radioactive and/or mixed waste materials. This report demonstrates a thorough approach to documenting model applications in a consistent manner and is intended to assist technical staff responsible for identifying and implementing flow and transport models in support of cleanup decisions at radioactive and hazardous waste sites. It is hoped that adoption of the tenets in the report will enhance the understanding between modelers and their managers of what may be expected in model documentation; facilitate the peer-review process by ensuring that modeling documentation is complete; ensure the institutional memory is preserved; and institute greater consistency among modeling reports.

This document is one of several the working group is developing to bring a uniform approach to solving environmental modeling problems common to all federal agencies. The interagency working group has also prepared the following reports:

- Computer Models Used to Support Cleanup Decision-Making at Hazardous and Radioactive Waste Sites, EPA 402-R-93-005, March 1993.
- Environmental Characteristics of EPA, NRC, and DOE Sites Contaminated with Radioactive Substances, EPA 402-R-93-011, March 1993.
- Environmental Pathway Models—Ground Water Modeling in Support of Remedial Decision-Making at Sites Contaminated with Radioactive Material, EPA 402-R-93-009, March 1993.
- A Technical Guide to Ground Water Model Selection at Sites Contaminated with Radioactive Substances, EPA 402-R-94-012, June 1994.

The Project Officers of the Interagency Working Group (Beverly Irla—EPA, Paul Bean—DOE, Sam Nalluswami—NRC) acknowledge the cooperation and insight of many staffers in preparing this document from organizations including EPA Regions 2, 3, 4, 5, 6, and 8; EPA Office of Emergency and Remedial Response; EPA Office of Underground Storage Tanks; EPA Robert S. Kerr Environmental Research Center; EPA Office of Radiation Programs/Las Vegas; EPA National Air and Radiation Environmental Laboratory; EPA Office of Radiation and Indoor Air Criteria and Standards Division; DOE Office of Environmental Restoration; and NRC Office of Material Safety and Safeguards, who graciously agreed to provide review and comment. We also thank their managers who permitted them the time to provide us with valuable input.

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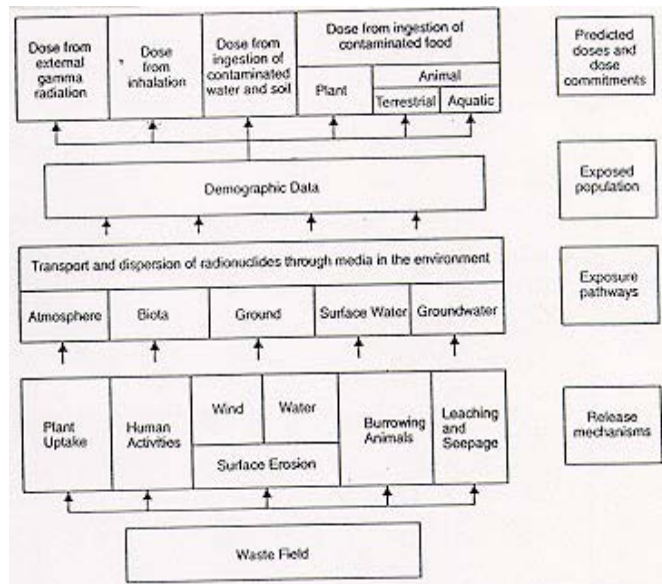
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## EXECUTIVE SUMMARY

This joint EPA/DOE/NRC program is concerned with the selection and use of mathematical models that simulate environmental behavior and the impacts of radionuclides via all potential pathways of exposure, including the air, surface water, ground water, and terrestrial pathways. Figure ES-1 gives an overview of these various exposure pathways.

Though the joint program is concerned with all pathways, this report focuses on ground-water pathways. Ground-water pathways were selected for first consideration for several reasons. At many sites currently regulated by EPA and NRC or managed by DOE, the principal concern is the existence of, or potential for, contamination of the underlying aquifers. Compared to the contamination of air, surface water, and terrestrial pathways, ground-water contamination is more difficult to sample and monitor, resulting in greater dependence on models to predict the locations and levels of environmental contamination.

The types of models used to simulate the behavior of radionuclides in ground water are generally more complex than models for surface water and atmospheric pathway transport. The additional complexity is necessary to address the complexity and diversity of settings associated with different sites. The methods used to model ground water are not as standardized as the methods for surface water and air dispersion modeling, and there is considerably less guidance on appropriate methods for such modeling. The information presented in this report is consistent with recent standards on ground-water modeling published by the American Society for Testing and Materials (ASTM). ASTM is a private organization that publishes consensus standards for a variety of fields, including ground-water modeling. The ASTM Subcommittee D18.21 on Ground-Water and Vadose Zone Investigations has approved seven new standards related to ground-water modeling. These standards have been written in the form of guides (not rigid standards) and include the following publications:



**Figure ES-1. Exposure pathways**

- D-5447 Standard Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem
- D-5490 Standard Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information
- D-5609 Standard Guide for Defining Boundary Conditions in Ground-Water Modeling
- D-5610 Standard Guide for Defining Initial Conditions in Ground-Water Modeling
- D-5611 Standard Guide for Conducting a Sensitivity Analysis for a Ground-Water Flow Model Application
- D-5718 Standard Guide for Documenting a Ground-Water Flow Model Application
- D-5719 Standard Guide for Simulating Subsurface Air Flow using Ground-Water Flow Modeling Techniques

This report describes a process by which ground-water flow and transport modeling can be systematically reviewed during each phase of the remedial process. The phases include the initial scoping phase, the detailed characterization of the site, and the selection and implementation of remedial alternatives.

The proper application of the selected model(s) is as important, if not more important, than its selection. No matter how well a model is suited to a particular application, it could give erroneous and highly misleading results if used improperly or with incomplete or incorrect input data. Conversely, even a model with very limited capabilities, or a model used at a site which has not been well characterized, can give very useful results if applied properly with a full appreciation of the limitations of both the model and the input data. This report describes the methods for applying ground-water flow and transport models to sites contaminated with radioactive materials. The model application process is described in terms of the objectives, data availability, and

various site characteristics and processes requiring modeling.

A review by EPA of 20 site-specific modeling studies (LEE95) cited modeling mistakes in all aspects of the modeling process including: (1) misunderstanding of the selected model, (2) improper application of boundary conditions and or initial conditions, (3) misconceptualization, (4) improper or unjustifiable estimation of input data, (5) lack of or improper calibration/verification, (6) omission of or insufficient sensitivity/uncertainty analysis, and (7) misinterpretation of simulation results. Any of these errors can lead to the use of faulty assumptions as the basis for remedial and risk decisions.

This model review guide is designed to provide, at a minimum, a means to determine whether proper modeling protocol has been followed. In some cases, the guide provides sufficient information to ensure that common modeling pitfalls are avoided. For example, one of the errors indicated by LEE95 was that, in at least one of the investigations, ground-water extraction well(s) had been placed too close to the model boundary, which resulted in an underestimation of the ground-water capture zones predicted for these wells. The section of this guide dedicated to model construction discusses the correct placement of wells relative to model boundaries and provides a simple means for determining if the well has been placed too close to the boundary.

However, the goal of this review guide is not to detail exactly how ground-water modeling is performed. Instead, the intention is to provide a means to ensure that all modeling reports are properly documented and provide sufficient detail to allow a comprehensive peer review.

A checklist containing the major review steps is presented. With this checklist, the analyst for a specific project can identify potential problem areas in applying and documenting the model activities. The major steps in evaluating the model are listed in Table ES-1. The first step is to identify the objectives of the modeling study. Do



the objectives correspond to the project's objectives?

The second step is to examine in detail the site characterization data provided by the modeler. Are there sufficient data to characterize the site? Are there sufficient data to match its history? Were aquifer tests and tracer tests performed? If so, how were they analyzed? Does the distribution of wells give a sufficient vertical as well as horizontal picture? Are the wells deep enough to delineate the greatest depths to which contaminants are expected to migrate? Do the data provide information on the soil profile as well as the water levels?

The next step is to review the conceptual approach used by the modeler to represent the ground-water flow and contaminant transport processes occurring at the site. Here, the modeler should attempt to identify and list the key assumptions used in developing the conceptual ground-water flow and transport models. The justifications for the individual assumptions should be carefully examined, in conjunction with a general review of field information or data on site characterization provided by the modeler. The key objective of the examination should be to determine if the modeler's conceptual approach is consistent with the field data and the objectives. Specific questions that should be addressed include:

- Can a steady flow system be assumed, or must transient flow conditions be considered?
- What transport processes are important?
- Which of these processes are not considered in the conceptual model?
- What are the features of site characterization that support or repudiate the conceptual modeling assumptions?
- Can two-dimensional horizontal flow be assumed or must three-dimensional flow conditions be considered?

Assuming the conceptual approach is appropriate, the reviewer should then examine the methodology selected by the modeler to solve the flow and transport problems. The objective at this stage is to identify the particular analytical or numerical model used by the modeler and determine if it can reliably predict solutions to the ground-water flow and transport problems identified during the conceptual stage. Specific questions that should be addressed include:

- Can the model treat all of the important components or features identified in the conceptual model?
- Does the model provide the type of results that are necessary to satisfy the objectives set forth at the beginning of the study?
- If a series of flow and transport models are selected, how do they fit together?
- Is the computer code well-documented and has it received thorough testing?

If a numerical model is used in obtaining the solution, the following question pertaining to spatial and temporal approximations also should be asked:

- Are the grids and time increments selected for the flow and transport simulations sufficiently refined to give results of acceptable accuracy?
- Are the grids free of numerical instability caused by rapid changes in grid spacing or time step size?

Next, the critical input parameters and boundaries of the model should be identified and the rationale for selecting the parameter values and boundary conditions assessed. Are the parameter values based on site-specific data or on previous studies? What data support the selected boundary conditions? It is the modeler's responsibility to insure that this result is consistent with field evidence. Specific questions may include:

- Are the boundary conditions consistent with the conceptual model and with natural hydrologic boundaries? (Watch for arbitrary boundaries, such as geographic boundaries)
- Will the selected boundaries influence model predictive simulations because they are too close to the area of interest?
- Are the parameter values consistent with the conceptual model and within the range of reported or measured values?
- Are the parameter values assigned in a patchwork pattern? (A common problem is that parameters are adjusted on a block-by-block basis to achieve a good calibration without regard for geologic evidence)

If the model is calibrated to the field data, the comparison of the observed and simulated results should be examined. History matching or model calibration refines estimates of hydrologic parameters and boundary conditions by comparing the model results with observed data. Estimates of parameters are changed to improve the comparison. It is important to constrain the changes so that physically realistic parameters are specified; this generally requires an experienced ground-water hydrologist. The history matching procedure can be done either by a trial and error or by automatic regression. No matter which approach is selected, sensitivity analysis will be part of the matching phase. If the model is not calibrated, clear justification should be provided. Specific areas to evaluate in model calibration include:

- Have calibration criteria been established and have these criteria been met by the calibration?
- Are calibration errors (differences between measured and computed heads/concentrations) spatially biased? (e.g., too high in one area of the model and too low in another)
- Were model parameters varied beyond a

reasonable range in order to achieve the calibration goals?

- Does the model report discuss the rationale for selection of the final calibrated model parameters?

In the final phase of the study, the future behavior of the system is predicted. Generally, this is the shortest part of a study. Predictions are based on the results using the best estimate of the system's parameters obtained by history matching. Because the set of parameters is not unique, it is important to assess the uncertainty in the predicted results, which is usually accomplished by using a sensitivity analysis. The model's predictive results and the sensitivity analysis should be examined to determine if sufficient conservatism has been made in the simulation. Any numerical error that may have been introduced as a result of inappropriate solution techniques or poor choice of grid spacing and time increment should be assessed carefully.

Finally, the validity of the modeler's conclusions should be reviewed. Do these conclusions satisfy the original objectives? The modeler should trace back each conclusion to ensure that the conclusion is valid and follows from supporting documentation. Is there sufficient information to allow the modeling study to be reproduced?

It is the reviewer's responsibility to review data and modeling results. It is critical that the reviewer has sufficient experience to interpret data and assess the conceptualization as well as to evaluate the results.

**Table ES-1. Major Steps in Modeling Evaluation Procedures**

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
<b>CHAPTER 2 OBJECTIVES AND DATA REQUIREMENTS</b>			
<i>Are the purpose and scope outlined?</i>			
<i>Are the objectives consistent with decision-making needs?</i>			
<i>Are the objectives satisfactory?</i>			
<i>Are a site description and waste disposal history provided?</i>			
<i>Are the data requirements for the proposed modeling outlined?</i>			
<i>Are the sources of data adequately presented?</i>			
<i>Are data uncertainties discussed?</i>			
<i>Is the probable sensitivity of the future modeling results presented for the data?</i>			
<i>Are the potential data limitations and weaknesses provided?</i>			
<i>Are the plans to resolve data limitations discussed?</i>			
<b>CHAPTER 3 CONCEPTUAL MODEL DEVELOPMENT</b>			
<i>Is the physical framework discussed in detail? Both regional and local?</i>			
<i>Is the hydrogeologic framework described in detail? Both regional and local?</i>			
<i>Is the nature of the contaminant source term described?</i>			
<i>Are the hydraulic boundaries described in detail?</i>			
<i>Are data base deficiencies clearly identified and modeling implications discussed?</i>			
<i>Is the conceptual model consistent with the field data?</i>			
<i>Are the uncertainties inherent in the conceptual model discussed?</i>			
<i>Are the simplifying assumptions outlined?</i>			
<i>Are the assumptions justified?</i>			
<i>Are the natural boundaries or the aquifer system described?</i>			
<i>Are the following figures and/or tables<sup>1</sup> included:</i>			
<ul style="list-style-type: none"> <li>• Map showing location of study area.</li> </ul>			
<ul style="list-style-type: none"> <li>• Geologic map and cross sections indicating the areal and vertical extent of the system.</li> </ul>			

In some instances tabular representation of the data may be appropriate.

**Table ES-1 (Continued)**

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
• Topographic map with the surface water bodies.			
• Contour maps showing the tops and/or bottoms of the aquifers and confining units.			
• Isopach maps of hydrostratigraphic units.			
• Maps showing extent and thicknesses of stream and lake sediments.			
• Maps indicating discrete features (e.g., faults), if present.			
• Maps and cross sections showing the unsaturated zone properties (e.g., thickness, $K_{sat}$ ).			
• Potentiometric surface maps of aquifer(s) and hydraulic boundaries.			
• Maps and cross sections showing storage properties of the aquifers and confining units. <sup>1</sup>			
• Maps and cross sections showing hydraulic conductivity of the aquifers, confining units and stream and lake sediments.			
• Maps and hydrographs of water-budget information.			
• Maps and cross sections indicating transport parameters (e.g., $K_d$ ). <sup>1</sup>			
• Areal and cross sectional isoconcentration maps of primary contaminants in soil and ground water.			
• Time-series graphs of contaminant concentrations.			
• Relevant source-term inventory information.			
<b>CHAPTER 4 MODEL APPLICATION</b>			
<b>Section</b>			
(4.1) SCOPING ANALYSIS			
<i>Are scoping analyses performed?</i>			
<i>Do scoping results lead to proposed modeling approach?</i>			
(4.2) SITE CHARACTERIZATION MODELING			
(4.2.1) Code Selection			
<i>Is the rationale for the selection clearly presented for proposed code(s)?</i>			
<i>Are the general features of the code(s) presented?</i>			
<i>Are the assumptions and limitations of the code(s) presented and compared to the conceptual model?</i>			
<i>Is the basis for regulatory acceptance presented?</i>			
<i>Is the source documentation for the code included?</i>			
<i>Is an executable version of the code included?</i>			

**Table ES-1 (Continued)**

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
<i>Is the source code readily available for inspection?</i>			
<i>Does the code have a history of use?</i>			
<i>Is the code well documented?</i>			
<i>Is the code adequately tested?</i>			
<i>Are the hardware requirements compatible with those available?</i>			
(4.2.2) Model Construction			
(4.2.2.1) Layering and Gridding:			
<i>Is the domain of the grid large enough so that the boundaries will not interfere with the results?</i>			
<i>Do the nodes fall near pumping centers on existing and potential future wells and along the boundaries?</i>			
<i>Is the grid oriented along the principal axes of hydraulic conductivity?</i>			
<i>Is the grid discretized at the scale appropriate for the problem?</i>			
<i>Are areas of sharp contrasts (e.g., hydraulic conductivity, concentration, gradient) more finely discretized?</i>			
<i>Is the Peclet number less than 2?</i>			
<i>Do adjacent elements vary in size by a distance less than a factor of 1.5?</i>			
<i>Are strong vertical gradients within a single aquifer accommodated by multiple planes or layers of nodes?</i>			
<i>If matrix diffusion is important, are the confining units adequately discretized in the relevant regions of the model?</i>			
<i>Is the grid more finely spaced along the longitudinal direction of simulated contaminant plumes?</i>			
<i>Is the aspect ratio less than 100:1?</i>			
<i>Are the following figures included:</i>			
<ul style="list-style-type: none"> <li>• Grid presented as an overlay of a map of the area to be modeled.</li> </ul>			
<ul style="list-style-type: none"> <li>• A vertical cross section(s) which displays the vertical layering of the model grid.</li> </ul>			
(4.2.2.2) Boundary and Initial Conditions			
<i>Is justification provided for the selection of all boundary and initial conditions?</i>			
<i>Are model boundaries consistent with natural hydrologic features?</i>			
<i>Are the boundary and initial conditions consistent with the conceptual model?</i>			

**Table ES-1 (Continued)**

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
<i>Are the uncertainties associated with the boundaries and initial conditions addressed?</i>			
<i>Are the boundaries far enough away from any pumping/injection centered to prevent "boundary effects"?</i>			
<i>Are transient boundaries discussed?</i>			
<i>Is the rationale given for simplifying the boundaries from the conceptual model discussed?</i>			
<i>Are the values for the assigned boundaries presented?</i>			
(4.2.2.3) Specification of Time Steps			
<i>Is the Courant criterion satisfied?</i>			
(4.2.2.4) Model Parameterization			
<i>Are data input requirements fully described?</i>			
<i>Is the discussion of the data well founded with respect to Objectives and Data Review Section?</i>			
<i>Are the interpretation and extrapolation methods (e.g., Kriging) adequately presented?</i>			
<i>Do the figures and tables completely describe the data input with respect to discrete components of the model?</i>			
<i>Are the model parameters within the range of reported or measured values?</i>			
(4.2.3) MODEL CALIBRATION			
<i>Has calibration been attempted?</i>			
<i>Is the rationale for model calibration approach presented?</i>			
<i>Are the calibration procedures described in detail?</i>			
<i>Are the calibration criteria presented?</i>			
<i>Does the calibration satisfactorily meet specified criteria?</i>			
<i>Is the rationale presented for selecting convergence criteria?</i>			
<i>Are code convergences and numerical instabilities discussed?</i>			
<i>Do the calibrated parameters fall within their expected ranges?</i>			
<i>Are discrepancies explained?</i>			
<i>Has the calibration been tested against actual field data?</i>			
<i>Are the differences between steady-state and transient calibrations presented?</i>			
<i>Could other sets or parameters have calibrated the code just as well? Is this discussed?</i>			

**Table ES-1 (Continued)**

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
<i>Are areal and cross-sectional representations of the final calibrated results included for both hydraulic heads and radionuclide plume(s)?</i>			
<i>Does calibration of the model take into account the inconsistency between point measurements at wells and areal averages of model output?</i>			
<i>Is the match between the calibration targets and final parameters shown diagrammatically?</i>			
<i>Were calibrating errors presented quantitatively through the use of descriptive statistics?</i>			
<i>If particle-tracking was performed, are these results shown?</i>			
<i>Is the calibrated model consistent with the conceptual model?</i>			
<i>Are any changes to the conceptual model discussed and justified?</i>			
<i>Is non-uniform areal recharge applied? Is this approach justified?</i>			
<i>Does the calibration properly account for vertical gradients?</i>			
<i>Is the calibrated hydraulic conductivity field consistent with the geologic logs and aquifer stress tests?</i>			
<i>Are the convergence criteria appropriate?</i>			
<i>Was a mass balance performed?</i>			
<i>Is the water-balance error less than 1%?</i>			
<i>Are the mass balance results for the calibrated model discussed?</i>			
<i>Is the model's water balance consistent with known flows of rivers and levels of lakes?</i>			

**Table ES-1 (Continued)**

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
<b>(4.2.4) SENSITIVITY ANALYSES</b>			
<i>Was a sensitivity analysis performed?</i>			
<i>Is the approach to the sensitivity analysis detailed?</i>			
<i>Were all input parameters selected for investigation? If not, was rationale presented for excluding parameters?</i>			
<i>Was a sensitivity analysis performed on the boundary conditions?</i>			
<i>Are the ranges of parameters appropriate?</i>			
<i>Were sufficient simulations performed? Was justification provided?</i>			
<i>Was the relevance of the sensitivity analysis results to the overall project objectives discussed?</i>			
<i>Are the results presented so that they are easy to interpret?</i>			
<i>Were sensitivity analyses performed for both the calibration and the predictive simulations?</i>			



# CHAPTER 1 —INTRODUCTION

## 1.1 Purpose of This Manual

A review by EPA of 20 site-specific modeling studies (LEE 95) cited modeling mistakes in all aspects of the modeling process including: (1) misunderstanding of the selected model, (2) improper application of boundary conditions and or initial conditions, (3) misconceptualization, (4) improper or unjustifiable estimation of input data, (5) lack of or improper calibration/verification, (6) omission of or insufficient sensitivity/uncertainty analysis, and (7) misinterpretation of simulation results. All of these errors could lead to the use of faulty assumptions as the basis for remedial and risk decisions.

This manual is designed to provide, at a minimum, a means to determine whether proper modeling protocol has been followed. In some cases, the guide provides sufficient information to ensure that common modeling pitfalls are avoided. Specific goals of this manual include:

- Enhance understanding between managers and modelers of what is expected in terms of modeling documentation.
- Facilitate the peer review process by ensuring that the modeling documentation is complete.
- Ensure that institutional memory is created and/or utilized.
- Institute greater consistency among modeling reports.

It is not the goal of this manual to detail exactly how ground-water modeling is performed. Instead, it is intended to provide a means to ensure that all modeling reports can be properly documented and provide sufficient detail to allow a comprehensive peer review. Furthermore, this document is not intended to be used as a sole reference for reviewing modeling application studies. Rather it is intended to be used along with other published general references (e.g., EPA87, 88a, 88b, 94a, 94b, 94c, 94d, ASTM93, 94, 95).

## 1.2 How to Use This Manual

This manual has been designed to provide a basic understanding of modeling terminology, modeling approaches, and documentation requirements to facilitate the peer review process. The content's of its five chapters and three appendices are outlined below.

## Chapter 2 — Modeling Objectives and Data Review

The goal of Chapter 2 is to illustrate the connection between the modeling objectives and data requirements for each phase in the remedial process. Specifically, it should allow the reviewer to ensure that the modeling report identifies:

- the data needed for modeling.
- the origins of data.
- how the data will be used to meet modeling objectives.

## Chapter 3 — Conceptual Model Development

This chapter is designed to ensure that the reviewer has sufficient information to assess the adequacy of the conceptual model presented in the modeling report.

## Chapter 4 — Model Application

This chapter discusses model application in each phase of the remedial process (i.e., scoping, site characterization, remedial selection and design).

Before designing the field investigation, it is advisable, that at a minimum, a series of scoping calculations be made to assess the potential importance of the ground-water pathway. The scoping section in Chapter 4 is closely linked to calculational methods presented in Appendix B and is intended to provide a means for making preliminary estimates of the rate of contaminant migration and the expected down-gradient contaminant concentrations using a calculator. General equations, data requirements, and example problems are given. An integral part of the discussion is a description of the dominant physical and chemical processes that may affect the fate and transport of radionuclides. A basic understanding of these processes will give a general appreciation of the complexity of the controlling processes, and of the limitations inherent in the scoping calculations.

Application of the model during the site characterization and remedial phases generally is fairly sophisticated and typically will be undertaken by experienced modelers. Therefore, these sections emphasize the overall modeling approach and methods that can be used as simple reality checks on modeling performed by others. Guidelines are given as to which information should be requested to facilitate a peer review.

## Chapter 5 — Report Presentation Guidelines

This chapter summarizes the previously presented guidelines for the presentation of reports and provides a step-by-step checklist to facilitate the review of the modeling activities.

### Appendix A - Fate and Transport of Radionuclides

This appendix consists of a discussion of ground-water flow and physical and chemical transport processes that affect the mobility of radionuclides in ground water.

### Appendix B - Scoping Analysis Procedures

This appendix discusses in detail a series of screening calculations that can be used to estimate radionuclide transit times and concentrations.

### Appendix C - Default Parameter Values

Typical values of parameters that are frequently used in modeling studies are presented.

## 1.3 Key Terms

The key terms and concepts that are fundamental to understanding this report are explained below.

*Conceptual Model.* The conceptual model of a site is a flow diagram, sketch, and/or a description of a site and its setting. The conceptual model describes the subsurface physical system including the nature, properties, and variability of the aquifer system (e.g., aquifers, confining units), and also the types of contaminants or wastes at a site, where they are located, and how they are being transported off site by runoff, percolation into the ground and transport in ground water, or suspension or volatilization into the air and transport by the prevailing meteorological conditions. The conceptual model also attempts to visualize the direction and path followed by the contaminants, the actual or potential locations of the receptors, and the ways in which receptors may be exposed, such as direct contact with the source, ingestion of contaminated food or water, or inhalation of airborne contaminants.

As information about a site accumulates, the conceptual model is continually revised and refined, in order to consolidate site and regional hydrogeologic and hydrologic data into a set of assumptions and concepts that can be evaluated quantitatively. More specifically, the conceptual model identifies and describes important aspects of the physical hydrogeologic system or subsystem for a given purpose. At a minimum, the system conceptualization should include: the geologic

and hydrologic framework, media type (e.g., fractured or porous), the nature of relevant physical and chemical processes, time dependence, dimensionality of the system, initial and boundary conditions, hydraulic properties, and sources and sinks (water budget). The conceptual model should not only be consistent with the physical system but also must be internally consistent. Each of the components typical of the hydrogeological conceptual model is briefly discussed below.

*Geologic framework.* The geologic framework is the distribution and configuration of the transmissive (e.g., sands and gravels) and nontransmissive (e.g., clay) geologic units. Of primary interest are the thickness, continuity, lithology, and geologic structure of those units relevant to the study.

*Hydrologic framework.* The hydrologic framework in the conceptual model includes the physical extent of the flow system, hydrologic features that affect or control the ground-water flow system, analysis of ground-water flow directions, and media type. The conceptual model must address the degree to which the system behaves as a porous media. If the system is significantly fractured or solution channeled, the conceptual model must address these issues.

*Hydraulic properties.* The hydraulic properties include the transmissive and storage characteristics of the geologic units (aquifers) and properties of the fluids. Specific examples of aquifer and fluid properties include transmissivity, hydraulic conductivity, storativity, fluid viscosity, and densities.

*Sources and sinks.* Sources and/or sinks of water and/or gas affect the pattern and rate of flow and therefore will affect the transport of radionuclides from the source. The most common examples of sources and sinks include pumping or injection wells, infiltration, evapotranspiration, drains, and flow from surface water bodies.

*Boundary and initial conditions.* Boundary conditions are the conditions the modeler specifies, typically on the perimeter of the model domain, as known or estimated flux, head, or concentration values in order to solve for the unknowns in the problem domain. These values may be associated with either the ground-water flow or the contaminant transport aspects of the problem. Ground-water boundaries may be described in terms of where water and/or radionuclides are flowing into or out of the ground-water system. Many different types of boundaries exist, including surface water bodies, ground-water divides, rainfall, wells, and geologic features such as faults and sharp contrasts in lithology. These real-world boundaries must be

translated into their mathematical counterparts which include fixed-head or concentration, constant flux, or head-dependent flux. The most common contaminant-source type boundaries either specify the source concentration or prescribe the mass flux of contamination entering the system. Initial conditions are defined as values of ground-water elevation, pressure, flow volumes, or contaminant concentrations which are initially assigned to interior areas of the modeled regions at the start of the simulation.

*Transport processes.* Various mechanical and geochemical processes affect the transport of radionuclides by flow through either a porous matrix or a fracture system in a porous matrix. The dominant mechanical processes are advection, dispersion (hydrodynamic dispersion, channeling) and diffusion. The chemical processes potentially affecting radionuclide transport include radioactive decay, adsorption on mineral surfaces (both internal and external to the crystal structure), speciation, precipitation, colloidal transport, radiolysis, biofixation, natural organic matter interactions, anion exclusion, and complexation.

*Spatial dimensionality.* Ground-water flow and contaminant transport are seldom constrained to one or two dimensions. However, in some instances, it may be appropriate to restrict the analysis to one or two dimensions. The particular number of dimensions should be chosen based on the modeling objectives and the availability of field and/or laboratory data.

*Temporal dimensionality.* Either steady-state or transient flow simulations can be performed. At steady-state, it is assumed that the flow field remains constant with time, whereas a transient system changes with time. Steady-state simulations produce average or long-term results and generally require that a true equilibrium case be physically possible. Transient analyses are typically performed when boundary conditions vary through time or when study objectives require answers at more than one time. It is also possible to mix temporally dimensionality in a modeling study. A common technique is to use a steady-state flow model and a transient transport model.

A conceptual model describes the present condition of the system. To predict future behavior, it is necessary to develop a dynamic model, such as physical scale models, analog models, or mathematical models. Laboratory sand tanks are physical scale models that simulate ground-water flow directly. The flow of ground water can also be implied using electrical analog models. Mathematical models, including analytical and numerical methods, which are discussed

below, are more widely used because they are easier to develop and manipulate.

*Model application.* The model application is the process of choosing and applying the appropriate software algorithm, or other analysis techniques, capable of simulating the characteristics of the physical hydrogeologic system, as identified in the conceptual model. To enhance understanding and facilitate implementation of the model application criteria developed in this report, the evolution of the computer model is traced from the inception of the conceptual model, its progression through to the mathematical model, and finally to the development of the computer code where computer instructions for performing the operations that are specified in the mathematical model are programmed.

*Mathematical Model.* A mathematical model is essentially a mathematical representation of a process or system conceptual model. For example, the mathematical model for ground-water flow is derived by applying principles of mass conservation (resulting in the continuity equation) and conservation of momentum (resulting in the equation of motion). The generally applicable equation of motion in ground-water flow is Darcy's Law for laminar flow, which originated in the mid-nineteenth century as an empirical relationship. Later, a mechanistic approach related this equation to the basic laws of fluid dynamics. In order to solve the flow equation, both initial and boundary conditions are necessary.

*Solution Methodology.* Solution methodology refers to the strategy and techniques used to solve a set of mathematical equations. In ground-water modeling, the equations are normally solved for head (water elevations in the subsurface) and/or contaminant concentrations.

Mathematical methods developed to solve the ground-water flow and transport equations can be broadly classified as either deterministic or stochastic. Deterministic methods assume that a system or process operates such that the occurrence of a given set of events leads to a uniquely definable outcome, while stochastic methods presuppose the outcome to be uncertain and are structured to account for this uncertainty.

Most stochastic methods are not completely stochastic in that they often utilize a deterministic representation of soil processes and derive their stochastic nature from their representation of inputs and/or spatial variation of soil characteristics and resulting chemical movement. While the deterministic approach results in a specific

value of a soil variable (e.g., solute concentration) at pre-specified points in the domain, the stochastic approach provides the probability (within a level of confidence) of a specific value occurring at any point.

The development of stochastic methods for solving ground-water flow is a relatively recent endeavor. It occurred as a result of the growing awareness of the importance of the intrinsic variability of the hydrogeologic environment and the fact that the variability cannot be fully characterized. Stochastic methods are still primarily research tools; however, as computer speeds continue to increase, the use of stochastic methods will spread from the research community into mainstream management applications. This discussion focuses primarily on deterministic methods, due to their more widespread use.

*Deterministic Methods.* Deterministic methods may either be broadly classified as either analytical or numerical. Analytical methods usually involve approximate or exact solutions to simplified forms of the differential equations for water movement and solute transport. Simple analytical methods are based on the solution of applicable differential equations which make a simplified idealization of the field and give qualitative estimates of the extent of contaminant transport. Such methods are simpler to use than numerical methods and can generally be solved with the aid of a calculator, although computers are also used. Analytical methods are restricted to simplified representations of the physical situations and generally require only limited site-specific input data. They are useful for screening sites and scoping the problem to determine data needs or the applicability of more detailed sophisticated methods.

Analytical methods are used in ground-water investigations to solve many different kinds of problems. For example, aquifer parameters (e.g., transmissivity, storativity) are obtained from aquifer tests through the use of analytical methods, and ground-water flow and contaminant transport rates can also be estimated by analytical methods.

Analytical methods that solve ground-water flow and contaminant transport equations in porous media are comparatively easy to use. However, because the governing equations are relatively simple, analytical solutions are generally restricted either to radial flow problems or to cases where velocity is uniform over the area of interest. Except for some radial flow problems, almost all available analytical solutions are developed for systems having a uniform and steady flow. This means that the magnitude and direction of the velocity

throughout the system are uniform with respect to time and space, which requires the system to be homogeneous and isotropic with respect to the hydraulic conductivity.

Unfortunately, the equations of flow and continuity in the form of partial differential equations do not lend themselves easily to rigorous analytical solutions when boundaries are complex. Therefore, if a realistic expression for hydraulic head or concentration as a function of space cannot be written from the governing equations and boundary and initial conditions, then analytical methods are generally abandoned, and more sophisticated numerical methods are used to solve the set of equations.

Numerical methods provide solutions to the differential equations describing water movement and solute transport using approximate methods such as finite differences and finite elements. Numerical methods can account for complex geometry and heterogeneous media, as well as for dispersion, diffusion, and chemical retardation processes (e.g., sorption, precipitation, radioactive decay, ion exchange, degradation). These methods always require a digital computer, greater quantities of data than analytical modeling, and an experienced modeler.

A numerical model for ground-water flow consists of the mathematical framework for the solution of the material balance equations that govern laminar flow through porous media. These mass balance equations depend on physical constraints and constitutive relationships. The constraints simply state conditions that components of the mass balance equations must satisfy, whereas the constitutive relationships describe the dependence of parameters, in the mass balance equations, on other physical processes. Furthermore, the mass balance equations are composed of both spatial and temporal terms, both of which require discretization within the model domain. These terms describe the head or concentration in space and time. The numerical methods mentioned above (i.e., finite element and finite difference) are used as discretization methods for the spatial term, whereas finite-difference methods are generally used to discretize the temporal term.

The mass balance equations, physical constraints, and constitutive relationships lead to a series of equations that must be solved in space and time. The means by which the equations are discretized, linearized (e.g., Newton-Raphson), organized (i.e., matrix construction), and solved via either direct or iterative methods are all part of the numerical model.

Following the formulation of the numerical model, the computer program is developed. The program consists of the assembly of numerical techniques, bookkeeping, and control language that represents the model from acceptance of input data and instructions to delivery of output.

In summary, the conceptual model is an interpretation or working description of the characteristics and dynamics of a physical system. Model construction is the process of transforming the conceptual model into a simplified, mathematical description of the physical system, coded in computer programming language, together with a quantification of the simulated system (in the form of boundary and initial conditions, system and process parameters, and system stresses). An intermediate step in the model transformation process is the mathematical model which consists of two aspects: a process equation and a solution technique to solve the process equation. An analytical solution solves a very simple process equation analytically by hand calculations. An analytical model solves a more complex, but still relatively simple, process equation analytically with a computer program. A numerical model solves a simple or complex process equation numerically with a computer program. In the context of this document, mathematical model refers to all three solution techniques of a process equation. The complexity of the process equation dictates the solution technique required. The model formulation process concludes with the coding of the mathematical model into computer programming language for performing a specified set of operations.

#### 1.4 Conceptual Approach

One of the primary goals of mathematical modeling is to synthesize the conceptual model into mathematical expressions, which, in turn, are solved by selecting and applying an appropriate computer code. This section discusses how the different components of the conceptual model, in conjunction with the modeling objectives, influence the model selection and ultimately the model application.

The underlying premise of model application is that the various aspects of the conceptual model may be simulated in a variety of ways, but the selected approach must remain consistent with the objectives. That is, the physical system cannot be overly simplified to meet ambitious objectives, and less demanding objectives should not be addressed with highly sophisticated modeling approaches.

Table 1-1 presents an overview of how the overall approach to modeling a site differs as a function of the

stage of the remedial process. The most common code application mistakes are applying codes that are more sophisticated than are appropriate for the available data or the level of the result desired, and the application of a code that does not account for the flow and transport processes that dominate the system. For example, a question that often arises is: when should three-dimensional codes be used as opposed to two-dimensional or one-dimensional codes? Inclusion of the third dimension requires substantially more data than one- and two-dimensional codes. Similar questions involving underlying assumptions need to be considered in the selection of a modeling approach and the physical processes which are to be addressed. If the modeler is not practical, sophisticated approaches may be used too early in the problem analysis. In other instances, the complexity of the modeling is commensurate with the qualifications of the modeler. An inexperienced modeler may take an unacceptably simplistic approach. One should begin with the simplest code that will satisfy the objectives and progress toward the more sophisticated codes until the modeling objectives are achieved.

#### 1.5 Standardization in Ground-Water Modeling

On October 26, 1993, the Office of Management and Budget (OMB) issued a revised version of OMB Circular A-119, "Federal Participation in the Development and Use of Voluntary Standards." The revised circular encourages greater agency use of voluntary standards. It reaffirms the basic federal policy that voluntary standards should be given preference over nonmandatory government standards

unless the use of such voluntary standards would adversely affect performance or cost, reduce competition, or have significant disadvantages. Even before this circular was revised, the American Society for Testing and Materials (ASTM), U.S. EPA, the USGS, and the U.S. Navy entered into a cooperative agreement in 1988 (the Navy joined in 1990) to accelerate the development of voluntary consensus standards by ASTM. The cooperative agreement funds eleven task groups within ASTM's Subcommittee D18.21 on Ground-Water and Vadose Zone Investigations. Task Group 10 (D18.21.10) was formed to develop standards on subsurface fluid-flow modeling and has produced a total of seven standards to date, with numerous standards in draft form. The information presented in this report is consistent with these recent standards on ground-water modeling published by ASTM. These standards have been written in the form of guides (not rigid standards) and include the following publications:

- D-5447 Standard Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem
- D-5490 Standard Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information
- D-5609 Standard Guide for Defining Boundary Conditions in Ground-Water Modeling
- D-5610 Standard Guide for Defining Initial Conditions in Ground-Water Modeling
- D-5611 Standard Guide for Conducting a Sensitivity Analysis for a Ground-Water Flow Model Application
- D-5718 Standard Guide for Documenting a Ground-Water Flow Model Application
- D-5719 Standard Guide for Simulating Subsurface Air Flow using Ground-Water Flow Modeling Techniques

**Table 1-1. General Modeling Approach as a Function of Project Phase**

<b>Attributes</b>	<b>Scoping</b>	<b>Characterization</b>	<b>Remediation</b>
Accuracy	Conservative Approximations	Site-Specific Approximations	Remedial Action Specific
Temporal Representation of Flow and Transport Processes	Steady-State Flow and Transport Assumptions	Steady-State Flow/Transient Transport Assumptions	Transient Flow and Transport Assumptions
Dimensionality	1-Dimensional	1,2-Dimensional/ Quasi-3-Dimensional	Fully 3-Dimensional/ Quasi-3-Dimensional
Boundary and Initial Conditions	Uncomplicated Boundary and Uniform Initial Conditions	Nontransient Boundary and Nonuniform Initial Conditions	Transient Boundary and Nonuniform Initial Conditions
Assumptions Regarding Flow and Transport Processes	Simplified Flow and Transport Processes	Complex Flow and Transport Processes	Specialized Flow and Transport Processes
Lithology	Homogeneous/ Isotropic	Heterogeneous/ Anisotropic	Heterogeneous/ Anisotropic
Methodology	Analytical	Semi-Analytical/Numerical	Numerical
Data Requirements	Limited	Moderate	Extensive

## CHAPTER 2 —MODELING OBJECTIVES AND DATA REQUIREMENTS

Successful ground-water modeling must begin with an approach that is consistent not only with the site characteristics but also with the modeling objectives, which depend strongly on the stage of the remedial process (i.e., scoping vs. site characterization vs. the selection and implementation of a remedy).

The most common mistakes in applying models are in using models that are more sophisticated than are appropriate for the available data or the level of the result desired, and in using a model that does not accurately account for the flow and transport processes that dominate the system. The simplest model that will satisfy the objectives should be used first, progressing toward more sophisticated ones as understanding of the system improves and objectives change.

The remedial process is generally structured in a way that is consistent with this philosophy (i.e., as the investigation proceeds, additional data become available to support more sophisticated ground-water modeling). The data available in the early stage of remediation may limit the modeling to one or two dimensions. In certain cases, this may be sufficient to support decision-making. If the modeling objectives cannot be met in this manner, additional data will be needed to support more complex models. The selection of more complex models in the later phases often depends on the results obtained with simpler models during the early phases.

Generally, in the later phases of the investigation, enough data have been collected to meet more ambitious objectives through complex three-dimensional modeling. The necessary degree of sophistication of the modeling effort can be evaluated in terms of both site-related issues and objectives, as well as the qualities inherent in the computational methods available for solving ground-water flow and transport.

Modeling objectives for each stage of the remedial investigation must be very specific and well-defined early within each phase. All too often modeling is carried out without a clear rationale to meet the objectives, and only after modeling is completed are the weaknesses in the approach discovered.

The objectives must consider the decisions that the results are intended to support. The selected approach should not be driven by the availability of data, but by

the modeling objectives which should be defined in terms of what can be accomplished with the available data; also, the objectives should be reviewed and possibly revised during the modeling process. Furthermore, ground-water modeling should not be thought of as static or linear process, but rather one that can be continuously adapted to reflect changes in modeling objectives, data needs, and available data.

### 2.1 Scoping Phase

A large part of ground-water modeling in this early phase is understanding the decisions that need to be made and determining which of these, which can be assisted by using specific calculations when the data are limited and the controlling hydrogeologic processes at the site are not completely understood.

In the scoping phase, the objectives generally focus on establishing order-of-magnitude estimates of the extent of contamination and the probable maximum radionuclide concentrations at actual or potential receptor locations. At most sites, the migration rates and contaminant concentrations are influenced by several parameters and flow and transport processes that typically are not fully characterized in the early phase of the investigation. The parameters include recharge, hydraulic conductivity, effective porosity, hydraulic gradient, distribution coefficients, thicknesses of the aquifer and confining unit, and source concentrations. During this early phase, questions pertaining to flow and transport processes typically are limited to general considerations, such as whether flow and transport are controlled by porous media or fractures, and whether the wastes are undergoing transformations from one phase to another (e.g., liquid to gas).

At this point in the remedial program, one of the most useful analyses is to evaluate the potential effects of the controlling parameters on flow and transport. One objective of the early analyses is to assess the relationships among the parameters. How do changes in one parameter affect the others and the outcome of the modeling exercise? A better understanding of such interdependencies assists in properly focusing the site-characterization activities and ensuring that they are adequately scoped. Also, it is desirable to evaluate the effects that various processes have on flow and transport; however, this generally has to be deferred until additional information is obtained during site



characterization. Furthermore, some caution is needed: if simplistic assumptions have been made in the model, the results may not be valid (i.e., transferable) to a more refined model that incorporates more realistic or complex boundary conditions, initial conditions, or variations in parameters.

In general, the uncertainty associated with each of the parameters is expressed by a probability distribution, which yields a likely range of values for each parameter. At this early phase in the modeling process, it is important to use a modeling approach where values for individual parameters can be selected systematically from the probable range and easily substituted into the governing mathematical equations describe the dominant flow and transport processes at the site. In this manner, the effects that a single parameter, or a multitude of parameters, have on the rate of movement and concentrations of contaminants may be evaluated. This technique of substituting one value for another from within a range of values is called a sensitivity analysis. It is important to ensure that the range of individual values and combinations of parameters selected allow for a conservative analysis of the flow and transport processes.

In many cases, the potential range of values of important parameters is unknown or very large. Consequently, the analyst has little alternative but to evaluate the sensitivity of the results to a very broad range of possible values for the parameters. Many of these results will be unrealistic but cannot be ruled out until reliable site data are obtained during site characterization. These types of analyses are useful because they help to direct the field work. However, they also can be used incorrectly. For example, individuals not familiar with the scoping process could come reach grossly inappropriate conclusions about the potential public health impacts of the site based on these results. Accordingly, care must be taken to assure that the results of scoping analyses are used to support the decisions for which they were intended.

An alternative to a detailed sensitivity analysis is a conservative bounding approach. In this less demanding analysis, values are selected from the range of parameters to provide the highest probability that the results are conservative (i.e., that the contaminant migration rates and concentrations would not be underestimated). For example, high values of hydraulic conductivity combined with low effective porosities and low distribution coefficients would maximize the predicted migration rates of the contaminant, although the higher flow rates may dilute the concentrations predicted to reach the receptors.

Even though efforts are made to ensure a conservative analysis, natural as well as anthropogenic influences may adversely affect the migration of radionuclides. For instance, published distribution coefficients are frequently determined at neutral pH values. However, even values conservatively selected from the low range could be too high if acidic wastes were also discarded with the radioactive material. Burrowing animals and construction activities also have been responsible for moving radioactive wastes beyond the boundaries predicted by ground-water flow and transport models.

Other processes that could invalidate an otherwise conservative analysis include facilitative transport and discrete features, such as soil macropores. Facilitative transport is a term used to describe the mechanism by which radionuclides may couple with either naturally occurring material or other contaminants and move at much faster rates than would otherwise be predicted by their respective distribution coefficients. Furthermore, discrete features are rarely considered in early analyses, even though it is well known that some, such as soil macropores, can allow the movement of contaminants on the order of meters per year in the vadose zone. Such features can result in a gross underestimate of the time of arrival and concentration of contaminants downgradient. Nonetheless, the lack of site-specific data will generally preclude the mathematical modeling of anomalous flow and transport processes during the project's scoping phase. Therefore, it's possible that what normally would be considered conservative modeling results actually underestimate the velocities and concentrations of the contaminant. This possibility highlights the need to confirm the modeling results with site-specific field data, even when a conservative approach has been taken.

In the scoping phase, the data generally available have been collected over relatively short intervals. Therefore, modeling objectives would be limited to those which could be met without a detailed understanding of the temporal processes affecting flow and transport. For example, a typical analysis that may not require detailed knowledge of the temporal nature of recharge, source release rates, and other flow and transport mechanisms would be an estimate of the distance that radionuclides have traveled since the beginning of waste management activities. This analysis would use yearly average values for the input parameters, such as infiltration and source release rates. However, without accommodating the transience of these processes, predictions of peak concentrations of contaminants arriving at

downgradient receptors would be associated with a high degree of uncertainty.

Site-specific information is often limited in the scoping phase. Therefore, modeling during the early planning phase of most remedial investigations generally is designed to support relatively simple objectives that can be easily linked with more ambitious goals developed during later phases of the investigation. The iterative process of data collection, analysis, and decision-making itself dictates that the preliminary objectives must evolve to meet the needs of the overall program. That is, it would be unreasonable to assume that initial modeling based upon limited data would do little more than direct future activities.

## 2.2 Site Characterization

In the site characterization phase, the plans developed during the scoping phase are carried out. The collected field data are used to characterize more fully the nature and extent of the contamination at the site, to define environmental and demographic characteristics, and to support assessments of the actual or potential impacts. The results of the site characterization are analyzed to determine compliance with applicable regulations and to begin to define strategies for remediation.

The site characterization phase typically provides the first opportunity to gain a detailed understanding of the overall behavior of the system. This improved understanding leads to a refinement of the conceptual model and, in turn, allows more ambitious objectives to be entertained.

The primary reasons for ground-water modeling in the site characterization phase of the remedial process are to: (1) refine the existing conceptual model; (2) optimize the effectiveness of the site characterization program; (3) support the baseline risk assessment; and (4) provide preliminary input into the remedial approach. To accomplish these goals, it is generally necessary to apply relatively complex ground-water models to simulate flow and transport in the saturated zone and, in some instances, the unsaturated zone.

A properly designed site characterization program will expand the data base to address very specific, often demanding objectives. Consequently, the simplified modeling approaches undertaken in the scoping phase give way to more sophisticated means of evaluating the data, but also convey far more complications in developing the proper approach.

In many instances, several different approaches to modeling will be taken to accomplish these objectives. For example, the output of analytical modeling of the unsaturated zone, in the form of radionuclide concentrations at the interface between the saturated and unsaturated zone, may be used as input to numerical models of the saturated zone. Regardless of the phase of the remedial process, the simplest modeling approach that meets the objectives should be taken.

The site characterization program is the first time in the investigation that detailed flow and transport processes are identified and investigated. Before site characterization, the investigator could only evaluate the effects of various parameter values on flow and transport. In the scoping phase, the modeling focused on estimating the dominant parameters rather than on the effects that more complex chemical and physical flow mechanisms have on the fate and transport of contaminants. Examples of these mechanisms include fractures, time-dependence of physical and chemical processes, phase transformations, and changes in the geochemical environment.

It is important to gain an appreciation for the governing geochemical processes, as they may have a significant impact on the transport of radionuclides, and can be simulated indirectly in the analysis by assuming a specified retardation of the contaminant. Direct means (computer codes) for simulating geochemical processes are available; however, a detailed discussion of these methods is beyond the scope of this report.

As additional data are acquired during the site characterization program and the system boundary conditions and hydrogeology become better understood, the modeling approach becomes more involved. Without the data limitations that constrained the choice of methods in the scoping phase, the number of possible alternatives in the modeling approach increases dramatically.

## 2.3 Data Requirements

At most sites, the parameters that influence migration rates and concentration, flow, and transport processes of the contaminant would not have been fully characterized in the early phase of the investigation. These parameters are the basis upon which the early conceptual model is formulated, and include variables such as recharge, hydraulic conductivity, effective porosity, hydraulic gradient, distribution coefficients, aquifer thicknesses, and source concentrations. As the

site characterization proceeds additional data are obtained to support more advanced modeling. The following information is generally required to estimate the concentrations of contaminants released, although the precise data needs will depend on the modeling objectives:

#### Release Concentration

1. Curies of radionuclide(s)
2. Water solubility of radionuclide(s) (optional)
3. Half-life of the radionuclide
4. Distribution coefficient(s) of radionuclide(s)
5. Saturated hydraulic conductivities of soil
6. Source dimensions
7. Soil bulk densities
8. Total porosities
9. Volumetric water content(s)
10. Infiltration rates
11. Soil-specific moisture-release curve

#### Volumetric Release Rate

1. Percolation rate (evapotranspiration, precipitation, runoff)
2. Area of contributing source
3. Water solubility of radionuclide(s)
4. Hydraulic conductivities
5. Hydraulic gradient

To estimate the velocity of ground water through the unsaturated zone, the following information is needed:

1. Average percolation or recharge rate
2. Average volumetric water content

To estimate the velocity of ground water through the saturated zone, the following information is needed:

1. Hydraulic conductivities (vertical and horizontal)
2. Hydraulic gradient
3. Effective porosities

To estimate migration of radionuclides through the saturated or unsaturated zones, the following information is needed:

1. Pore-water velocity
2. Concentration in the liquid phase (optional)
3. Dispersion coefficients in the x, y, and z directions (optional)
4. Decay coefficients (half-life)
5. Retardation factors (bulk density, distribution coefficient, effective porosity)

Table 2-1 shows the data typically required for ground-water modeling at each stage in the remedial process. For convenience, the data have been grouped into three general categories: the Physical Framework, the Hydrogeologic Framework, and Source Characteristics. Data in the physical framework category define the geometry of the system, including the thickness and areal extent of each hydrostratigraphic unit. Hydrogeologic data include information on the system's boundary conditions as well as the properties of the aquifer. Source characteristics pertain to the contaminated zone, which is the below-ground region within which radionuclides are present in above-background concentrations. Sometimes referred to as the source term, it serves as the starting point for all pathways.

The following is a brief discussion of the relevance of the individual parameters to the overall conceptual models.

Table 2-1. Data Requirements

TYPICAL SOURCES OF INFORMATION		
	Scoping Calculations	Site Characterization/ Remedial Design
<b>PHYSICAL FRAMEWORK</b>		
Depth to Ground Water	Topographic Maps	Well Logs/Water-Level Data
Areal Extent and Thickness of Aquifer(s)	Literature Values	Monitoring Well Logs/Geophysics
Areal Extent and Thickness of Confining Unit(s)	Literature Values	Monitoring Well Logs/Geophysics
Elevation of Unsaturated Zone Base	Literature Values	Soil Borings/Elevation Survey
Elevation of Top and Bottom of Aquifer(s) and Confining Units	Literature Values	Monitoring Well Logs/Elevation Survey/Geophysics
Areal Extent and Thickness of Stream and Lake Sediments	Literature Values	Soil Boring
Location and Orientation of Discrete Features	Literature Values	Surface Mapping/Aerial Photo Interpretation
<b>HYDROLOGIC FRAMEWORK</b>		
<b>UNSATURATED ZONE</b>		
Hydrodynamic Dispersion	Literature Values	Literature Values
Infiltration Rate	Literature Values	Field Measurements
Moisture-Release Curve Parameters	Table C-2	Laboratory Test
Saturated Hydraulic Conductivity ( $k_{sat}$ )	Table C-3	Laboratory Analyses
Soil Water Content	Table C-1	Laboratory Analyses
Gradient	Unit Gradient Assumed	Unit Gradient Assumed
Total Porosity	Table C-9	Laboratory Analyses/Field Analyses
Bulk Density	Literature Values	Laboratory Analyses/Literature Values
Distribution Coefficients ( $k_d$ )	Table C-5	Laboratory Analyses/Literature
<b>SATURATED ZONE</b>		
Gradient	Topographic Map	Water Level Measurements/ Elevation Surveys
Hydraulic Conductivity	Table C-4	Aquifer Stress Tests
Storage Properties	Literature Values	Aquifer Stress Tests
Effective Porosity	Table C-10	Field Tracer Tests/Laboratory Analyses/Literature

Table 2-1 (Continued)

TYPICAL SOURCES OF INFORMATION		
	Scoping Calculations	Site Characterization/ Remedial Design
HYDROGEOLOGIC FRAMEWORK		
Bulk Density	Literature Values	Laboratory Analyses/Literature Values
Dispersivity	Table C-11	Literature Values/Field Tracer Tests
Distribution Coefficients	Table C-5	Laboratory Analyses/Literature Values/Field Tracer Tests
Diffusion Coefficients	Literature Values	Literature Values/Laboratory Experiments
Receptor Location(s)	Literature Values	Field Survey
HYDRAULIC BOUNDARIES		
Precipitation	Literature Values	Field Measurements/Literature Values
Evapotranspiration/Runoff	Literature Values	Independent Calculations/ Literature Values
Surface-Water/Ground-Water Interactions	Literature Values	Field Measurements
Ground-Water Pumping	Assumed Rates	Field Measurements
SOURCE CHARACTERISTICS		
Areal and Vertical Extent	Assumption Guidelines	Radiation Surveys/Soil Borings/ Immunoassays
Composition	Historical Site Activities	Chemical Analyses
Release Mechanism	Calculations (Appendix C)	Soil Borings/Ground-Water Monitoring Data/Site History
Concentration	Assumption	Field Data
Radioactive Decay	Literature Values	Literature Values

## Physical Framework

The physical framework of the system defines the geometry of the system and includes the depth to water, areal extent of hydrostratigraphic units and fluvial deposits, and discrete features. The relevance of each of these data to ground-water flow and contaminant transport is discussed below.

*Areal Extent and Thickness of Hydrogeologic Units.* In heterogeneous formations, hydraulic properties change spatially. These properties may include the aquifer and/or confining unit (i.e., aquitard) thickness. The thickness of the units directly impacts the volume of flow and therefore, mass transport through the system. Furthermore, areas where the confining units are thin or discontinuous would provide avenues for radionuclides to move more freely among aquifers. For these reasons, the determination of the areal extent and thicknesses of the hydrogeologic units is one of the primary objectives during the site characterization program.

The thickness of the aquifer is generally not a required parameter for the scoping calculations, although it does set upper bounds on the maximum amount of vertical mixing that could potentially occur as is discussed in Appendix B.

*Areal Extent and Thickness of Stream and Lake Sediments.* The physical properties (e.g., hydraulic conductivity, sorption properties) of fluvial deposits are typically different from the underlying aquifer. Therefore, ground-water flow and radionuclide transport into and out of the ground-water system may be very sensitive to the degree of interconnection of the aquifer system with surface-water bodies.

*Location and Orientation of Discrete Features.* The presence of discrete features, such as fractures, faults and macropores could have a significant effect on the ground-water flow and radionuclide transport.

Modeling flow through the unsaturated zone is generally based on the assumption that the soil is a continuous unsaturated solid matrix that holds water within the pores. Actual soil, however, has a number of cracks, root holes, animal burrows, etc., where the physical properties differ enormously from the surrounding soil matrix. Under appropriate conditions, these flow channels have the capacity to carry immense amounts of water at velocities that

greatly exceed those in the surrounding matrix. At present, there is no complete theory describing water flow through these structural voids or macropores. There is uncertainty regarding the significance of subsurface voids in water flow, since, if large, they should fill only when the surrounding soil matrix is close to saturation. Nonetheless, studies have shown that contaminants can migrate to substantial depths with only a small amount of water input.

Ground-water flow and radionuclide transport in the saturated zone may be strongly influenced by the presence of fractures. When a radionuclide is introduced into a fractured porous medium, it migrates through the fracture openings by means of advection as well as hydrodynamic dispersion. The radionuclide may also diffuse slowly into the porous matrix. Molecular diffusion dominates flow and transport within the porous matrix because the fluid velocity in the porous matrix is usually very small. Upon introduction of the radionuclide into a fractured aquifer, the radionuclide moves rapidly within the fracture network. As time progresses, the zone of contamination will diffuse farther into the porous matrix. Since the porous matrix has a very large capacity to store the contaminant, it plays a significant role in retarding the advance of the concentration front in the fractures. If the source of contamination is discontinued and the aquifer is flushed by fresh water, the contaminant mass in the fractures will be removed relatively quickly, whereas the contaminant in the porous matrix will be removed very slowly via diffusion back to the fracture openings.

## Hydrogeologic Framework

The hydrological data have been divided into those associated with the unsaturated zone and saturated zones. These data include information on aquifer properties, hydrologic stresses, and hydraulic heads. The relevance of each of these to ground-water flow and contaminant transport is discussed below.

### **Unsaturated Zone**

The unsaturated zone is the zone between the land surface and the water table including the capillary fringe. In the subsurface environment, contaminants migrate through this partially saturated zone (i.e., unsaturated zone) prior to reaching the saturated zone. In this zone, flow is usually assumed to be in the vertical direction. The flow is generally one-

dimensional: therefore, scoping calculations are also performed in one dimension. Generally, water in this zone is under less than atmospheric pressure, and some of the voids may contain air or other gases at atmospheric pressure. Beneath flooded areas or in perched water bodies the water pressure locally may be greater than atmospheric.

The volumetric flux of liquid moving under isothermal and isosmotic conditions through a partially saturated, natural hydrogeologic unit, regarded as an equivalent porous-medium continuum system, is determined by the spatial gradients of matrix and gravitational potentials and by the hydraulic properties. This functional dependence obeys "Darcy's Law" for unsaturated liquid flow (Appendix B).

The means by which water transports radionuclides through the unsaturated zone is a complex process. The passage of water is dynamic and depends on detailed variations of the hydraulic properties of the soil through which the water passes. Water storage by a soil profile is characterized by water content distribution, which ultimately depends on the detailed spatial variability of hydraulic properties. Infiltrating water that exceeds the soil water-holding capacity will contribute to the net recharge of the underlying aquifer.

A rigorous analysis of the flow and transport processes through the unsaturated zone is accompanied by demanding data requirements. However, rarely in the scoping phase of the investigation would detailed data be available. Even during the site characterization phase, these data are rarely available. A discussion of the data that are required for both scoping and site characterization modeling of the unsaturated zone are presented below.

*Infiltration Rate (Recharge).* Water from a precipitation event moves downward through the soil under the influence of gravity and matric pressures. Water is extracted from the unsaturated zone as surface evaporation and as plant transpiration; together these processes are termed evapotranspiration. The rates of both extraction processes depend primarily on available solar energy, surface winds, and plant and soil type.

A number of simple methodologies are available to estimate the fraction of precipitation that recharges into the aquifer (i.e., precipitation minus

evapotranspiration and runoff). Recharge estimates are described by DAS77, FEI75, and THO55, and 57. In areas drained by perennial streams, recharge may be estimated by base-flow separation methods.

A somewhat more sophisticated method is incorporated in the Hydrologic Evaluation of Landfill Performance (HELP) model (SCH83 and 84). HELP is a quasi-two-dimensional model that computes the daily water budget for a landfill represented as a series of horizontal layers.

As a first, rough approximation, net recharge can be estimated by subtracting pan evaporation from precipitation rates, both of which are generally readily available. This approach would overestimate net recharge because runoff is assumed to be negligible. Typically, higher infiltration rates result in greater health risks, but there are exceptions to this guideline. When radium is a concern, the risk associated with direct exposure to radium is generally greater than the radium risk associated with the ground-water pathway. Therefore, higher infiltration rates tend to flush the radium from the source and, in turn, reduce the direct exposure.

*Soil Type.* The soil type (e.g., sand, silt, clay) may be used to obtain qualitative estimates of saturated hydraulic conductivities, porosities, and the moisture release information. In conjunction with infiltration rates, the soil type can be used to make preliminary estimates of moisture content. The moisture content is assumed to fluctuate between field capacity and saturation with the effective hydraulic conductivity based on an empirical equation (Appendix B). Typical values for these parameters are presented in Appendix C. Appendix B describes how these parameters are used to solve radionuclide transport.

*Hydraulic Gradient.* After water infiltrates beneath the ground surface, it generally travels vertically downward under the influence of gravity and matric (i.e., suction) forces until it reaches the water table. The gravity and capillary forces make up the hydraulic gradient. Under partially saturated conditions, liquid water is bound to the solid within the pore and fracture openings either by surface-tension (capillary) forces or, at very low saturations, by physical or chemical adsorption. The strength of the bonding force is measured in terms of an equivalent negative pressure, or pressure head, designated as the matric potential.

Since the gravitational head gradient has the value of unity, it follows that scoping calculations will not require site-specific information pertaining to the partially saturated zone hydraulic gradient. For more complex site characterization modeling, however, capillary pressure relationships are used to determine hydraulic gradients.

Matric potential is a function of liquid-water saturation. Typically, an analytic or graphical representation of the functional relationship defines the moisture-retention curve for the porous medium. Moisture-retention curves for most media are not unique; they display hysteresis in which the precise relation between matric potential and saturation depends on the wetting and drying history of the medium.

Standard techniques, using mercury intrusion, pressure-plate apparatus, thermocouple psychrometers, and centrifuges are used to measure the moisture-retention curves for small soil and rock samples.

*Thickness.* The thickness of the unsaturated zone or depth to water affects the travel time of radionuclides leached from the surface to the ground water. Typically, very little dilution occurs in the unsaturated zone and radionuclide concentrations will be diminished only through radioactive decay and volatilization. The depth to ground water has no direct influence on transport mechanisms other than to create a relatively thin region known as the capillary fringe which is above the water table and has a higher moisture content, and therefore, a higher relative hydraulic conductivity.

Depth to ground water can also influence the extent of upward water flow occurring to a surface layer which has been evaporating without water input for an extended period of time. It has been shown both theoretically and experimentally that finer textured soils can move water and radionuclides upward from much greater depths than can coarse textured soils.

If site data are unavailable, approximate depth to water estimates may be made based on land surface topography, the elevation of nearby surface water bodies, and the tendency of the shallow water table to mirror the land surface topography. Detailed modeling, however, cannot be performed without a good understanding of the vadose zone geometry.

*Distribution Coefficient.* A distribution or partitioning coefficient (designated  $K_d$ ), which describes the degree of sorption, is used to calculate the partitioning of species such as radionuclides between the ground water and aquifer and, thereby, calculate the sorption capacity or retardation. The standard convention for recording concentration units for soil samples is to express the concentration in mass of constituent per dry mass of soil. Based on this convention, the dissolved liquid and absorbed-solid concentrations can be expressed as follows:

$$C = \frac{CS_{TOT}\rho}{(\theta + \rho K_d)}$$

$$S = \frac{(CS_{TOT}\rho)}{(\theta + \rho K_d)} K_d$$

in which  $S = K_d C$

and

$$K_d = \frac{S}{C}$$

where:

$C$  = dissolved-liquid phase concentration, expressed as mass per volume of liquid (Ci/ml or g/ml)

$CS_{TOT}$  = total contaminant concentration, expressed in weight of dry soil (Ci/g or g/g)

$\rho$  = bulk density of the soil ( $\text{g/cm}^3$ )

$\theta$  = moisture content

$K_d$  = equilibrium (partition of distribution) coefficient (ml/g)

$S$  = particulate concentration, expressed in weight of dry soil (Ci/g or g/g)

This expression assumes that there is a direct, linear relationship between the amount of a solute sorbed onto soil,  $S$ , and the concentration of the solute,  $C$ . Therefore, the adsorption isotherm of  $C$  as a function of  $S$  will graph as a straight line. The assumptions regarding this linear relationship are presented in



## Appendix A.

If the soil contaminant concentrations are presented on a per unit volume basis (i.e., mass of contaminant per total volume of sample), the dissolved liquid and absorbed-solid concentrations can be expressed as follows:

$$C = \frac{C_T}{(\theta + \rho K_d)}$$

$$S = \frac{C_T K_d}{(\theta + \rho K_d)}$$

where:

$C_T$  = total contaminant concentration, expressed in activity or mass per unit volume (Ci/cm<sup>3</sup> or g/cm<sup>3</sup>)

These relationships are used in Appendix B to estimate the radionuclide release leaching into the subsurface environment and migrating with the ground water.

In the literature, distribution coefficients measured from adsorption conditions abound; however, the  $K_d$  values depend not only on the soil's physical and chemical properties but also on the chemical properties of the ground water. Because of its dependence on many site-specific properties, the value of the distribution coefficient for a specific radionuclide in soils can range over several orders of magnitude under different conditions.

Of particular significance in the unsaturated zone is that sorption, rather than being dependent upon effective porosity as in the saturated zone, is a function of the moisture content as described by the following:

$$R_f = 1 + \frac{K_d \rho}{\theta}$$

where:

$R_f$  = Retardation Factor  
 $K_d$  = Distribution Coefficient  
 $\theta$  = Moisture Content  
 $\rho$  = Bulk Density

This relationship indicates that retardation will increase as moisture content decreases. Furthermore,

because moisture content is transient in space and time, the retardation factor will also exhibit these characteristics.

Unless data are available to the contrary, scoping calculations will generally use the same distribution coefficient for the unsaturated zone and for the source term. Whereas the distribution coefficient in the source term is used to predict leaching concentrations and rates, the distribution applied to the unsaturated zone dictates the rate at which the radionuclide will be transported as described in Appendix B. Typical distribution coefficients are presented as Table C-5 in Appendix C. However, the modeling results are typically very sensitive to the distribution coefficient, and caution should always be used when applying non-site-specific data.

*Hydrodynamic Dispersion.* Since soil water flux is represented as a continuous quantity which is volume-averaged over many pores, the individual travel paths around soil grains are mathematically replaced by an equivalent one-dimensional flow. When this one-dimensional flow of water is multiplied by the dissolved solute concentration, the resulting mass flux does not take into account the additional spreading of solute which occurs by three-dimensional mass flow at the pore scale in the actual system. This apparent solute spreading arising from the mass flux effects which are obscured by mathematical volume averaging is called hydrodynamic dispersion.

*Saturated Hydraulic Conductivity.* Saturated hydraulic conductivity is the proportionality coefficient between the saturated water flux and the hydraulic head gradient. In cases where water is ponded on the soil surface, either through irrigation, rainfall or natural lakes or man-made storage ponds or lagoons, hydraulic conductivity will have a dominant influence on the amount of water infiltrating into the soil and, therefore, will strongly affect mass flow and transport.

Hydraulic conductivity and permeability are often used synonymously in ground-water modeling; however, they have different meanings. Hydraulic conductivity combines the properties of the aquifer and of the fluid, while permeability is a property of only the aquifer material. The two parameters are related by the following equation:

$$K = \frac{k\rho g}{\mu}$$

where:

- $K$  = hydraulic conductivity (m/s)
- $k$  = permeability ( $m^2$ )
- $\rho$  = fluid (water) density ( $kg/m^3$ )
- $g$  = acceleration due to gravity ( $m/s^2$ )
- $\mu$  = fluid (water) viscosity (Pa-s)

Most saturated ground-water flow models require hydraulic conductivity as input, while multi-phase models require permeability data.

*Soil Water Content.* Volumetric soil water content has a significant influence on the flow and transport mechanisms. The curies of radionuclide moved per unit time from one point to the next is inversely proportional to the distance between the two points. The actual path length in soil followed by a radionuclide is strongly affected by water content. Therefore, water content increases, the cross-sectional area for flow increases, and the path length decreases as liquid replaces air in the medium. Since flux of radionuclide is proportional to water flux multiplied by the dissolved radionuclide concentration, it is not directly affected by water content. However, because increasing the water content of a given soil will result in a higher mass flux, some correlation between radionuclide movement and water content may be found.

The soil water content can influence adsorption in two ways: it can modify the solution pathway leading to the adsorption sites and thus increase or decrease the accessibility of the surface to the solute, and it may also affect the physical-chemical properties of the adsorbent by increasing or decreasing the hydrolysis of the clay lattice. However, the influence of soil water content on adsorption is slight until the soil is extremely dry. In dry soil, the preferential coverage of water molecules on the soil's adsorbing surfaces is removed, and solute adsorption increases dramatically.

*Total Porosity.* The porosity of a rock or soil is its property of containing interstices or voids. This may be expressed quantitatively as the ratio of the volume of its interstices to its total volume.

Flow and transport are indirectly affected by porosity since regions of low porosity are likely to have lower permeability to transport water. Although no reliable models exist to describe the relationships between porosity and permeability, permeability of a given soil type strongly decreases as porosity decreases because the pore sizes contract. However, finer-textured soils such as clays generally have a higher porosity and lower permeability than sandy soils.

Porosity is an important parameter in computing ground-water velocity in both the saturated and unsaturated zones. Velocity is inversely proportional to porosity. Another way that porosity affects transport is that decreasing soil porosity increases the density of mineral adsorption sites and thus causes increased adsorption of radionuclides with a corresponding decrease in solution concentration.

*Bulk Density.* The soil or dry density is the ratio of the mass of the solid phase of soil (i.e, dry soil) to its total volume (solid and pore volumes together).

The influence of increasing bulk density on adsorption is to increase the density of adsorption sites per unit volume which will directly increase adsorption capacity. However, the correlation between adsorption and bulk density for a group of soils will be small because clay and organic soils tend to be found at lower bulk density than coarser textured soils which are low in organic matter. Thus, the effect of increasing bulk density on adsorption refers to compressing a given soil volume.

### **Saturated Zone**

The saturated zone is that part of the earth's crust beneath the regional water table in which all voids, large and small, are filled with water under pressure greater than atmospheric. The saturated zone may depart from the ideal in some respects. A rising water table may cause entrapment of air in the upper part of the zone of saturation. The shallowest aquifer typically would be under unconfined conditions or a water-table aquifer. The ground water flowing within a water-table surface is in immediate contact with the atmosphere and is directly recharged through the overlying unsaturated zone. This water-table surface is free to rise and fall within the aquifer in response to varying amounts of recharge (e.g., rain). The water-table aquifer generally follows land-surface

topography and is frequently revealed in the form of surface-water bodies such as lakes and rivers. This connection between the ground water and the surface water also creates potential surface-water pathways. Scoping calculations generally focus on contaminant releases to the shallowest aquifer, whereas site characterization modeling would tend to include all aquifers and aquitards in the hydrogeologic flow system. The data required to describe ground-water flow and radionuclide transport through the saturated zone are presented below.

*Potentiometric Surface Maps.* The potentiometric surface is a way of depicting the static head in an aquifer. It is defined by the levels to which water will rise in tightly cased wells. In cases where the head varies appreciably with depth (i.e., upward or downward gradients) in the aquifer, a potentiometric surface is meaningful only if it describes the static head along a particular specified surface or stratum in that aquifer. More than one potentiometric surface is then required to describe the distribution of head. The water table is a particular potentiometric surface for an unconfined aquifer.

With respect to ground-water flow and contaminant transport, the potentiometric surfaces define the hydraulic gradients, which in turn, are used to calculate the direction and volume of flow through the system, as well as the ground-water and contaminant velocities.

*Hydraulic Gradient.* The hydraulic gradient will play a significant role in estimating the velocity at which the radionuclides are migrating (Appendix B). If site-specific data are not available for the scoping calculations, hydraulic gradients may be approximated from the land-surface topography. However, in the site characterization modeling, water levels from at least three wells screened in the aquifer are needed to determine the direction and magnitude of the gradient.

*Hydraulic Conductivity.* The hydraulic conductivity of a soil or rock is a measure of the soil's ability to transmit water under a hydraulic gradient. The values of hydraulic conductivity in soils and rocks vary within a wide range of several orders of magnitude, depending on the grain size, the structure of the soil matrix, the type of soil fluid, and the relative amount of saturation present in the soil or rock matrix.

Aquifer tests are often performed for the purpose of

determining field values of aquifer hydraulic conductivities. Analyses of the field test data are based upon analytical solutions for radial flow towards wells under a variety of conditions. The analytical methods used are very straightforward and generally do not require the use of a computer.

Before site characterization, only the most general assumptions can be made about the relative flow properties of the aquifers. For example, as a rule of thumb for sedimentary deposits, it is often assumed that the hydraulic conductivity in the horizontal direction is ten times greater than that in the vertical direction. In the absence of site-specific values, literature values may be used for the scoping calculations (Table C-6, Appendix C). For site characterization modeling, hydraulic conductivity values should be site specific.

*Storage Properties.* The storativity of a saturated confined aquifer can be defined as the volume of water that an aquifer releases from storage per unit surface area of aquifer per unit decline in the component of hydraulic head normal to that surface.

The storage term for unconfined aquifers is known as the specific yield. It is defined as the volume of water that an unconfined aquifer releases from storage per unit surface area of aquifer per unit decline in the water table.

Storage properties are required only for transient ground-water flow simulations. If flow is assumed to be steady state, the storativity of the aquifer is assumed to be zero: in flow is equal to outflow with no change in storage.

*Effective Porosity.* The effective porosity is the ratio of the volume of interconnected pore spaces available for transport to the total system volume. It is used to estimate the velocity at which ground water and radionuclides travel through a porous medium (Appendix B). The smaller the effective porosity the higher the ground-water velocity and the more rapidly the transport of radionuclide(s) or other solubles. Total porosity is the ratio of the total pore volume to the total system volume and includes dead pore space. Therefore, it is important not to confuse effective porosity with total porosity, as total porosity will always be greater than effective porosity.

In natural porous systems, such as subsurface soil,

where the flow of water is caused by capillary, molecular, and gravitational forces, the effective porosity can be approximated by the specific yield, which is defined as the ratio of the volume of water drained by gravity from a saturated sample of soil to the total volume of soil.

The most accurate means of obtaining effective porosity data is by conducting site-specific field tracer tests. These tests, however, are time consuming and may not significantly reduce the uncertainty associated with the effective porosity. Since the greatest source of uncertainty relative to transport is typically the distribution coefficient, it is generally best to estimate effective porosities from the literature (Table C-10). An analysis can be performed to evaluate the sensitivity on flow and transport results (Section 4.1.4).

*Bulk Density.* The bulk density of the soil or rock is used to determine the retardation factor as derived in Appendix B. The soil or dry density is the ratio of the mass of the solid phase of soil (i.e., dry soil) to its total volume (solid and pore volumes together). The dry density of most soils varies within the range of 1.1 - 1.6 gr/cm<sup>3</sup>. In sandy soils, dry density can be as high as 1.6 gr/cm<sup>3</sup>, in clayey soils and aggregated loams, it can be as low as 1.1 gr/cm<sup>3</sup>. Although laboratory measurements may be made to obtain accurate bulk density values, it is rarely worth the effort as the potential range is relatively narrow, and the modeling results are typically insensitive to bulk density.

*Dispersion Coefficients.* The equations of solute transport that are solved in contaminant-transport codes are derived assuming that the solute migration is due to advection and hydrodynamic dispersion. Hydrodynamic dispersion is caused by the tendency of the solute to spread out from the path that it would be expected to follow if transported only by advection. This spreading of the contamination over an ever-increasing area is called hydrodynamic dispersion and has two components: mechanical dispersion and diffusion. Hydrodynamic dispersion causes dilution of the solute and occurs because of spatial variations in ground-water flow velocities and mechanical mixing during fluid advection. Molecular diffusion, the other component of hydrodynamic dispersion, is due to the thermal kinetic energy of solute molecules and also contributes to the dispersion process. Thus, if hydrodynamic dispersion is factored into the solute transport processes, ground-water contamination will

cover a much larger region than in the case of pure advection, with a corresponding reduction in the maximum and average concentrations of the contaminant. Typical dispersivity values, obtained from tracer tests, are presented in Table C-11.

Because hydrodynamic dispersion is the sum of mechanical dispersion and diffusion, it is possible to divide the hydrodynamic dispersion term into the two components and have two separate terms in the equation. Under most conditions of ground-water flow, diffusion is insignificant and is frequently neglected in many of the contaminant transport codes. However, this artificial exclusion of the diffusion term may create problems in certain instances (see Section 3.3 under the topic of matrix diffusion).

Representing dispersion adequately in computer codes is difficult, because dispersion is related to spatial scale and variations in aquifer properties that are generally not explicitly simulated in the code (e.g., tortuosity). Furthermore, dispersion coefficients are very difficult to measure in the field and have been shown generally to increase with scale of observation. These difficulties are generally addressed by using dispersivity values from the published literature and refining these estimates during the model calibration process.

*Distribution Coefficient.* As with the unsaturated zone, the distribution coefficient assigned to the saturated zone will help determine the rate at which the radionuclides migrate. This distribution coefficient should be consistent with the rock or soil types that make up the aquifer or water-bearing unit.

A detailed discussion of distribution coefficients is presented in Appendix A. The use of literature values for site characterization modeling is rarely defensible. Furthermore, modeling results are typically very sensitive to the magnitude of the distribution coefficients. Therefore, site-specific distribution coefficients should be obtained during the site characterization program.

The two most common experimental techniques for the determination of the distribution coefficient are the batch and column methods. The batch method is used to measure the distribution coefficient under saturated equilibrium conditions. The column method is used to obtain a more representative value as the soil has not been altered (e.g., grinding, agitated) as much as in

the batch experiments.

*Precipitation/Irrigation.* The characteristics of the precipitation or rainfall events (i.e., intensity and distribution) greatly affect the extent of radionuclide transport. Precipitation will have a dominant influence on flow because the rainfall rate is directly related to the water flow rate in the soil. Therefore, soils that receive intense, frequent rainfall will have high water fluxes and hence high radionuclide activity fluxes. Furthermore, extremely intense rainfall might induce saturation which could result in a greatly enhanced mass transport through soils of high permeability. That is, the saturated hydraulic conductivity may be reached. These same characteristics may be observed in aquifers underlying irrigated fields.

*Evapotranspiration.* Evapotranspiration represents the amount of applied water which is removed by plants or water loss from surfaces via evaporation and hence is unavailable for drainage. Thus, the extent of evapotranspiration will strongly affect the water flux below the root zone and therefore, the extent of radionuclide leaching by mass flow. For soils not receiving water input by irrigation, rainfall minus evapotranspiration and runoff determines the net amount of water infiltrating beyond the root zone.

*Surface-Water/Ground-Water Interactions.* Water resource development has frequently been based on the predominant use of either surface or ground water. These two components of the total water resource, however, are interdependent. Changes in one component can have significant effects on the other. In streams that are termed "gaining," stream flows are sustained by ground water influx, whereas "losing" streams replenish the ground water by seepage through the stream bed. The hydraulic conductivity of the stream bed sediments will be a contributing factor to the rate at which water moves into or out of a stream.

*Ground-Water Pumping/Injection.* The injection or withdrawal of water into or out of an aquifer can have a pronounced effect on the hydraulic gradients. In the case of withdrawal wells, capture zones are created which will not allow contamination to migrate beyond this zone.

#### Source Characteristics

The accurate portrayal of the contaminant source term is one of the most difficult tasks in the modeling process. All too often, there are no data that characterize the nature and extent of the contamination or the release history.

Some knowledge of the history of the waste disposal activities can often provide valuable insight into the probable nature of the contaminant source term. In general, the longer the site has been active, the more likely it is that the wastes have been discarded in many different forms and dispersed over a larger area. The presence of product and waste lines immediately suggests that line-type sources are present. Absorption beds and storage tanks indicate potential point sources, whereas mill tailings, large lagoons, and air emissions that carried and subsequently deposited contaminants in the site vicinity would generally represent area sources.

The distribution of measured contaminants in the soil and ground water will also provide clues as to their source. Contaminants that are wide-spread and of similar concentrations suggest an areal source (or non-point), while narrowly defined areas of contamination indicate a more localized or point source.

As a general rule, it is best to keep initial assumptions regarding the source term as simple as possible. The large uncertainties of the initial scoping phase dictate that the sensitivity analysis become a critical component of the analysis to quantify associated uncertainties. As more data become available during the site characterization, source term characteristics can be more accurately modeled. The characteristics typically associated with the source term are discussed below and include: source dimensions, release mechanisms, radionuclide concentrations, and leaching rates.

*Areal and Vertical Extent.* The vertical and areal extent of contamination is a site-specific parameter that will potentially have a high degree of associated uncertainty for the scoping calculations. In practice, scoping calculations often assume the source to be a point source that includes 1 m<sup>3</sup> of material. This volume is subsequently scaled upwards to analyze larger areas.

One of the primary objectives of the site characterization program is to define the geometry of

the contaminant source. Most numerical models allow the source geometry to be accurately portrayed to the degree desired.

*Release Mechanism.* Computer codes can simulate the introduction of contaminants to the ground water as an instantaneous pulse or as a continuous release over time. A continuous release may either be constant or vary with time. The two most common means of simulating continuous or pulse releases are by either specifying release concentrations or by specifying the contaminant mass entering the system. In general, both approaches have drawbacks and limitations and require considerable thought and possibly a number of independent calculations prior to selecting and implementing the most appropriate method for the modeling exercise. Furthermore, most ground-water flow and transport codes do not explicitly account for the physical degradation of waste containers, and therefore, anticipated release rates must be estimated through other means (e.g., waste package codes) and input as boundary conditions into the flow and transport model.

*Concentration.* The source term concentration is one of the most critical parameters. It is recommended that site-specific data be obtained because the initial concentration will directly impact the predicted concentration at a receptor. Source term concentrations should also be varied as an integral part of the sensitivity analysis. Frequently, the source concentration is normalized: that is, the concentration is set to one. This practice allows the predicted results presented in terms of percentages of the actual concentration.

*Radioactive Decay.* Radionuclides either decay to stable products or to another radioactive species called a daughter. In some species, several daughter products may be produced before the parent species decays to a stable element. In considering this process over the transport path of radionuclides, one transport equation must be written for each original species and each daughter product to yield the concentration of each radionuclide (original species and daughter products) at points of interest along the flow path.

Radioactive source terms present special considerations in that the activity of the parent isotopes will diminish with time due to radioactive decay. However, if the radionuclide release is solubility

controlled, or if the half-life is extremely long, the concentration of the leachate may remain constant despite the decay of the source term. The release concentrations may remain constant until the source term has decayed to concentrations where solubility limits no longer dictate the amount of radionuclides that may go into the solution.

*Distribution Coefficient.* As mentioned previously, the distribution coefficient describes the soil-water partitioning for a given compound. This relationship is frequently used to predict the rate at which radionuclides will leach from the source term, as described in Appendix B.

## 2.4 Remedial Design and Implementation Phase

As the site characterization process ends and the Remedial Design and Selection Phase is entered, data that will assist in defining the remedial alternatives have been acquired. The various remedial alternatives can be conveniently grouped into the following three categories:

- Immobilization
- Isolation
- Removal

This section briefly describes each category, the types of processes that need to be modeled to support each category, and the special information needs for each of these categories. The information is required not only for implementation of the remedial design but also to evaluate its effectiveness through numerical modeling.

### Immobilization

Immobilization of the radioactive wastes refers to physical, chemical, and/or biological processes used to stabilize the radionuclides and preclude their transport. A number of treatment options exist, each having its own associated modeling needs, including:

- Physical
  - vapor extraction
  - in-situ coating
  - grouting of fissures and pores
  - in-situ freezing
  - in-situ vitrification

- Chemical
  - induce secondary mineralization
  - induce complexation
  - alter oxidation-reduction potential
- Biological
  - in-situ microbial activity
- Physical/Chemical
  - alter surface tension relationships
  - alter surface charges
  - in-situ binding
  - adsorbent injection
  - radionuclide particle size augmentation through clay flocculation

The following are the types of physical, chemical, and biological processes that may need to be modeled to support alternative remedies based on immobilization:

- Physical Properties and Processes
  - unsaturated zone flow and transport\*
  - heat energy transfer\*
  - multiple layers\*
  - vapor transport\*
  - extreme heterogeneity\*
  - temperature-dependent flow and transport\*
- Chemical Properties and Processes
  - density-dependent flow and transport\*
  - oxidation-reduction reactions
  - system thermodynamics
  - chemical speciation\*
  - ion-exchange phenomena
  - precipitation
  - natural colloidal formation
  - radiolysis
  - organic complexation
  - anion exclusion
- Biotic Properties and Processes
  - biofixation

\* indicates modeling codes are readily available

It would be ideal if these processes and properties could be reliably described and modeled with conventional and available models. However, many of these properties and processes are not well understood, and, in these instances, models do not

exist that yield reliable results.

The specialized data required to support ground-water modeling of immobilization techniques include:

- Determination of temperature-dependent flow and transport parameters
- Characterization of the geochemical environment
- Determination if the physical rock properties that govern flow and transport have been altered
- Characterization of the microbial environment

#### Isolation

A common remedial alternative is to emplace protective barriers either to prevent contaminated ground water from migrating away from a contaminated site or to divert incoming (i.e., clean) ground water from the source of contaminants. These barriers include walls, caps and lines. Several types of materials are being used to construct such barriers, including soil and bentonite, cement and bentonite, concrete, and sheet piling. An alternative to the physical emplacement of protective barriers is the use of hydraulic containment which involves controlling the hydraulic gradient through the use of injection and/or withdrawal wells or trenches in order to contain and treat the contaminant plume. Examples of potential barriers include the following:

- Physical
  - hydraulic containment
  - grout curtains, sheet piling, bentonite slurry walls
  - low permeability caps (clay and/or synthetic)
  - liners
- Chemical
  - ion-exchange barriers
- Biological
  - microbial barriers

If properly designed and emplaced, such barriers can last for several decades, barring any geological disturbances, such as tremors, ground settling, significant changes in hydraulic gradients, etc.

Accordingly, such barriers can be useful in mitigating the impacts of relatively short-lived radionuclides, or to control the migration of long-lived radionuclides until a more permanent remedy can be implemented.

Several mechanisms or processes can affect the long-term integrity of such barriers. Once the installation is complete, failures can occur due to cracking, hydrofracturing, tunneling and piping, and chemical disruption. Changes in the site's geological or hydrological characteristics can also lead to catastrophic failures, such as partial collapse, settling, and breaking. If a barrier should fail following installation, water may infiltrate the site, and contaminated leachates may move beyond the site. This type of failure could result in the dispersion of contaminants in the environment.

The modeling approaches to simulating the effects of flow barriers on the fate and transport of radionuclides are closely tied to the ability of the code to accommodate factors, such as: high permeability contrasts, transient boundary conditions, and possibly chemical and biological reactions. These considerations will be discussed in greater detail in the following sections.

The following are the types of physical, chemical, and biological processes that may need to be modeled to support alternative remedies based on isolation. Many of these processes are very complex, and attempts at modeling will meet with varying degrees of success.

- Physical Properties and Processes
  - unsaturated zone flow and transport\*
  - runoff\*
  - multiple layers\*
  - vegetative cover\*
  - transient source term\*
  - extreme heterogeneity\*
  - areal recharge and zero flux capability\*
- Chemical Properties and Processes
  - localized ion exchange phenomena
- Biotic Properties and Processes
  - localized biofixation
  - microbial population modeling

\* indicates modeling codes readily available

Typical characterization data needs related to barrier emplacement include:

- Barrier dimensions
- Barrier hydraulic conductivity
- Geochemical environment
- Structural integrity of barrier/barrier degradation
- Microbial environment
- Detailed hydrogeology

### Removal

Radioactively contaminated soil can result from the disposal of both solid and liquid waste. Solid wastes may have been buried in the past without sufficient integrity of containment so that, eventually, radioactivity intermingled with the contiguous soil. Percolation of rain water through shallow burial sites can contribute further to the migration of radionuclides to lower depths as well as to some lateral movement. Wider areas of contamination have occurred when waste, stored temporarily at the surface, has lost containment and has been dispersed by the wind. The most common technologies for removing radionuclides in solid, liquid, and vapor (e.g., tritium) form include the following:

- Physical
  - soil excavation (solid)
  - pump and treat (liquid)
  - in-situ vaporization (vapor)
- Biological
  - injection and removal of biomass foam

The following are the types of physical, chemical, and biological processes that may need to be modeled to support alternative remedies based on removal. Most of these processes and properties are readily described in mathematical terms and can be modeled reliably. Obviously, modeling the biological activity associated with the injection of a biomass will have the same limitations that are common to other types of biological modeling.

- Physical Properties and Processes
  - transient source term\*
  - unsaturated zone flow and transport\*
  - matrix diffusion\*
  - desaturation and resaturation of the aquifer\*



- vapor transport\*
- Biological Properties and Processes
  - physical injection and withdrawal of the biomass
  - microbial population modeling

*\* indicates modeling codes readily available*

Typical characterization needs related to radionuclide removal include:

- Air permeability of the unsaturated zone
- Unsaturated zone flow and transport parameters
- Areal extent of contaminated wastes
- Depth to ground water
- Saturated zone flow and transport properties

The degree to which these factors are addressed in the modeling relies heavily upon the objectives as well as the availability of the required data.

## CHAPTER 3 —CONCEPTUAL MODEL DEVELOPMENT

### 3.1 Preliminary Conceptual Model

In the scoping phase, site-specific information is often limited. Therefore, the modeling performed during the early planning phase of most remedial investigations is generally designed to support relatively simple objectives which can be easily tied to more ambitious goals developed during the later phases of the investigation. The very nature of the iterative process of data collection, analysis, and decision making dictates that the preliminary objectives will need to evolve to meet the needs of the overall program. That is, it would be unreasonable to assume that simplified modeling based upon limited data would do little more than provide direction for future activities.

An important issue that often arises during the scoping phase is whether remediation and decommissioning strategies can be selected during the scoping phase based on limited data and simple screening models. Such decisions can be costly at complex sites where the nature and extent of the contamination and transport processes are poorly understood. However, at relatively simple sites, early remediation decisions can help avoid the unnecessary delays and costs associated with a possibly prolonged site characterization and modeling exercise.

The formulation of a conceptual model is an integral component of the modeling process. Sometimes, components of the conceptual model may be simplified to meet either limited objectives or limitations in the data. That is, it is often useful to simulate only certain components of the conceptual model. For instance, even if there are data that indicate separable property zones in the aquifer, it is common during the scoping phase to evaluate ground-water flow and contaminant transport as a function of average values using homogeneous soil and rock properties. This simplification of the conceptual model is a valid approach because, in practice, early modeling focuses upon assessing the significance of specific parameter values and their effects on flow and transport, rather than on modeling specific hydrogeologic transport processes. Figure 3-1 illustrates typical conceptual models in the early phase of the investigation.

While different aspects of the conceptual model may be simulated in a variety of ways, the selected

approach must remain consistent with the objectives. That is, the physical system cannot be overly simplified to meet ambitious objectives, and less demanding objectives should not be addressed with sophisticated models. Hence, the development and acceptance of a conceptual model is an evolutionary process that depends upon the modeling goals and availability of data. An important part of model application in the early phase of the investigation is understanding the project decisions that need to be made, and identifying which of these decisions can be supported by the use of specific codes when limited data and the controlling hydrogeologic processes at the site are incompletely understood.

Because general trends, rather than accuracy, are most important during the scoping phase, the ground-water modeler typically makes the following simplifying assumptions early in the investigation:

- Steady-State Assumptions
- Restricted Dimensionality
- Uncomplicated Boundary and Initial Conditions
- Simplified Flow and Transport Processes
- System Homogeneity

These conceptual assumptions, discussed in greater detail below, generally translate into modeling approaches that are consistent with the available data. They are discussed in greater detail next.

#### *Steady-State Solutions*

In the scoping phase, the data generally available have been collected over relatively short time intervals. Therefore, modeling objectives would be limited to those that could be met without a detailed understanding of the temporal nature of processes affecting flow and transport. For example, a typical analysis not requiring detailed knowledge of the temporal nature of recharge, source release rates, and other flow and transport mechanisms would be the estimation of the distance that radionuclides have traveled since the beginning of waste management activities. This analysis would use yearly average

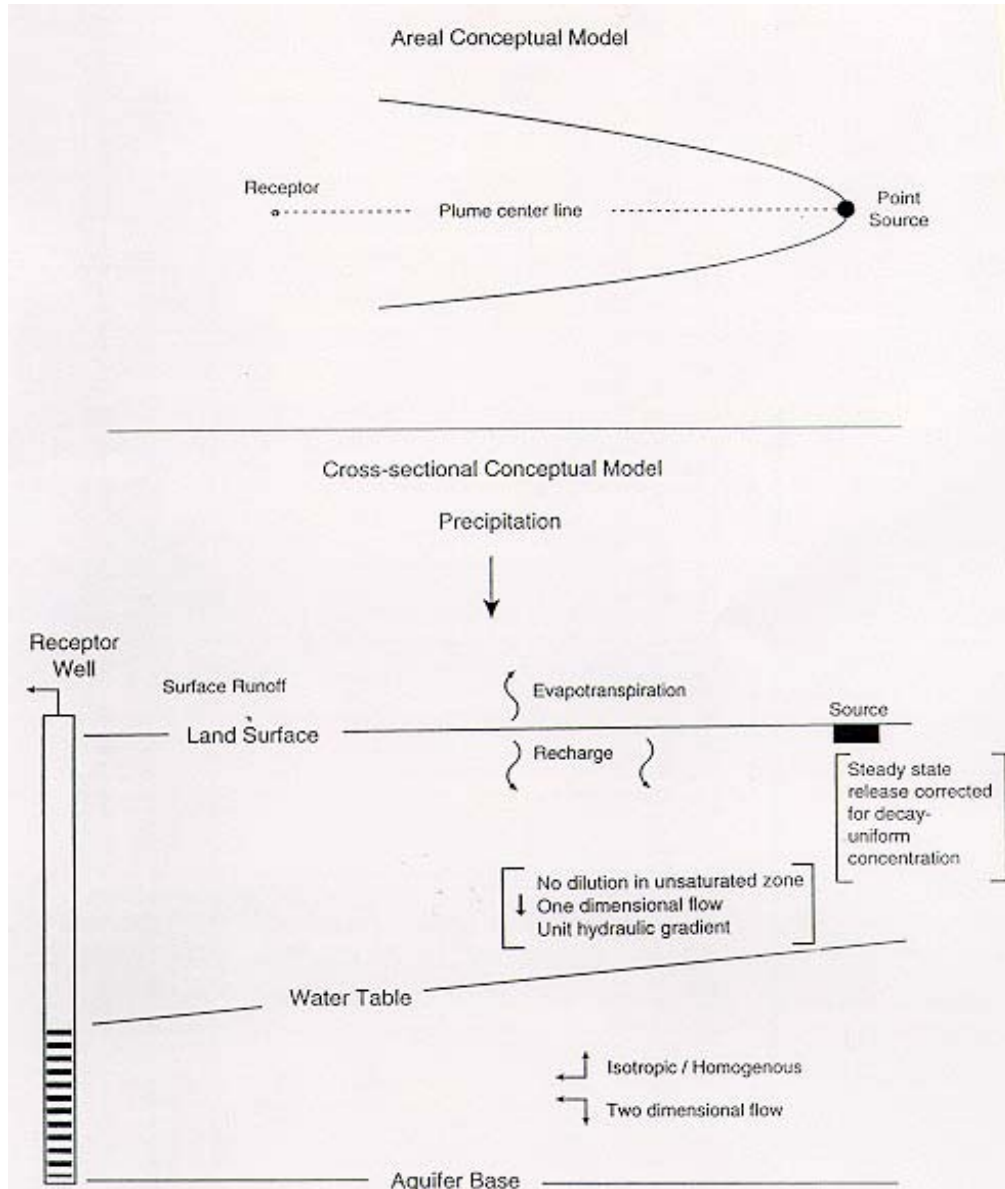


Figure 3-1. Typical conceptual model(s) in the scoping phase

values for the input parameters, such as ambient recharge, stream flow stages, and source concentration release rates. However, without accommodating the transient nature of these processes, predictions of peak contaminant concentrations arriving at downgradient receptors would have a high degree of uncertainty. The conceptual model could, therefore, be simplified to a translation of the physics of the system into relatively simple mathematical terms such as those described by analytical expressions.

#### *Restricted Dimensionality*

Ground-water flow and contaminant transport are seldom constrained to one or two dimensions. However, during scoping, modeling objectives and conceptual model development must take into account that information is rarely sufficient to describe mathematically the controlling flow and transport processes in three dimensions. In reality, most of the modeling analysis in the preliminary investigation will focus upon centerline plume concentrations which are essentially one- and two-dimensional analyses. One-dimensional analyses of the unsaturated zone are customarily performed in a cross-sectional orientation because flow and transport are predominantly vertically downward. Similarly, in the saturated zone, vertical gradients are generally much smaller than lateral gradients and, as a result, vertical transport need not always be explicitly modeled. Therefore, the assumption that flow is two-dimensional may be appropriate for areal analyses.

#### *Uncomplicated Boundary and Uniform Initial Conditions*

Boundary conditions are the conditions that the modeler specifies as known values in order to solve for the unknowns. Ground-water boundaries may be described in terms of where water is flowing into the ground-water system and where water is flowing out. Many different types of boundaries exist, including: surface-water bodies, ground-water divides, recharge, wells, and geologic features such as faults and sharp contrasts in lithology. Initial conditions are defined as values of ground-water elevation, flow volumes, or contaminant concentrations initially assumed to be present in the area of interest.

Because of the lack of site-specific data in the scoping phase, the system boundary and initial conditions usually cannot be accurately defined; only very limited

calculations of approximate travel distances and contaminant concentrations can be made.

#### *Uniform Properties*

Homogeneity describes a system where all of the characteristics spatially are uniform within the aquifer, whereas isotropy means that the hydraulic properties are identical in all directions. A homogeneous system may have anisotropic flow properties; for example, an otherwise homogeneous sandstone aquifer may have a greater hydraulic conductivity in the horizontal direction than in the vertical. Therefore, hydrogeologic units may have anisotropic qualities but still be considered spatially homogeneous throughout, provided the anisotropy does not vary within the unit.

Before site characterization, only the most general assumptions may be made about the relative flow properties of the aquifers. For example, it is often assumed that the hydraulic conductivity in the horizontal direction is ten times greater than that in the vertical direction for sedimentary deposits. These types of simplifying assumptions regarding the aquifer properties would form the basis of the conceptual model.

#### *Simplified Flow and Transport Processes*

Site-specific information describing the flow and transport processes that dominate the migration of radionuclides would not be available before detailed site characterization occurs. Therefore, modeling objectives would need to be limited to those that can be addressed with only limited knowledge of the site hydrogeology and geochemistry. In practice, this means that uniform porous media flow would be assumed in the conceptual model, and all of the geochemical reactions that affect the radionuclide transport would be lumped together as a single parameter termed the distribution coefficient.

Discrete features, such as macropores, fractures, and faults, would generally have to be excluded from the mathematical expression of the conceptual model, and conservative distribution coefficients would be selected from conservative values found in the literature. Movement through the unsaturated zone would be simulated with simplified versions of more complex equations describing the unsaturated flow and transport.

To demonstrate the potential effects that simplifying assumptions may have on modeling results, the discussion in Appendix B outlines the physical and chemical processes that may affect the transport of radionuclides (estimates of moisture content).

### 3.2 Evolution of the Conceptual Model

The conceptual model is based on the modeler's experience and technical judgment and represents the modeler's understanding of the system framework and behavior. The conceptual model will naturally become more complex as more processes are identified and interrelationships of important components within the systems are considered. The transformation of the conceptual model into a mathematical model which, in reality, is only an extrapolation of a basic understanding of the system, will result in intrinsic simplifications of the system. For example, the mathematical models assume that there is a direct scaling between the model simulations and the scale at which the data are collected. The lack of knowledge about the system resulting from limited information also contributes to inevitable simplifications between the conceptual and mathematical models.

Besides the simplifications inherent in the process, there are deliberate simplifications in which the modeler selects the physical characteristics and processes relevant to the model's application. Examples of these simplifying assumptions include:

- Flow through the unsaturated zone is vertical and in one dimension.
- Chemical reactions are reversible and instantaneous.
- Soil or rock medium is isotropic and/or homogeneous.
- Flow field is uniform and under steady-state conditions.

As more and more of these simplifying assumptions are found to be significant, the complexity of the model increases. Thus, the development of a dynamic model allows for the neglected components of the conceptual model to be integrated systematically.

Components of the conceptual model may be simplified, either because of limited objectives or because of constraints on data availability. Even when

the available data support the use of a more sophisticated model, simplifications are sometimes advisable. For instance, the site characterization modeling described in Section 4.2 discusses the application of complex numerical models. However, after applying these complex models, it is frequently possible to simplify the assumptions again and use less sophisticated models to meet the objectives of the risk assessment. This iterative process ensures that the mathematical model is consistent with the modeling objectives.

As discussed in Chapter 1, formulating a conceptual model is an integral component of the modeling process. The data obtained during site characterization provides an opportunity to remove some of the simplifications made in the scoping phase. Generally, in the site characterization phase, sufficient data are collected to formulate relatively complex conceptual models. Therefore, the degree to which the conceptual model is simplified frequently depends more on the objectives, than on limitations in the data. Figures 3-2 and 3-3 illustrate typical conceptual models in the site characterization phase of the investigation.

The following assumptions are typical of the conceptual model in the site characterization phase:

- Steady-State Flow/Transient Transport
- Multi-Dimensionality
- Steady-State Boundary and Non-uniform Initial Conditions
- Complex Flow and Transport Processes
- System Heterogeneity

These conceptual model assumptions generally translate into modeling approaches that are consistent with the data available during the site characterization phase. They are discussed in greater detail next.

#### *Steady-State Flow/Transient Transport*

The data obtained during the site characterization program are generally collected over a relatively short time and frequently do not reflect the temporal nature of the hydrogeologic system. Unfortunately, objectives in the site characterization phase often involve the prediction of temporal trends in the data.

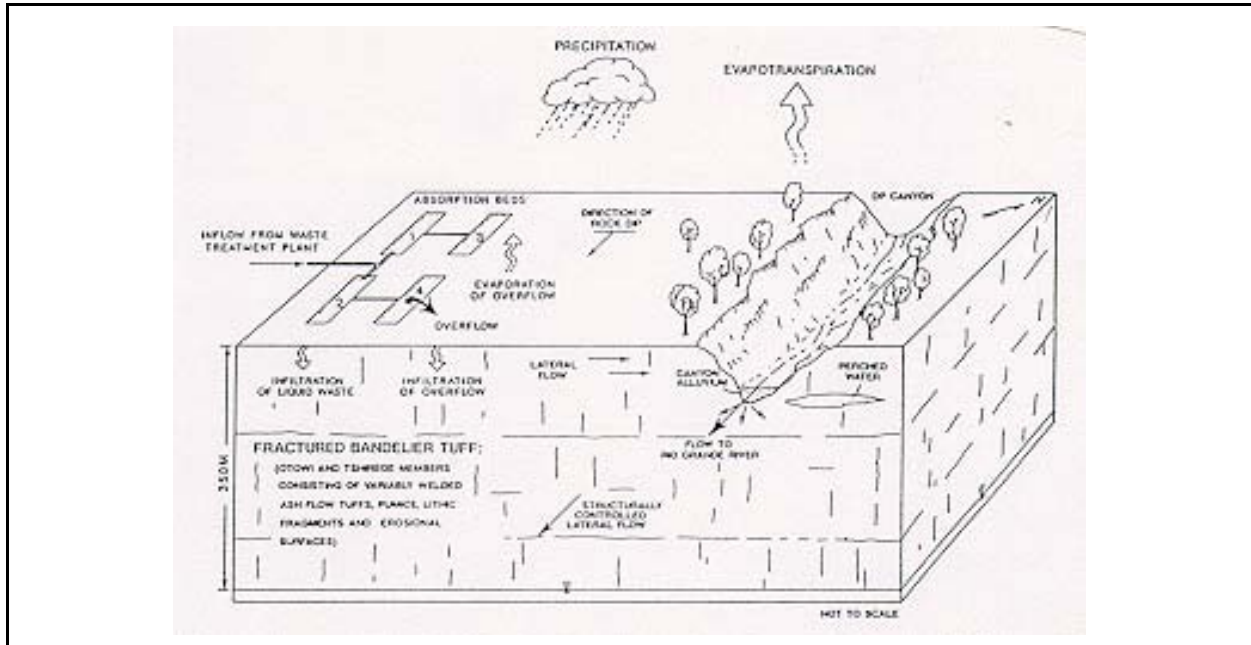


Figure 3-2. Representative conceptual model of the unsaturated zone.

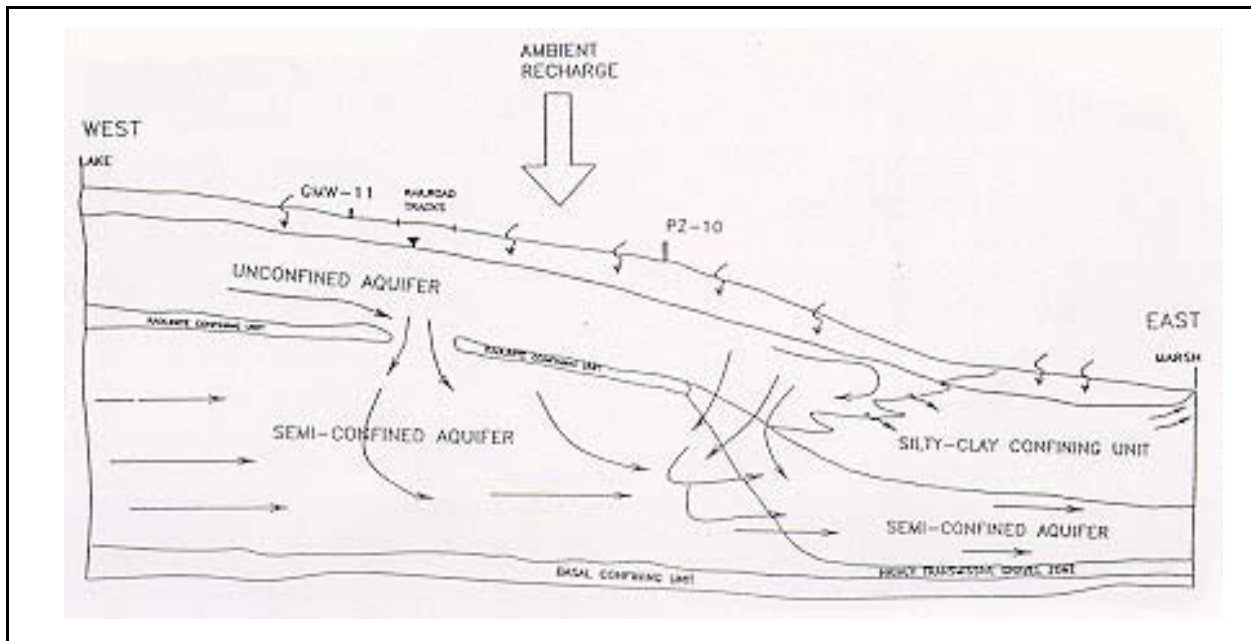


Figure 3-3. Representative conceptual model of the saturated zone.

For instance, the risk assessment generally includes an analysis of the peak arrival times of radionuclides at downgradient receptors. This incompatibility between the objectives and the data available gives rise to some of the greatest uncertainties associated with the entire remedial investigation. However, one of the principal utilities of mathematical models is their ability to extrapolate unknown values through time.

The modeling approach during site characterization generally assumes a steady-state flow field and accommodates the transient nature of the system through the contaminant transport analysis. Steady or transient leaching rates are used in conjunction with the existing plume concentrations for initial conditions. Therefore, the system is actually modeled as a steady flow system with possibly a transient or pulse-like source term. However, the transient nature of the plume is generally used as a model calibration parameter and is not carried forward into the predictive analysis for future radionuclide concentrations. That is, rarely are there sufficient data to describe the temporal nature of the source release. Exceptions to this occur when records are available pertaining to the volumes of radioactive liquids that were dumped over time into infiltration, recharge or evaporation trenches or when correlations between rainfall events and source leaching rates may be extrapolated.

The validity of the steady-state assumption depends on the features of the flow pattern, which are in turn dictated by the nature of boundary conditions and sinks or sources existing in the flow domain. Whether or not such an assumption is justified also depends on the time scale of interest and, perhaps most important, the conservative objectives of the modeling study.

For example, as mentioned above, ground-water flow modeling performed in conjunction with contaminant transport modeling is usually based on an assumption of steady-state flow. This is done to reduce the complexity and cost of the time-dependent transport simulation. Indeed, all analytical solutions and most of the numerical solutions of the contaminant transport equation likely to be used in the modeling study will be based on the assumption of a steady-state velocity field. Such an assumption is valid, provided that during the time period of the transport simulation the flow pattern or velocity distributions do not change significantly. A common pitfall is a situation where the modeler deals with the ground-water flow system

containing internal sinks or sources (e.g., pumping or injection wells) but ignores drastic changes in the velocity distribution due to changes in the well operation or flow rates. Another situation involves gradual or sudden changes in conditions at the flow boundaries which lead to reversal of flow directions during the period of the transport simulation. Such changes must be taken into account to obtain reliable predictions of contaminant migration.

As a cautionary note, one modeling report identified in the EPA CSMoS study (LEE95) assumed steady-state conditions based on only several months of ground-water monitoring data. This assumption resulted in a predicted ground-water gradient to the west, whereas contaminant data indicated that the plume was migrating northward. Obviously, steady-state assumptions must be based on a sufficient monitoring period.

#### *Multi-Dimensionality*

The site characterization program should be designed to gather sufficient data to develop a three-dimensional conceptual model. It is only after the three-dimensional system is relatively well understood that it can be determined whether one-, two-, or three-dimensional modeling is necessary. If one or two dimensions are eliminated from the analysis, careful consideration needs to be given to what impact restricting the dimensions will have on the model's capability to simulate existing field conditions.

The magnitude of flow and transport in any direction relative to the other directions provides the criteria for which dimension(s) should be included or excluded. In most instances, flow and transport in the unsaturated zone are assumed to be predominantly downward with smaller horizontal components. If the flow components are found to have two dominant flow directions, a two-dimensional cross section may allow for an adequate representation of the flow field.

Modeling and field validation studies of the vadose zone (the unsaturated zone) have yielded mixed results both in model calibration and in the comparison of transport predictions against measured field values. In modeling the vadose zone, as well as the saturated zone, the question is always how much uncertainty in the results is acceptable, considering the objectives.

Two-dimensional simulations of the saturated zone are

usually performed when the horizontal flow components are far greater than the vertical flow components, allowing the vertical components to be ignored. However, in much of the modeling performed for site characterization, the vertical components of flow are important because many natural features, such as surface water bodies, often have strong vertical flow components associated with them. Furthermore, particular care must be taken in eliminating the third dimension because attempts to simulate three-dimensional processes in two dimensions can lead to difficulties in model calibration, as well as in producing defensible modeling results.

Water-level data collected from closely spaced wells that penetrate the same aquifer and are screened at different depths provide excellent information on vertical hydraulic gradients. This information may be used during the site characterization program to determine the effective hydraulic basement of any contamination present, as well as recharge and discharge areas. If there are strong vertical gradients, the capability to simulate the vertical movement of ground water within the hydrogeologic system becomes very important in defining the nature and extent of the contaminant plume.

It should also be kept in mind that two-dimensional planar modeling will average the contaminant concentrations over the entire thickness of the aquifer, and the vertical definition of the contaminant plumes will be lost. This vertical averaging of contaminants will result in lower downgradient concentrations and may not provide a realistic or conservative baseline risk assessment. Again, this example illustrates that the decision as to how many dimensions to include in the modeling must be related to the objectives and the need to be aware of the limitations in the results if one or more dimensions are eliminated.

The recent development of more sophisticated pre- and post-processors greatly facilitates data entry and processing. These advances, in conjunction with the rapid increase in computer speeds over the past several years, have greatly reduced the time involved in performing three-dimensional modeling. In general, it is better to include the third dimension, even if many of the parameters in the third dimension have to be estimated than to constrain the analysis to two dimensions.

Two-dimensional analyses during the site characterization program are most valuable for modeling the unsaturated zone and for performing sensitivity analyses of selected cross-sections through a three-dimensional model. Two-dimensional approaches are also useful for performing regional modeling from which the boundary conditions for a more site-scale modeling study may be extrapolated.

#### *Steady-State and Non-uniform Initial Conditions*

In general, boundary conditions are known or estimated values that are assigned to surfaces and planes that either frame the perimeter of the modeled area or define the nature of release from the contaminant source. The different types of flow boundary conditions are: (a) head (ground-water elevation) is known for surfaces or planes bounding the modeled region; (b) ground-water flow volumes are known for surfaces or planes bounding the modeled region; and (c) some combination of (a) and (b) is known for surfaces or planes bounding the region. Boundary conditions could also be assigned to interior features of the modeled region where ground-water elevations or flow volumes are known, such as lakes, rivers, canals, lagoons, or marshes.

The most common types of contaminant source boundaries either specify the source concentration or prescribe the mass flux of contamination entering the system. The concentration is generally prescribed when the solubility limits of the contaminant largely controlled the release. The mass flux type boundary is typically used when a leaching rate is known or estimated. Specialized source boundaries have also been formulated which allow for radioactively decay in the source. The ability of the code to treat source decay may not be important if the parents and daughters have a relatively long half-life compared to the expected travel time to the nearest receptor.

One of the primary objectives of the site characterization program is to identify the presence and location of ground-water flow and contaminant source boundaries so that they may be incorporated into the conceptual model. These boundaries are generally quantified in terms of the volume of ground water and contamination moving through the system. The physical boundaries are then translated into mathematical terms as input into the computer model.



Initial conditions are defined as values of ground-water elevation, flow volumes, or contaminant concentrations, which are initially assigned to interior areas of the modeled regions. At least for the flow modeling performed during the site characterization, initial conditions are generally set to uniform values. This is because the temporal nature of the flow system is usually poorly defined. In addition, if the flow analysis is performed to steady-state, which is usually the case, the initial conditions assigned to the model domain are irrelevant as identical solutions will be reached for these values regardless of the values initially assigned. This occurs because these steady-state values depend solely on the values assigned to the boundaries of the model.

Non-uniform initial values (i.e., contaminant concentrations) are routinely used in the contaminant transport analysis to depict the geometry and varying contaminant concentrations within the plume, as well as to define the contaminant concentrations leaching from the contaminant source. The ability of a code to allow non-uniform initial conditions would be essential to a full description and simulation of the contaminant plume(s).

#### *Complex Flow and Transport Processes*

Site-specific information describing the flow and transport processes that dominate the migration of radionuclides is not available during the scoping phase of the investigation. As the site characterization activities progress, greater attention is focused on the physical, chemical, and biological processes that affect ground-water flow and contaminant transport. Up until this time, attention has been paid primarily to estimating parameter ranges and variances within these ranges via sensitivity analyses. This approach has limitations and needs to be broadened during the site characterization phase if ground-water flow and contaminant transport are to be well described. This parameter-based approach is expanded by using computer codes that mathematically accommodate the dominant flow and transport processes. These processes could include flow and transport through fractures, density-driven flow, matrix diffusion, fingering, surface-water/ground-water interactions, and geochemical reactions. If active, each of these processes can invalidate the output of models based on the assumption that uniform flow and transport are occurring through a homogeneous porous media.

Even at this stage, all of the geochemical reactions that affect radionuclide transport are likely to be lumped together into a single parameter, termed the distribution coefficient. However, a better delineation of any geochemical facies would allow for the distribution coefficient to vary from layer to layer as well as within the units themselves. If this simplified means of simulating geochemical processes is found to be inadequate, it may be necessary to use thermodynamically based geochemical models in order to address specific geochemical reactions.

Movement through the unsaturated zone can be simulated in a number of different ways, depending upon the objectives. If the unsaturated zone is relatively thin and travel times are short, simplified versions of more complex equations describing the unsaturated flow and transport may suffice. However, if the travel time through the unsaturated zone is significant and accurate flow and transport predictions are required, then mathematical methods, which account for complex processes associated with flow and transport through the unsaturated zone, may be necessary.

The modeling objectives need to be defined prior to the characterization; only then can the modeler be sure that data are sufficient to perform modeling at the necessary level of complexity. All too often, limitations in the data, rather than the modeling objectives, drive the sophistication of the modeling.

#### *System Heterogeneity*

One of the primary objectives of the site characterization program is to identify heterogeneity within the system and to delineate zones of varying hydraulic properties. System heterogeneity is one of the leading causes of a poor understanding of the physical system controlling flow and transport.

If an accurate simulation of heterogeneous rocks is required to meet the modeling objectives, a modeling approach which allows for zones with different porous rock properties is required; however, relatively few codes can simulate discrete features, such as faults, fractures, solution features, or macropores.

### 3.3 Remedial Design and Implementation

As the site investigation proceeds into the remedial phase, data are acquired that will be useful in identifying feasible remedial alternatives. In combination with models, these data are used to simulate flow and transport. By predicting the behavior of ground-water flow and the transport of radionuclides the data and models in the selection and design of the remedy and can be used to demonstrate that the chosen remedy will achieve the remedial goals.

Once remedial action alternatives have been identified, their design may be refined as part of the development of a conceptual design. Optimizing a design involves evaluating alternative screen depths, pumping rates, and well locations to identify the most effective configuration.

Numerous studies have demonstrated the benefits of using models to evaluate the flow of ground water and the transport of radioactive substances. Models have been used in the detailed analysis of alternative actions to identify actions that would be ineffective or would fail to meet the site's remediation goals. The quantitative measures of performance derived from simulation provide a useful basis for comparison with other factors like the costs of remedial action. However, if the travel time through the unsaturated zone is significant and accurate predictions of flow and transport are required, then mathematical methods may be necessary to account for the complexity of flow and transport through the unsaturated zone.

The modeling objectives associated with remedial alternative design generally are more ambitious than those associated with the site characterization phase. Therefore, it often is necessary either to select an advanced computer code or to modify the existing model to simulate the more complex conditions. The following are specific examples of processes that may not be important to assessing baseline risk or to site characterization but are often essential to the remedial design:

- three-dimensional flow and transport
- matrix diffusion (pump-and-treat)
- desaturation and resaturation of the aquifer (pump-and-treat)

- heat-energy transfer (in-situ vitrification/freezing)
- sharp contrasts in hydraulic conductivity (barrier walls)
- multiple aquifers (barrier walls)
- movement from confined to unconfined conditions (pump-and-treat)
- simulation of complex flow conditions (pumping wells, trenches, injection wells)

From a modeling standpoint, the remedial design and implementation is the most challenging phase of the investigation. Frequently, it is the first time that data are sufficient to verify the model's predictions. The many potential remedial actions (e.g., pump and treat) provide excellent information on the temporal response of the flow and transport to hydraulic stresses. These data allow continuous refinement to the calibration, making the model a powerful management tool.

The modeling approaches taken at various sites generally would have the following characteristics of the conceptual model in common:

- Transient Flow and Transport
- Multi-Dimensionality
- Prescribed Boundary and Non-uniform Initial Conditions
- Specialized Flow and Transport Processes
- System Heterogeneity

#### *Transient Solutions*

By the time of the remedial design phase, the available data usually span a relatively long period, which often allows the temporal nature of the hydrogeologic system to be well defined. The objectives of remedial design can involve many criteria that could not be met during the site characterization phase. Many of these additional criteria may require that the code simulate transient flow and transport which is necessary to evaluate the effectiveness of remedial alternatives. One such alternative is the placing of earthen covers and a broad range of natural and synthetic barriers, which are engineered to cap the surface and subsurface soil. The cover prevents rainwater from percolating through contaminated soil and carrying

radionuclides to the ground water. In the site characterization program, the objectives could probably have been met by assuming a constant areal recharge over the modeled area. However, this steady-state approach would not account for varying recharge rates, which would be needed to simulate the deterioration of the cap and the subsequent effect on the leaching rates of radionuclides.

Excavation of radioactively contaminated soil will leave some residual radioactivity in the soil contiguous to the removal operations. It also could redistribute contaminants in the unsaturated zone. Without the ability to perform transient simulations, with the source now largely removed, it would not be possible to determine how long it would take for the remedial actions to have a noticeable effect on downgradient receptors.

#### *Multi-Dimensionality*

The need to perform three-dimensional modeling during the remedial phase will largely depend on the remedial alternatives being considered and how their effectiveness will be evaluated.

The remedial alternatives that are most commonly supported by three-dimensional and quasi-three-dimensional modeling are those that impart a strong artificial stress to the hydraulic flow field, such as pumping wells and extraction trenches. Often, before these stresses are imposed, vertical ground-water gradients are up to several orders of magnitude less than the horizontal gradients and, therefore, can be ignored; this simplification allows the system to be modeled using a one- or two-dimensional flow analysis. However, when imposed stresses significantly alter on the hydraulic gradients, three-dimensional flow fields generally develop. Without the ability to simulate a three-dimensional flow field, it would be very difficult to determine capture zones and influent contaminant concentrations largely because vertical leakage from units above and below the screened interval of the extraction well would be ignored, as would vertical concentration gradients.

Another remedial alternative that generally creates three-dimensional flow fields is installation of physical barriers to ground-water flow. Whether the barriers consist of grout injection techniques, sheet pile cutoff

walls, or bentonite slurry walls, all have a common problem: the hydraulic head builds up behind the structures and induces vertical gradients, allowing ground water to flow under the barriers. In these cases, the analysis of vertical flow component is essential in determining probable leakage rates and the volume of water that would potentially flow beneath the structure.

#### *Transient Boundary and Non-Uniform Initial Conditions*

Most of the analysis up until the remedial phase can be modeled with steady-state boundary conditions; i.e., physical features, such as the water elevations of surface water bodies and areal recharge, can be simulated with values that are constant in time. The objectives of the remedial phase, however, may demand that the transiency of these boundaries be considered in the analysis. Time-weighted averages may no longer apply. For instance, water bodies, such as radioactively contaminated waste lagoons, probably would have been treated as constant boundaries, and their water-surface elevations would have been held constant. However, if one of the remedial activities involved withdrawing contaminated water from one or more of the lagoons, the effect that the change in water-surface elevations would have on the ground-water gradients could be evaluated only by simulating the drop in surface elevations with time. This would be simulated by prescribing progressive changes in the lagoon water level over time.

The ability to prescribe boundaries within the model domain also would be important in the evaluation of in-situ soil flushing techniques, which are used to enhance the mobility of contaminants migrating towards recovery points. In this case, recharge would be varied with time to reproduce the effects that various rates of flushing would have on the ground-water flow and transport of contaminants.

Protective barriers to ground-water flow are constructed of very low permeability material and emplaced either to prevent contaminated ground-water from migrating away from a site or to divert incoming clean ground water away from the source of contaminants. Potentially, barriers can last for several decades, barring any geological disturbances, such as tremors, ground settling, or significant changes in hydraulic gradients. However, if a barrier should fail,

water may infiltrate the site, and contaminated leachate may move beyond the site. Therefore, the effects of failure of a barrier to ground-water flow and transport should be evaluated. The failure of the barrier can be simulated in several ways. The most straightforward method is to use transient boundaries to simulate additional flow through the barrier as well as a reduction in the difference between water-level elevations in front of and behind the barrier. Therefore, the selected code should be able to incorporate transient boundaries.

#### *Specialized Flow and Transport Processes*

The design and evaluation of remedial alternatives frequently involve consideration of flow and transport processes that probably were not explicitly modeled during site characterization. These processes include complex geochemical reactions, matrix diffusion, heat flow, and possibly, biological reactions.

As discussed, few numerical models satisfactorily couple ground-water flow and contaminant transport to complex geochemical reactions. The complex geochemical models are based upon the laws of thermodynamics, so they predict the potential for a particular reaction to occur within a closed system. Consequently, it is important that the controlling geochemical reactions are examined, possibly in laboratory benchscale or field studies. This is particularly significant when physical/chemical stabilization processes are considered as a remedial alternative. In these processes, physical or chemical agents are added to and mixed with a waste (typically sludge in pits, ponds, and lagoons), to improve the handling or leaching characteristics of the waste destined for land disposal.

A detailed understanding of geochemistry also can be very useful in estimating leach rates for uranium mill tailings which otherwise might be associated with unacceptably high uncertainties.

Matrix diffusion is the process by which concentration gradients cause contaminants either to move into or be drawn out of low-permeability areas where diffusion rather than advection and dispersion governs contaminant transport. Pump-and-treat systems tend to draw water from the more permeable units, which may leave large volumes of contaminants stored in the clays and other fine-grained materials, which will

eventually diffuse out. Many computer codes do not adequately simulate this very slow process. If matrix diffusion is not accounted for, the movement of the contaminant will be based solely on ground-water velocities rather than the diffusion term. Ground-water velocity generally will move the contaminant much more rapidly than diffusion, and clean-up times may be dramatically underestimated.

In-situ vitrification (ISV) of soils is a destructive thermal treatment that converts contaminated soil and waste into a chemically inert, stable glass and crystalline product that resembles obsidian. Predicting the effectiveness of ISV requires the modeling of several specialized processes. One such process would be vapor transport of radionuclides, such as tritium, which would be an important health consideration if the media was heated.

Microbial fixation appears to affect the transport of radionuclides under some conditions. Radionuclides may be either immobilized or mobilized by organisms or plants. Immobilization may occur if radionuclides are incorporated in the cells of microorganisms or plants that are relatively stationary. On the other hand, radionuclides may be mobilized by forming biocolloids with bacteria, spores, and viruses. Modeling microbial processes requires a code that, at a bare minimum, allows a degradation rate to be assigned to the contaminant(s).

#### *System Heterogeneity*

The ability of a code to accommodate severe contrasts in the properties of soils and rocks is particularly important in designing and evaluating physical barriers for protecting ground water. If the application involves extending the barrier down to a low-permeability strata to form a seal and deter underflow leakage, it is important that the code can incorporate multiple stratigraphic layers, as well as sharp contrasts in hydraulic conductivity. Only in this way can the modeler show how contaminant flow and transport affects leakage through the barrier wall and basement strata.

## CHAPTER 4 —MODEL APPLICATION

Figure 4-1 shows the three primary sources of ground-water contamination by radioactivity that lead to four possible contamination scenarios: (1) placing wastes beneath the water table in direct contact with the ground water, (2) placing wastes above the water table, (3) disposing of wastes in surface impoundments and seepage basins, and (4) recharge from surface water bodies (streams, rivers, lakes) to the ground water. Once the radioactivity reaches the ground water, it may be reintroduced to the ecosystem in the following ways: (1) discharge to rivers, lakes, and other surface water bodies, (2) pumped to the surface, (3) brought to the surface through plant transpiration (phreatophytes), and (4) transport of vaporized radionuclides undergoing phase transformations (e.g.,  $^3\text{H}$ ,  $^{14}\text{C}$ ,  $^{85}\text{Kr}$ , and  $^{222}\text{Rn}$ ).

The complexity of the analysis of the fate and transport of radionuclides will depend upon the objectives of the evaluation as well as on the availability of the necessary data. It is important to understand the uncertainty associated with the data used for the analysis because this uncertainty will play a role in evaluating the results of the analysis. As a general rule, it is best to start with the simplest means of evaluating the data and progress towards more complex techniques. Appendix B presents simplistic but useful calculations that may be made for release rates, and the fate and transport of ground water and radionuclides. Appendix B also gives some examples of problems where common analytical methods, which are less complex than numerical methods, have been used to estimate the fate and transport of radionuclides.

Prior to scoping calculations, the appropriate release mechanisms for the movement of radionuclides to the ground water must be determined. If it is relatively certain that one or more components of the conceptual model (e.g., unsaturated zone) is unimportant, then it may be neglected. The physical and chemical processes affecting the fate and transport of radionuclides at the site (e.g., fracture flow, vapor transport) also needs to be determined. An earlier report issued as part of this interagency agreement outlines how to determine what site-related characteristics may be important (EPA94a).

After these determinations have been made, it must then be decided how accurate the results need to be and what level of analysis is appropriate to obtain the desired results. If the physical and chemical processes at the site are too complex to be satisfactorily predicted by simplistic data analysis, then experts in the field should be consulted regarding how to proceed. It is not practical to perform complex analyses without the use of computer programs and considerable expert help.

The calculational methods presented in this chapter and Appendix B are focused on scoping level analyses. They have been divided into two parts: the release analysis and the fate analysis. The equations given in the release analysis section are used to estimate contaminant release concentrations and volumetric release rates. The fate analysis section deals with the processes influencing radionuclide transport and how to estimate radionuclide concentrations in the ground water.

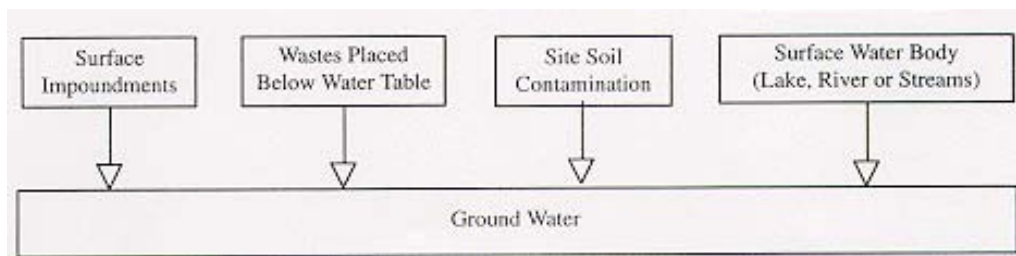


Figure 4-1. Modes in which ground water may become contaminated

## 4.1 Scoping Calculations

One of the primary goals of mathematical modeling is to synthesize the conceptual model, as discussed in Chapter 3, into mathematical expressions, which in turn are solved with either a hand calculator or a microcomputer. However, accurate modeling of all aspects of the conceptual model is not always necessary; only certain components require modeling. In practice, early modeling focuses upon assessing the significance of specific parameter values and their effects on flow and transport, rather than modeling specific hydrogeologic transport processes. For instance, it is common during the scoping phase to evaluate transport as a function of a range of hydraulic conductivities; however, it is unlikely that more complex processes, such as flow and transport through fractures, would be considered.

This section, in conjunction with Appendix B, describes methods used to calculate the volume and concentration of radioactivity that may be expected to reach the ground water from several types of contaminant sources (Figure 4-1). Also described are methods for estimating transit times and concentrations of radionuclides. To impart a sense of the uncertainties inherent in the calculations, the primary mechanisms that affect the fate and transport of radionuclides are discussed. In particular, it is important to keep in mind that all of the complex geochemical reactions that influence radionuclide transport generally are lumped into a single parameter termed the distribution coefficient ( $K_d$ ). Without a basic understanding of how these processes can affect radionuclide transport, even the most simplistic analysis may have fundamental flaws. Therefore, the geochemical processes affecting radionuclide transport are discussed briefly in Appendix A. In Appendix B, a series of screening calculations are given with several examples of problems illustrating the mathematical methods that may be used to estimate radionuclide transit times and concentrations.

### 4.1.1 Release Analysis - Ground Water

When analyzing a radionuclide release to ground water, the potential release mechanisms should be evaluated first. This evaluation involves a qualitative screening approach aimed at determining the sources of release. The factors and mechanisms that may significantly affect the potential for release are then analyzed; this may require more detailed field investigations or numerical modeling.

Several mechanisms may release radionuclides to the ground water either directly or indirectly, as follows:

- Direct discharge (e.g., on-site release from treatment processes)
- Generation of leachate (e.g., from buried wastes, surface impoundments, and absorption beds)
- Overland flow (e.g., from impoundment overflow or failure, drum leakage)

Generation of leachate and direct discharges are the mechanisms most likely to affect ground water directly. Overland flow might affect ground water indirectly, and is discussed in Appendix B.

Several factors affect leachate release:

- Physical/chemical/radiological properties of the radionuclides;
- Type of waste form and container (e.g., steel drums, wooden or cardboard boxes, plastic bags, absorption beds);
- Length of time that the wastes have been stored or buried;
- Hydrogeologic framework of the system (e.g., depth to water table, soil/rock properties);
- Quantity of wastes;
- Climatological considerations (e.g., precipitation).

Information about the physical, chemical, and radiological properties of the radionuclides may help to determine the associated disposal practices, which may, in turn, assist in estimating the potential for release. Furthermore, the physical and chemical properties of a particular radionuclide will dictate its fate and transport processes.

A clear understanding of the physical system (e.g., climatology, hydrogeology) is necessary as a basis from which to predict migration rates and exposure pathways.

Information about when the wastes were disposed or emplaced and the quantities involved is important

when estimating concentrations of radionuclides that could potentially reach sensitive receptors.

Ground-water contamination results from radionuclides leaching from surface or subsurface soils; from treatment, storage, and disposal areas; and from the direct migration of liquid wastes. Radionuclides can be leached from disposal areas by precipitation and runoff that percolates through the soil or by direct submersion of the waste in ground water. Unlined lagoons and surface impoundments may introduce contaminants directly into ground water. The containers for radioactive materials stored above ground may leak and percolate to ground water. The potential for release from all of these sources must be evaluated; any that are significant generally undergo a more quantitative assessment.

Estimation of release involves two quantifications: (1) of radionuclide concentrations in waste and/or leachate, and (2) of the volume of the leachate or direct-discharge release rates. The procedures vary, depending upon the characteristics of the release site. Section B.1 of Appendix B describes procedures to calculate steady-state releases of radionuclides to ground water. The calculations focus on release concentrations and volumetric release rates. For ponds or lagoons, the concentration of the radionuclide in the lagoon or impoundment is considered to be the concentration of the leachate. This assumption ignores the geochemical reactions that may be occurring at the base of the pond where sediments may tie up high concentrations of radionuclides when oxidizing conditions prevail (summer) and release pulse concentrations of contaminants when reducing conditions are favored (winter). Methods for estimating volumetric release rates are presented for both solid and liquid wastes.

#### 4.1.2 Fate Analysis - Ground Water

The nature of the ground-water environment restricts the number of processes that control the fate of radionuclides as they are transported from their source to the receptor area. These processes fall into two categories: transport processes and radioactive decay. Transport-related processes (i.e., sorption, ion exchange, and precipitation of solids) can facilitate or retard the movement of ground-water contaminants, but radioactive decay always results in a loss of activity (disintegrations or decays per second) of the original radionuclide. However, as the parent

radionuclide disintegrates, radioactive or chemically toxic daughter products can increase.

Calculational screening methods do not directly simulate fate processes that influence the transport of radionuclides. Generally, the effects of these processes on transport are combined into a single term, designated the distribution coefficient. In Appendix A, these fate processes are discussed qualitatively to provide a general understanding of distribution coefficients, which are later used in Section B.2 (Appendix B) to determine quantitative retardation factors. Fate processes associated with radionuclide transport must be explicitly simulated, geochemical and/or hydrochemical computer models will be needed.

#### 4.1.3 Analytical Methods for Aquifer Flow and Transport

Analytical ground-water transport models can be used for certain analyses where the available data do not warrant a more complicated numerical analysis. Such models are useful for scoping the transport problem and may frequently be adequate for regulatory needs if the model and corresponding input data are chosen conservatively.

Analytical transport solutions are generally able to simulate only systems that assume steady-state flow conditions. However, because the available data rarely support transient simulations during the scoping phases, common analytical methods may often be used more effectively than numerical methods. It is much easier to conduct bounding and sensitivity analyses with analytical rather than numerical models. Examples of such calculations are presented in Appendix B.

#### 4.1.4 Uncertainty Analysis

In the scoping phase, the uncertainty in the analysis should be emphasized. Uncertainty is inherent in models of the behavior of a hydrogeologic system because our knowledge is incomplete. Many parameters used as inputs to a model are obtained by data collection. Investigators knowledgeable about the data they collect make a finite number of observations, choosing the parameters, and, how, where, and when to measure them. However, the collection process itself can introduce uncertainty through errors in measurements, the system's inherent randomness, and

limited sampling of the variable physical, chemical, and biological properties of the system. In many aspects of data collection, the professional judgment of an analyst with expertise in the area of investigation often enters into the scientific process. For example, selecting methods to collect data, interpreting data, developing conceptual models, and selecting model's parameters all require professional analysis and judgment. Therefore, the uncertainty in input parameters used in predictive models may result from several sources, including incomplete data, intrinsic spatial variability of the property in question, uncertainties in measurement, and uncertainties resulting from differences in scale between acquisition of the data and application of the model.

In practice, much of the early modeling focuses on assessing the significance of the uncertainty associated with specific parameters and their effects on flow and transport, rather than on modeling specific processes of hydrogeologic transport. For instance, it is common during the scoping phase to evaluate transport as a function of a range of hydraulic conductivities; however, it is unlikely that more complex processes, such as flow and transport through fractures, would be considered.

In general, the uncertainty associated with each of the parameters is expressed by a probability distribution, which yields a likely range of values for each parameter. It is important to select a model where individual parameter values can be selected systematically from the range and easily substituted into the governing mathematical equations that describe the dominant flow and transport processes at the site. In this manner, the effects of a single parameter or a multitude of parameters on the rate of contaminant movement and concentrations may be evaluated. This technique of substituting one value for another from within a range of values is called a sensitivity analysis.

In many cases, the possible range of values of important parameters is unknown or very large. Consequently, the analyst has little alternative but to evaluate the sensitivity of the results to a very broad range of possible values. Many of these early results will be unrealistic but cannot be ruled out until reliable site data are obtained. These types of analyses are useful because they help to direct the field work. However, they also can be used incorrectly. For example, individuals unfamiliar with the scoping

process could reach grossly inappropriate conclusions about the potential public-health impacts of the site based on these scoping analyses. Accordingly, care must be taken to assure that the results of scoping analyses are used for their intended purpose.

Sensitivity analyses identify the main contributors to the observed variation in the results. These techniques typically are applied iteratively. The first iteration can include rather general assumptions leading to preliminary results that help focus these techniques in subsequent iterations. Thus, the resources required for the uncertainty reduction techniques can be directed at the areas of the site characterization where the benefits of understanding uncertainty and reducing it (where possible) are greater.

However, sensitivity analyses alone will rarely identify a flawed conceptual model. For example, the failure to identify and include a fault(s) in the conceptual model subsequently would not account for preferential pathways that could, potentially, underestimate receptor concentrations.

An alternative to the detailed sensitivity analysis is a conservative bounding approach. In this less demanding analysis, values are selected from the range of parameters to provide the highest probability that the results are conservative, i.e., that the migration rates and concentrations of the contaminant would not be underestimated. For example, high values of hydraulic conductivity combined with low effective porosities and distribution coefficients would maximize the predicted migration rates of the contaminant although its concentrations at receptors may be underestimated.

Tables 4-1 and 4-2 give preliminary guidance on the general effects that various parameters have on the modeling results. Table 4-1 indicates whether the high end or low end of the parameter's distribution should be used if a conservative estimate (i.e., maximum value) of the extent of contamination is desired. The same concept has been used in Table 4-2 to show the effect of various parameters on the maximum concentrations arriving at a downgradient receptor. As shown in these tables, when estimating the maximum extent of contamination, the dispersivity should be maximized. The opposite is true when estimating maximum concentrations; in this case dispersivity should be minimized.



**Table 4-1. Bounding Analyses: Extent of Contamination**

Parameter	Maximum	Minimum
Source Term		
Constant Concentration	Insensitive	
Mass Flux	Insensitive	
Unsaturated Zone		
Infiltration Rate	High	Low
Moisture Content	Low	High
Total Porosity	Low	High
Bulk Density	Low	High
Distribution Coefficient	Low	High
Saturated Zone		
Aquifer Thickness	Insensitive	
Gradient	High	Low
Distribution Coefficient	Low	High
Dispersivity	High	Low
Effective Porosity	Low	High
Hydraulic Conductivity	High	Low
Well Location and Intake Depth	Shallow/Plume Centerline	Deep/Off Plume Centerline

**Table 4-2. Bounding Analyses: Concentration of Contaminants**

Parameter	Highest	Lowest
Source Term	Constant Concentration	Mass Flux
Unsaturated Zone		
Infiltration Rate	High	Low
Moisture Content	Low	High
Total Porosity	Low	High
Bulk Density	Low	High
Distribution Coefficient	Low	High
Saturated Zone		
Aquifer Thickness	Thin	Thick
Gradient	Low	Low
Distribution Coefficient	Low	High
Dispersivity	Low	High
Effective Porosity	Low	High
Hydraulic Conductivity	Low	High
Well Location and Intake Depth	Shallow/Plume Centerline	Deep/Off Plume Centerline

4.2 Site Characterization Modeling

In the scoping phase of the investigation, data limitations impose a simple modeling approach which uses conservative parameter estimates. One of the primary objectives of the site characterization program is to obtain sufficient data to enable the conservative modeling approach to be replaced by a defensible and more realistic approach which incorporates site-specific data.

Conservative analysis by itself cannot meet many of the objectives defined for the site characterization phase of the investigation. If parameter values are not known, it may be necessary to make conservative estimates; however, the effects that a conservative approach may have on other aspects of the remedial program must be considered. For example, if, during the baseline risk assessment, conservatively high

hydraulic conductivities are used in order to ensure that the downgradient contaminant arrival times are not underestimated, several problems may occur. First, it would be difficult to calibrate the model to known parameters (e.g., potentiometric surface), and adjustments to other parameters would be required in order to match measured field values. The end result would be a model that poorly predicts system responses to hydraulic stresses (e.g., extraction wells). A second problem would involve contaminant concentrations. A conservative increase in hydraulic conductivity would predict more ground-water flow through the system than is actually occurring, which might result in an underestimate of the contaminant concentrations at downgradient receptors. More problems may arise during the remedial design. If the modeling results are used to estimate clean-up times, the model may predict that water and contaminants are flowing faster than they actually are and at lower

concentrations. This would result in an underestimate of both the amount of time required for remediation as well as the contaminant breakthrough concentrations.

The major impact that a more specific conceptual model of the site will have on model application is that now parameter ranges have been narrowed by additional data acquisition, and sensitivity analyses can become more focused. Refinement of the parameter values diminishes the need to perform so many sensitivity analyses. In view of the increased demand for more accurate simulation of the controlling flow and transport processes, the advantages of scoping type analyses are outweighed by their inability to simulate more complex conditions. Therefore, model application in the site characterization phase will generally be performed with numerical models.

After the conceptual model is formulated and the modeling objectives are clearly defined in terms of the available data, the investigator should have a good idea of the level of sophistication that the anticipated modeling will require. Now, one or more computer code(s) can be chosen that have the attributes necessary to describe mathematically the conceptual model at the desired level of detail. Selecting the code requires a detailed analysis of the conceptual model to determine the degree to which specific waste and site characteristics need to be explicitly modeled. The selection process and evaluation criteria are described in a joint agency publication (EPA 94).

During the site characterization phase, application of the model is generally quite sophisticated and typically experienced modelers are in charge of the modeling process.

Therefore, this section will not describe the modeling process step-by-step, but, rather, will provide the Remediation Manager and support personnel with sufficient information to allow the remedial team to make informed decisions about ground-water modeling.

Accordingly, this section has three goals:

1. to impart a general understanding of how ground-water modeling is carried out in the site characterization phase and what objectives are achievable.

2. to outline the topics that should be covered in the application report and how results should be presented to facilitate peer review.
3. to provide relatively simple methods that can be used as reality checks on modeling performed by others.

This section is organized into subsections that follow a path typical of model application strategies. Specific guidance for each subsection is tabulated in Table 5-1.

#### 4.2.1 Code Selection

After formulating the conceptual model, it is necessary to select one or more computer code(s). Three basic choices are available: analytical, semi-analytical, or numerical codes. Analytical and semi-analytical methods, which are limited to simplified representations of the physical setting and flow and transport processes, are ideally suited for performing sensitivity and conservative bounding analyses because they are computationally efficient (i.e., fast) and require relatively little data as input. As discussed in Section 4.1.3, analytical models are typically designed for easy performance of sensitivity analyses. In contrast, numerical methods do not lend themselves to the same kind of "simplified" applications. Primarily because numerical models are difficult to set up and require substantial data input to calibrate the model, and multiple parameter substitutions are generally very cumbersome. However, as the modeling objectives become more complex and can no longer be addressed by simple bounding and sensitivity analyses, additional field data and more sophisticated analysis methods (e.g., numerical models) become necessary.

The greatest difficulty in selecting the most appropriate computer code is not in determining which codes have specific capabilities, but rather, which capabilities are required to support remedial decision-making during each phase of the remediation at a specific site. The necessary degree of sophistication of the modeling can be evaluated in terms of both site-related issues and objectives, as well as the qualities inherent in the computational methods for solving ground-water flow and transport equations.

A contaminant fate and transport model results from the application of a previously written or new

computer code to a specific problem via the collection of input data and the parameterization of site characteristics. The resultant model is, therefore, a merger of a mathematical formulation, solution methodology, data, and ancillary information which enhances or controls the use of the model. In addition to selection criteria for the modeling objectives which were presented in the previous section, the code evaluation process must also consider attributes that are integral components of the computer code(s) including;

- Source Code Availability
- History of Use
- Code Documentation
- Code Testing
- Hardware Requirements

The development of selection criteria presented in this section takes an approach consistent with industry standards by relying on published reports pertaining to the quality assurance and quality control in the development and application of computer codes.

#### *Source Code Availability*

To facilitate a thorough review of the generic code, detailed documentation of the code and its developmental history is required. Also, the source code must be available for inspection. In addition, to ensure independent evaluation of the reproducibility of the verification and validation results, the computer source code as well as the compiled version of the code (i.e., computer code in machine language) should be available to the reviewer, together with files containing the original test data used in the code's verification and validation.

#### *History of Use*

Much of the information needed for a thorough code evaluation can be obtained from the author or distributor of the code. In fact, inability to obtain the necessary publications may indicate that the code is either not well documented or that the code is not widely used. In either case, the inaccessibility of the documentation and related publications should be strong grounds for deciding that the code is unacceptable.

The acceptance and evaluation process should rely on

user opinions and published information in addition to hands-on experience and testing. User opinions are especially valuable in determining whether the code functions as documented or has significant errors or shortcomings. In some instances, users independent of the developer have performed extensive testing and bench-marking or are familiar with published papers documenting the use of the code. Users will also have first-hand knowledge about how easy it is to use the code and what level of experience is required.

#### *Quality Assurance*

Code selection should be closely tied to the quality assurance criteria followed during the development of the computer code. These criteria will determine the adequacy of the code testing and documentation.

Quality assurance in modeling is the procedural and operational framework put in place by the organization managing the modeling study, to assure technically and scientifically adequate execution of all project tasks included in the study, and to assure that all modeling-based analysis is verifiable and defensible (TAY85).

The two major elements of quality assurance are quality control and quality assessment. Quality control refers to the procedures that ensure the quality of the final product. These procedures include the use of appropriate methodology in developing and applying computer simulation codes, adequate verification and validation procedures, and proper usage of the selected methods and codes (HEI92). To monitor the quality control procedures and to evaluate the quality of the studies, quality assessment is applied (HEI89).

Software quality assurance (SQA) consists of the application of procedures, techniques, and tools through the software life cycle, to ensure that the products conform to pre-specified requirements (BRY87). This requires that in the initial stage of the software development project, appropriate SQA procedures (e.g., auditing, design inspection, code inspection, error-prone analysis, functional testing, logical testing, path testing, reviewing, walk-through), and tools (e.g., text-editors, software debuggers, source code comparitors, language processors) need to be identified and the software design criteria be determined (HEI92).

Quality assurance for code development and maintenance implies a systematic approach, starting with the careful formulation of code design objectives, criteria, and standards, followed by an implementation strategy. The implementation strategy includes the design of the code structure and a description of the way in which software engineering principles will be applied to the code. In this planning stage, measures are to be taken to ensure complete documentation of code design and implementation, record keeping of the coding process, description of the purpose and structure of each code segment (functions, subroutines), and record keeping of the code verification process.

Records for the coding and verification process may include: a description of the fundamental algorithms describing the physical process(es) which are to be modeled; the means by which the mathematical algorithms have been translated into computer code (e.g., Fortran); results of discrete checks on the subroutines for accuracy; and comparisons between the codes' numerical solutions and analytical or other independently verified numerical solutions.

Code verification or testing ensures that the underlying mathematical algorithms have been correctly translated into computer code. The verification process varies for different codes and ranges from simply checking the results of a plotting routine to comparing the results of the computer code to known analytical solutions or to results from other verified codes.

Traceability describes the ability of the computer analyst to identify the software which was used to perform a particular calculation, including its name, date, and version number, while retrievability refers to the availability of the same version of the software for further use.

#### *Code Documentation*

Detailed guidelines for the preparation of comprehensive software documentation are given by the Federal Computer Performance Evaluation and Simulation Center (FEDSIM81). This publication discusses the structure recommended for four types of manuals providing model information for managers, users, analysts, and programmers. According to FEDSIM81, the manager's summary manual should contain a model description, model development

history, an experimentation report, and a discussion of current and future applications. Currently, ASTM (American Society for Testing and Materials) is developing a standard ground-water code description for this specific purpose (HEI92).

As discussed in van der Heijde (HEI92), the code documentation should include a description of the theoretical framework represented by the generic model on which the code is based, code structure and language standards applied, and code use instructions regarding model setup and code execution parameters. The documentation should also include a complete treatment of the equations on which the generic model is based, the underlying mathematical and conceptual assumptions, the boundary conditions that are incorporated in the model, the method and algorithms used to solve the equations, and the limiting conditions resulting from the chosen approach. The documentation should also include user's instructions for implementing and operating the code, and preparing data files. It should present examples of model formulation (e.g., grid design, assignment of boundary conditions), complete with input and output file descriptions, and include an extensive code verification and validation or field testing report. Finally, programmer-oriented documentation should provide instructions for code modification and maintenance.

An integral part of the code development process is the preparation of the code documentation. This documentation of QA in model development consists of reports and files pertaining to the development of the model and should include (HEI92):

- A report on the development of the code including the (standardized and approved) programmer's bound notebook containing detailed descriptions of the code verification process;
- Verification report including verification scenarios, parameter values, boundary and initial conditions, source-term conditions, dominant flow and transport processes;
- Orientation and spacing of the grid and justification;
- Time-stepping scheme and justification;

- Changes and documentation of changes made in code after baselining;
- Executable and source code version of baselined code;
- Input and output (numerical and graphical) for each verification run;
- Notebook containing reference material (e.g., published papers, laboratory results, programmer's rationale) used to formulate the verification problem.

Furthermore, the software should be documented in sufficient detail to (GAS79):

- record technical information that enables system and program changes to be made quickly and effectively;
- enable programmers and system analysts, other than software originators, to use and to work on the programs;
- assist the user in understanding what the program is about and what it can do;
- increase program sharing potential;
- facilitate auditing and verification of program operations;
- provide managers with information to review at significant developmental milestones so that they may independently determine that project requirements have been met and that resources should continue to be expended;
- reduce disruptive effects of personnel turnover;
- facilitate understanding among managers, developers, programmers, operators, and users by providing information about maintenance, training, and changes in and operation of the software;
- inform other potential users of the functions and capabilities of the software, so that they can determine whether it serves their needs.

The user's manual should, at a minimum, consist of:

- an extended code description;
- code input data description and format;
- type of output data provided;
- code execution preparation instructions;
- sample model runs;
- trouble shooting guide; and
- contact person/affiliated office.

The programmer's manual should, at a minimum, include:

- code specifications;
- code description;
- flow charts;
- descriptions of routines;
- data base description;
- source listing;
- error messages; and
- contact person/affiliated office.

The analyst's manual should, at a minimum, present:

- a functional description of the code;
- code input and output data;
- code verification and validation information; and
- contact person/affiliated office.

The code itself should be well structured and internally well documented; where possible, self-explanatory parameter, variable, subroutine, and function names should be used.

#### *Code Testing*

Before a code can be used as a planning and decision-making tool, its credentials must be established through systematic testing of the code's correctness and evaluation of the code's performance characteristics (HE189). Of the two major approaches available, the evaluation or review process is qualitative in nature, while code testing results can be expressed using quantitative performance measures.

Code testing (or code verification) is aimed at detecting programming errors, testing embedded algorithms, and evaluating the operational characteristics of the code through its execution on carefully selected example test problems and test data sets. ASTM84 defines verification as the examination

of the numerical technique in the computer code to ascertain that it truly represents the conceptual model, and that there are no inherent problems that prevent correct solutions.

At this point, it is necessary to point out the distinction between generic simulation codes based on an analytical solution of the governing equation(s) (Appendix C) and codes that include a numerical solution. Verification of a coded analytical solution is restricted to comparison with independently calculated results using the same mathematical expression, i.e., manual calculations, using the results from computer programs coded independently by third-party programmers. Verification of a code formulated with numerical methods might take two forms: (1) comparison with analytical solutions, and (2) code intercomparison between numerically based codes, representing the same generic simulation model, using synthetic data sets.

It is important to distinguish between code testing and model testing. Code testing is limited to establishing the correctness of the computer code with respect to the criteria and requirements for which it is designed (e.g., to represent the mathematical model). Model testing (or model validation) is more inclusive than code testing, as it represents the final step in determining the validity of the quantitative relationships derived for the real-world system the model is designed to simulate.

Attempts to validate models must address the issue of spatial and temporal variability when comparing model predictions with limited field observations. If sufficient field data are obtained to derive the probability distribution of contaminant concentrations, the results of a stochastic model can be compared directly. For a deterministic model, however, the traditional approach has been to vary the input data within its expected range of variability (or uncertainty) and determine whether the model results satisfactorily match historical field measured values. This code-testing exercise is sometimes referred to as history matching.

Konikow and Bredehoeft (KON92) argue compellingly that computer models cannot be truly validated but can only be invalidated. As reported by Hawking (HAW88), any physical theory is only provisional, in the sense that it is only a hypothesis that can never be

proven. No matter how many times the results of the experiments agree with some theory, there is never complete certainty that the next test will not contradict the theory. On the other hand, a theory can be disproven by finding even a single observation that disagrees with the predictions of the theory.

From a philosophical perspective, it is difficult to develop selection criteria for a model validation process which may be intrinsically flawed. However, the average strategy presented in this chapter provides some assurance that the code selected has the highest probability of most accurately representing the conceptual model.

#### *Hardware Requirements*

In general, hardware requirements should rarely be a discriminatory factor in the selection of a computer code. However, a number of the available codes require very sophisticated hardware, not so much because of the intrinsic requirements of the code but because the simulated processes may be very complex and require time-consuming solution methods. Therefore, hardware requirements should be clearly identified for the code itself and be consistent with the hardware available to the user.

An earlier report prepared by this interagency working group details the conditions under which specific features and capabilities of the model are needed to support remedial decision-making (EPA94).

A final consideration, true for all phases of the project, is the need to select codes that have been accepted by technical experts and used within a regulatory context.

#### 4.2.2 Model Construction

One primary goal of mathematical modeling is to synthesize the conceptual model into numerical terms from which flow and transport processes may be investigated under specified conditions. This process entails several discrete steps: (1) partitioning the conceptual model into units of time and space; (2) assignment of boundary conditions; and (3) specification of the values of parameters. The following sections discuss the relevance of each of these topics to the modeling process. Then guidelines for modeling and, where appropriate, modeling review

criteria are suggested.

#### 4.2.2.1 Layering and Gridding

In a numerical model the region of interest is partitioned into a series of blocks (i.e., elements) which are arranged in layers (Figures 4-2 and 4-3). This practice, termed discretization, effectively replaces the continuous problem domain with an array of blocks and nodes. The basic concept used is to divide up the section as realistically as practical. When possible, geologic logs and other information typically are used to identify geologic unit contacts. Information on formational dip, depositional, and erosional features may have a pronounced effect on unit contact elevations and, therefore, will also have a significant impact on ground-water flow and contaminant transport. To accommodate variations in unit thickness, some finite element models allow the use of curvilinear elements to allow the model's planes to trace the unit contacts more precisely.

The determination of how many layers to include depends on both the conceptual model and the objectives of modeling. Typically, multiple layers are used to accommodate the vertical variation of hydrologic parameters that represent the hydrogeologic units within the modeled region.

One of the critical steps in applying a ground-water model is selecting the size of the nodal spacing. The

more finely the grid is spaced, the more accurate the numerical solution. However, the desire for accuracy must be balanced against the impracticality of solving for large numbers of nodes and the long computer run times that may be involved.

The most quantitative guidance for selecting the nodal spacing applies only to modeling contaminant transport not to ground-water flow modeling. These criteria are related to the fact that the value of dispersion coefficients (Section 2.4) varies with the absolute value of the Darcy velocity (Section B.3).

This relationship, as expressed below, defines a dimensionless Peclet number.

$$P_e = \frac{V\Delta x}{D}$$

where:

$P_e$  = Peclet Number

$V$  = Darcy Velocity

$D$  = Dispersivity

The numerical solution of the transport equation becomes unstable if the Peclet number becomes too large. Price *et al* (PRI66) have shown that the stability of the transport solution is ensured if the Peclet number is less than 2.

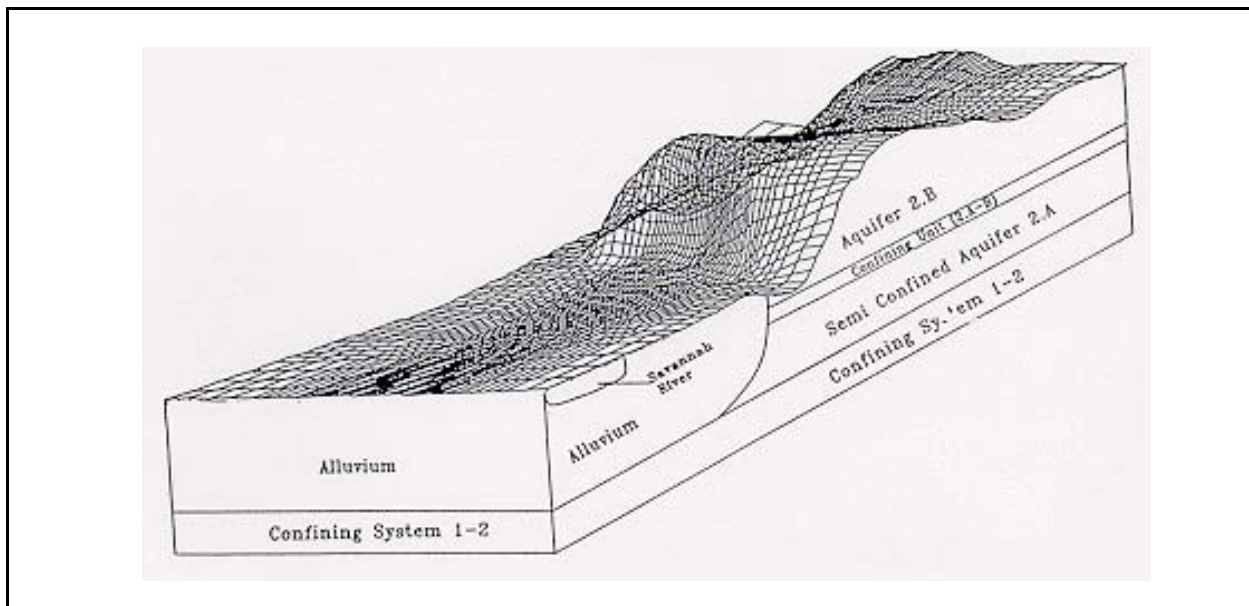


Figure 4-2. Three-dimensional view of model grid.



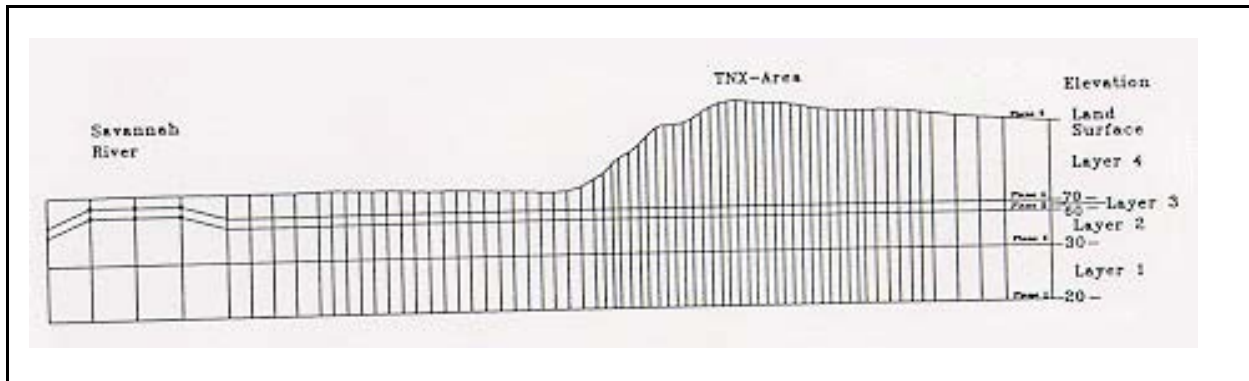


Figure 4-3. Cross-sectional view of model grid.

#### 4.2.2.2 Definition of Boundary and Initial Conditions

To obtain a unique solution for the governing equation of ground-water flow and contaminant transport, additional information is required about the physical state of the ground-water system. This information is described by boundary and initial conditions. Boundary conditions are the conditions the modeler specifies as known values to solve for the unknowns in the problem; these values may be associated with either ground-water flow or contaminant transport.

One of the primary objectives of the site characterization program is to identify the presence and location of ground-water flow and contaminant source boundaries so that they may be incorporated into the conceptual model. These boundaries generally are quantified in terms of the volume of ground water and contamination moving through the system. The physical boundaries are then translated into mathematical terms, as input into the computer model. The initial conditions are simply the values of hydraulic head or contaminant concentrations at a reference initial time. For steady-state problems, only boundary conditions are required, whereas for transient problems, both conditions are required.

#### Ground-Water Flow

##### *Boundary Conditions*

Ground-water boundaries may be described in terms of where water is flowing into and out of the ground-water system. There are many different types of boundaries, including: surface-water bodies, ground-

water divides, rainfall, wells, and geologic features, such as faults and sharp contrasts in lithology.

In general, boundary conditions are known or estimated values that are assigned to surfaces and planes that either frame the perimeter of the modeled area or define the release from the contaminant source. The different types of flow boundary conditions are: (a) head (ground-water elevation) is known for surfaces or planes bounding the modeled region; (b) ground-water flow volumes are known for surfaces or planes bounding the modeled region; and (c) some combination of (a) and (b) is known for surfaces or planes bounding the region. Boundary conditions could also be assigned to interior features of the modeled region where ground water elevations or flow volumes are known, such as lakes, rivers, or marshes. In practice, these types of boundaries result in three conditions including: (1) specified value of hydraulic head; (2) specified flux; and, (3) head-dependent flux. Table 4-3 briefly describes the three boundaries and their examples.

Just as the physical ground-water system is idealized as a continuum in deriving the mass balance differential equations, it also is expedient to idealize the conditions on the boundaries of the system so that they too can be approximated by a mathematical expression. In nature, the boundary conditions of ground-water systems are of several kinds. One of the most common would be at a well. Since the porous medium terminates at the well face, the aquifer not only has a boundary around its perimeter, but the outline of each well also is considered a

**Table 4-3. Boundary Conditions of Ground-Water Flow Equations**

Type	Description and Examples
I. Specified head	Value of hydraulic head is specified along the boundary. Typical examples include: (1) constant head condition on the boundary in direct hydraulic contact with a river or lake or spring outlets; and (2) boundary condition at a pumped well operating at constant or specified drawdown.
II. Specified flux	Flux or flow rate of water is specified along the boundary. The flux is usually expressed as $q_n = -K \partial h / \partial n$ , where $n$ refers to the direction perpendicular to the boundary. Typical examples include: (1) condition of zero flow across impermeable rock boundaries or across a water divide or a streamline; and (2) boundary condition on the water table receiving prescribed rate of accretion.
III. Head-dependent flux	Flux or flow rate of water is dependent on the head difference across a semi-impervious layer adjacent to the aquifer. This boundary condition is encountered when the flow domain is intercepted by a river bed clogged by a thin layer of silt or clay. The leakage flux is given by $q_n = K/b (h-H)$ where $K$ is the hydraulic conductivity, $b$ is the thickness of the thin layer, and $(h-H)$ is the pressure difference across the layer. A similar situation is encountered when the aquifer is overlain by a water table aquitard layer.

boundary to the aquifer. The boundary conditions at wells may also be treated as a constant or variable specified flux, or constant head, depending on which best describes the physical conditions.

Impermeable or nearly impermeable boundaries are formed by underlying or overlying beds of rock, by contiguous rock masses (as along a fault or along the wall of a buried rock valley), or by dikes or similar structures. Permeable boundaries are formed at the bottom of rivers, canals, lakes, and other bodies of surface water. These permeable boundaries may be treated as surfaces of equal head (specified) if the volume of surface water is large, so that its level is uniform and independent of changes in ground water flow. However, the uniform head on a boundary of this type may change with time due to seasonal variation in the surface-water level. Other bodies of surface water, such as streams, may form boundaries with non-uniform distributions of head which may be either constant or variable with time. For example, a small stream might be affected by a nearby withdrawal of ground water if that withdrawal occurred at a rate similar to the flow in the stream. Then, the boundary condition would depend on the ground-water flow; that is, it would be a head-dependent flux.

In an analysis of ground-water flow, it is common to assume a simple geometry for sinks and sources existing at the boundary, or inside the flow system. In areal flow simulations, points often are used to represent individual wells, whereas lines are used to represent rivers, lakes, and other surface-water bodies. These representations are justified, provided that detailed information about potentiometric head and velocity distributions in the immediate vicinity of the individual sources or sinks is not a concern. If such information is required, then the actual geometric features of the source or sink must be incorporated into the flow system. For instance, if the modeler is using flow analysis to assess the performance (e.g., specific capacity or maximum yield) of a pumping well or evaluate its drawdown versus time data, then the well must be represented as a cylindrical boundary of specified diameter and specified screened length.

Other assumptions related to sinks and sources are variations of volumetric flow rates of flux (flow rate per unit length) distributions. For a point source or sink, it is common to assume a constant flow rate unless the field data indicate drastic variations necessitating a more accurate treatment. For a line source or sink, uniform flux distribution along the line

also is assumed to simplify the analysis. Again, the justification of this assumption depends on actual field conditions.

#### *Initial Conditions*

Initial conditions are defined as values of ground-water elevation which are initially assigned to interior areas of the modeled regions. The initial conditions for steady-state flow models are generally set to uniform values because the temporal nature of the flow system is not simulated. The initial conditions assigned to the model domain are irrelevant as identical solutions will be reached regardless of the values initially assigned. This occurs because these steady-state values depend solely on the values assigned to the boundaries of the model.

The initial and boundary conditions for the variably saturated water flow equation can be stated in the same manner as those for the saturated ground-water flow equation. The solution of the former problem enables the analyst to obtain the head distribution, as well as the water saturation (or water content) distribution, and details of the velocities and flow rates for an analysis of the migration of contaminants in variably saturated porous media.

Initial conditions for a transient flow model may be interpolated from water-level data or may be set from a previous steady-state flow simulation. Ideally, the initial heads should come from a steady-state simulation. Interpolated initial conditions are often not consistent with the model boundary conditions and parameterization. In this case, heads computed during early time steps are inaccurate.

#### Contaminant Source

##### *Boundary Conditions*

The most common contaminant source boundaries either specify the source concentration or prescribe the mass flux of contamination entering the system. The former generally is prescribed when the release rate is largely controlled by the solubility limits of the contaminant. The mass-flux type boundary typically is used when a leaching rate is known or estimated. Specialized source boundaries also have been formulated which allow for radioactively decay in the source. The ability of the code to treat source decay

may not be important if the parents and daughters have a relatively long half-life compared to the expected time to travel to the nearest receptor.

Contaminant transport should not be analyzed until after the ground-water flow model has been calibrated (Section 4.2.3). As previously mentioned in assigning initial and boundary conditions to problems of ground-water flow, the solution of a contaminant transport problem is not unique unless the initial and boundary conditions associated with the governing transport equation are given. Generally, the initial concentration is specified for each node in the flow domain at some initial time,  $t = 0$ . This results in a concentration distribution that forms the basis of the initial conditions. In addition, boundary conditions must also be specified at all times. Three types of boundary conditions are commonly encountered in practice: (1) specified value of concentration; (2) zero normal concentration gradient; and (3) specified mass flux of solute. Table 4-4 briefly describes the three boundary conditions and gives examples.

In simulating areal transport, it also is common to assume a simple geometry for a contaminant's source (or sink). As in the areal simulation of ground-water flow, points are used to represent individual injection and pumping wells and waste disposal areas, such as landfills or recharge ponds. Lines are used to represent rivers, creeks, and leaking sewer or pipelines. Again, it is emphasized that point and line representations of sources are justified as long as attention is focused on contamination over an areal scale that is much larger than the area of the sources (greater than 10 or 100 times). If local information very near the sources is required, then the source geometry must be described more accurately as part of the flow region under consideration. Also, when analytical methods such as those given in Appendix B are used to simulate the transport problems, one of the following assumptions often is made about the source input: (1) the assumption of constant concentration during a continuous injection period or during a finite injection period; (2) the assumption of constant injection rate during a continuous injection period; or (3) the assumption of instantaneous injection of a slug of contaminant. The validity of these assumptions certainly depends on field conditions.

**Table 4-4. Boundary Conditions of Solute Transport Equations**

Type	Description and Examples
I. Specified concentration	Value of concentration is specified along the boundary. Typical examples include: (1) specified concentration condition on the boundary in direct hydraulic contact with a surface water body that is recharging into the aquifer system; (2) zero concentration condition on the boundary located at a great distance from the contaminant source; and (3) specified concentration condition at injection wells.
II. Zero concentration gradient, normal to the boundary	This type of boundary condition can be expressed as $dc/dn = 0$ . Typical examples include: (1) zero normal concentration gradient on impervious boundaries; and (2) zero normal concentration gradient on outflow boundaries (e.g., river and spring outlets, drains, and pumped wells) where the contaminant leaves the aquifer system.
III. Specified total mass flux of contaminant normal to the boundary	Total (advective and dispersive) flux is specified on the boundary. This boundary condition is usually expressed as $-(D_{ij}\delta c/\delta x_j)n_i = q_n(c^e - c)$ , where $n_i$ is the unit vector in the direction outward and normal to the boundary. $j$ is the index for the principal axis, and $c$ is the concentration. Typical examples include: (1) specified mass flux of contaminant at injection wells (in this case, $q_n$ corresponds to the volumetric fluid injection rate per unit area of the aquifer (L/T), and $c^e$ corresponds to concentration of injected fluid); and (2) specified mass flux of contaminant at the boundary receiving influx of contaminant from sources such as landfills and disposal ditches.

*Initial Conditions*

Initial conditions are defined as values of contaminant concentrations initially assumed to be present in the area. Non-uniform initial values (i.e., contaminant concentrations) are routinely used in the contaminant transport analysis to depict the geometry and varying concentrations of contaminant within the plume, as well as to define the concentrations leaching from the contaminant source. The ability of a code to allow non-uniform initial conditions is essential to fully describing and simulating the contaminant plume(s).

4.2.2.3 Specification of Time Steps

Transient simulations of flow and/or transport require the use of time steps. There is a direct relationship between numerical accuracy and stability, grid density, and time-step size. The time-step size should be selected to ensure that the Courant criterion is less than or equal to one as shown below:

$$C_r = \frac{V\Delta t}{\Delta x}$$

where:

- $C_r$  = Courant criterion
- $\Delta t$  = Time step interval
- $V$  = Darcy velocity
- $\Delta x$  = Grid spacing

That is, the time step should be selected so that it would take longer than the specified time to move the distance of the grid block.

4.2.2.4 Specifying Parameter Values in the Model

Table 2-1 shows the data typically required for modeling ground-water flow and transport, which can be obtained from previous and ongoing field studies. Data input into the numerical model is a painstaking process; therefore, to identify where a significant

effort should be made to ensure accuracy, the uncertainties inherent in the data must be considered. Such uncertainties will give an early indication of which data are most likely candidates for modification. For example, in all likelihood, the assumed recharge will be changed considerably from initial approximations when calibrating the model. Therefore, it would make sense to assign uniform values, rather than to estimate zones of recharge that most probably will be changed later. Modeling uncertainties include:

Measurements of flow and transport usually are taken at only a few sampling points. To obtain a complete picture, it is necessary to interpolate between these points, or make inferences from point data to apply to conditions over a larger area.

There may be an inherent difference between the scale on which the processes are mathematically described and the scale at which the data are obtained. For example, laboratory measurements may exhibit scale-dependence when extrapolated to a field site.

Data are never complete; in particular, those data pertaining to values of dispersivities and contaminant input rates usually are not available. Therefore, the modeling discussion should include a data limitation section. These gaps will have to be filled using estimates made during the calibration and sensitivity analyses.

The various methods for collecting samples and measuring parameters all have some error or uncertainty. Typical sources of error include an improper type of test, poor specification of test procedures, poor instrumentation, incorrect measurement, and incorrect interpretation of the results. Hence, the reliability of data obtained from various sources must be weighted.

#### 4.2.3 Calibration of the Model

Traditionally, the term "model calibration" is used to refer to the trial-and-error adjustment of parameters of the ground-water system by comparing the model's output (calculated values of hydraulic head or concentration) and the measured output (observed values of hydraulic head or concentration). In

essence, such a calibration procedure involves the following routines: (1) operating the model, using initial estimates of the values of parameters; (2) history-matching or comparing computed and observed values of hydraulic head or concentration; and (3) adjusting the values of the parameters and repeating the simulation.

Calibration of the model is aimed at demonstrating that it can produce realistic, and to a certain extent, accurate and reliable predictions. The model is calibrated by determining a set of parameters, boundary conditions, and hydraulic stresses that generate simulated potentiometric surfaces and fluxes that match field-measured values to within an acceptable range of errors.

The end result of the process of model calibration is an optimal set of values for parameters that minimize the discrepancy between the model's output and the observed data. Several major causes of discrepancy should be recognized; they are listed below, with general comments on actions that can be taken to rectify the problem.

1. Poor estimate of values for flow or transport parameters, or incorrect assessment of initial and boundary conditions of the ground-water system. In this case, the problem may be corrected by adjusting values of the physical parameters and rerunning the model.
2. Use of incorrect or inappropriate data on potentiometric head or concentration in the history-matching or the comparison of output. A common pitfall is comparing the potentiometric head computed for a point located at coordinates  $(x,y,z)$  in a three-dimensional flow field with data measured from an observation well located at  $(x,y)$  but screened over a significant portion of the aquifer thickness. Such a comparison is not valid unless the vertical flow component is negligible because the observed head represents the vertically averaged head over the screened length of the observation well, and not the head at the point  $(x,y,z)$ .

Such a discrepancy between the model's result and observed head can be avoided by carefully checking and interpreting the data.

3. Use of inadequate spatial and temporal discretizations. As pointed out earlier, it is important for the user of a numerical model to select grid and time steps that are sufficiently refined to give acceptable accuracy.
4. Use of an inappropriate conceptual model. In some instances, lack of information about some features of the ground-water system may have led to the use of an oversimplified or a wrong type of conceptual model, or to a poor definition of the flow and transport problems. Usually when this happens, it is necessary to return to the early stage of the simulation process and formulate a new conceptual model, or alter the existing model. Alternatively, additional data may be acquired that better define the flow and transport problems.

For a cost-effective calibration of the model, a systematic approach should be taken to the problem of identifying parameters. In general, a checklist should be kept of those parameters that are being varied and those that are being held constant. Various simplifying assumptions made in the conceptual model and formulation of the problem should be noted, together with the levels of uncertainties associated with all critical input parameters.

The iterative process of matching calculated values with observed (historical) data by adjusting the model's input can be a manual trial-and-error procedure or can be automated. The calibration process, also known as history-matching, is closely related to estimating parameters. This process might result in the refinement of initial estimates of aquifer properties (parameters), the establishment of the location of the boundaries (areal and vertical extent of aquifer), and the determination of flow and transport conditions at the boundaries. Trial-and-error calibration is a highly subjective, intuitive procedure. As the quantity and quality of data are often limited, no unique set of parameters results, leaving the modeler with a subjective choice. For example, the simulated potentiometric surface could be raised either by increasing areal recharge or by increasing the amount of leakage from a stream.

The success of such a procedure depends very much on the experience of the analyst. Another type of technique is based on the use of a formal optimization

procedure (e.g., Gauss-Newton parameter optimization algorithm), in conjunction with the ground-water flow model. Such techniques can be coded into a computer program that performs automatic history-matching, and calculates the optimal set of parameter values that minimize a certain objective function (e.g., the total sum of the square of the difference between computed and observed head values at all observation points).

Both the manual and automatic adjustment techniques may be categorized as the "indirect approach" to the problem of identifying parameters (See FRE79, pp. 357-359). This statement implies that calibration can be carried out via a "direct approach." Such an approach requires the inverse formulation of the problem of the ground-water flow. In other words, the flow problem is set up in such a way that the piezometric head and well discharges are known, but the transmissivity, storage, and recharge parameters are unknown. When posed in this manner, the identification problem is referred to specifically as the "inverse problem." Several techniques recently were developed to solve the inverse problem.

Automation calibration is based on the use of prescribed algorithms, which are completed when preset matching criteria are met. Because of the formal approach taken in adjusting input to the model, automatic procedures are less subjective than trial-and-error procedures. However, automatic procedures effectively eliminate the judgment of the modeler, and because the calibrated solution is not unique it may not be the best fit to the overall conceptual model. However, if numerous calibrations are required, it would make sense to use automated calibration tools to obtain probability distributions.

In contrast to the calibration of the ground-water flow model, calibration of a contaminant transport model usually is more subjective using the manual procedure of history-matching and trial-and-error adjustments of the parameter. There are several reasons for this; the most important is that data on concentration are usually completely lacking, or insufficient to permit an accurate calibration. Another important reason is that the transport equation contains more parameters and is more complex than the ground-water flow equation. Thus, it is more difficult to identify the parameters by an automatic estimation technique or by the direct (inverse formulation) approach.

Calibration can be performed to steady-state or transient data sets. Although most flow model calibration exercises involve steady-state data, in some hydrogeologic settings, assumption of steady-state conditions may be inappropriate due to large fluctuations in the water table or boundary conditions. In this case, the model may be calibrated against long- or short-term trends in water levels, stream and lake elevations, and possibly, system responses resulting from imposed stresses such as pumping wells. A transient flow calibration is necessary to calibrate values of storage parameters, which are needed if transient flow is to be modeled.

The results of the model calibration need to be evaluated both qualitatively and quantitatively. At present, no established protocol exists for determining whether a model has been satisfactorily calibrated. However, there are several common ways of reporting the calibration results. The simplest way is to list the measured and simulated heads together with their differences and some average of the differences.

Comparison between contour maps of measured heads versus contoured maps of simulated heads provides a visual means of assessing the "goodness of fit" and gives some idea of the spatial distribution of error in the calibration.

The simulated heads and concentrations will have some degree of error arising from how the model was discretized in both space and time. In some instances (e.g., if large mass balance errors are occurring), it may be necessary to perform a grid-convergence test to determine if the grid spacings in the model are fine enough; this can be time-consuming and painstaking unless a good pre-processor is available. The ready accessibility of high-speed computers may warrant over-discretizing the model grid at the beginning of the project, rather than having to redesign the grid during calibration. If a transient calibration is to be performed, the appropriateness of the selected time steps should be checked by comparing the model's results against an identical simulation with the time steps set at very small intervals. If the results with the large time steps do not diverge significantly from those with the smaller steps, the larger ones would provide a comparable result.

The mass balance error is calculated by comparing all of the water entering the modeled system with all of

the water exiting the domain. Transient simulations also will consider water going into and out of storage. The mass balance error should typically be less than one percent.

#### 4.2.4 Uncertainty and Sensitivity Analyses

After the model has been satisfactorily calibrated, sensitivity analyses should be performed to determine the sensitivity of the model's output to variations (or uncertainties) in physical parameters. For instance, what would be the effect of a 10 percent error in recharge values on the potentiometric head and velocity distributions?

The common practice for carrying out the sensitivity analysis is to repeat the simulations using a series of selected values for the physical parameters and to compare the results with those obtained using the calibrated values. Usually, the selected values of each varied parameter are within a range that depends on the degree of associated uncertainty. Output from the sensitivity runs can be expressed in actual units or in a dimensionless form. Using dimensionless variables often allows systematic conclusions to be drawn from the sensitivity study. In particular, if the model is an analytical model, important dimensionless parameters can often be easily identified by carefully examining the analytical solution.

Sensitivity analyses identify the main contributors to the observed variation in the results. These techniques typically are applied iteratively. The first iteration can include rather general assumptions leading to preliminary results that help focus the subsequent iterations.

Uncertainty in input parameters used in predictive models may result from several sources, including incomplete data, intrinsic spatial variability of a property, uncertainties in measurements, and uncertainties resulting from differences in scale between data acquisition and model application. However, uncertainty in input parameters is not the only potential source of uncertainty in modeling ground-water flow and contaminant modeling; additional uncertainty may enter the analysis through the choice of conceptual models used to represent the system.

The following definitions will be useful in this

discussion of uncertainty and sensitivity analyses.

*Conceptual Model:* A set of qualitative assumptions used to describe a system or subsystem for a given purpose. At a minimum, these assumptions concern the geometry and dimensions of the system, initial and boundary conditions, time-dependence, and the type of physical and chemical processes. The assumptions should be consistent with one another and with existing information within the context of the purpose.

*Alternative Conceptual Models:* Alternative sets of assumptions that describe the same system for the same purpose, where each set of assumptions is consistent with the existing information.

*Conceptual Model Uncertainty:* The lack of knowledge about the system resulting from the limited information available to support or refute alternative conceptual models.

Uncertainty also may exist in the computational models used for quantitative analyses, based on the chosen conceptual models. In this discussion, computational models refer to mathematical models used to represent the physical processes, numerical models used to solve the mathematical models, and computer codes used to implement the solution.

The selection of scenarios to be analyzed also may introduce uncertainty into the estimated performance. Still more uncertainty may exist in the completeness of the scenarios considered, in the way in which computational results are aggregated to represent the consequences of scenarios, and in the probabilities associated with their occurrence.

Sensitivity analyses identify the main contributors to the observed variation in the results. These techniques typically are applied iteratively. The first iteration can include rather general assumptions, leading to preliminary results that help focus these techniques in subsequent iterations. In this manner, the resources and techniques required to reduce the uncertainty can be directed at the areas of the modeling study where the benefits of understanding uncertainty and reducing it (where possible) are greater. However, sensitivity analyses alone will rarely identify a flawed conceptual model. For example, the failure to identify and include a fault(s) in the conceptual model would lead to an analysis that would not account for preferential

pathways that potentially could result in higher than predicted risks.

Modeling the behavior of a hydrogeologic system necessarily will be uncertain because knowledge about its real behavior is limited. Many of the parameters used as inputs to a model of the system are obtained only by collecting data. Investigators knowledgeable about the data they collect make a finite number of observations, choosing which parameters to measure and how, where, and when to measure them. However, the collection process itself can introduce uncertainty through errors in measurement, the system's inherent randomness, and limited sampling of the variable physical, chemical, and biological properties of the system. The professional judgment of an expert in the area of investigation often enters into the scientific process. For example, selecting methods to collect data, interpreting data, developing conceptual models, and selecting parameters all require professional analysis and judgment. The analyst's final data set is based on available data, use of the parameter in the computational model, behavior of analogous systems, and the analyst's own expert judgment.

Uncertainties arising from the numerical solutions of a mathematical model are resolved when verifying (checking for numerical accuracy) the computer programs. Uncertainty resulting from the scenarios selected for modeling is best addressed by a systematic, thorough examination of a scenario's possible components, based on probability, consequence, physical reasonableness, and regulatory guidance, and by assigning probability through techniques used for evaluation or estimation.

Monte Carlo techniques may be used for uncertainty and sensitivity analyses. Uncertainty analyses evaluate uncertainty in performance estimates that result both from the existence of alternative conceptual models and from imprecise knowledge input variables. Sensitivity analyses determine the contribution of individual input variables to the uncertainty in model predictions.

Monte Carlo analyses involve five steps: (1) selection of variables to be examined and the ranges and distributions of their values; (2) generation of the samples to be analyzed; (3) propagation of the samples through the analysis; (4) uncertainty analysis; and (5) sensitivity analysis.



### 4.3 Predictive Simulations

The final stage of the process is to perform predictive simulations using the optimal set of parameter values obtained from the model calibration. In general, these simulations address specific issues of the existing problem of ground-water contamination and provide guidance for policy decisions. Each simulation usually corresponds to one specified set of data pertaining to natural boundary conditions, pumping operation for the ground-water reservoir, or proposed remedial measures for the contamination. Typical objectives of the predictive simulation study are outlined below, along with pertinent comments.

1. To learn more about the existing contamination and to predict future behavior of the ground-water system under natural conditions. Among the questions that may be addressed are the following: Where is the contaminant plume located presently? In which direction is the plume moving? Will the contamination at the site pose serious danger to the public if no action is taken? Do the contaminant concentrations pose unacceptable risks? If the risks are unacceptable, how extensive must the clean-up be to reduce the concentration of the contaminant to an acceptable level?
2. To evaluate and compare alternative remedial schemes for the existing contamination. Typical remedial schemes that may be considered are (1) hydraulic barriers (e.g., pumping and recharge wells to flush the contaminant out of the aquifer, and (2) subsurface barriers to inhibit the contaminant from leaving the site. The predictive simulations are also aimed at the level of risk reduction offered by each alternative measure. Results from the comparative study are useful in the selection and implementation of a suitable remedial scheme for the site. These decisions usually are made in conjunction with economic considerations. In some instances, the predictive simulations can be directly incorporated into an economic analysis, allowing the most cost-effective remedy to be selected.
3. To predict the responses of the ground-water system to various management alternatives including, for example, different pumping or recharge operations that may be applied to the

wells existing at the site or groups of wells in the areas surrounding the site. The following are typical questions: How will different well operations affect the contaminant plume? Can the existing contamination problem be contained to the site and recovery efforts maximized by modeling review criteria for selecting a proper pumping schedule?

Modeling review criteria for the second two topics have been considered in previous chapters. The first topic is related to the baseline risk assessment, discussed in the next section.

### 4.4 Baseline Risk Assessment

The Baseline Risk Assessment typically accomplishes the following three objectives:

- Assesses the magnitude and sources of current and potential future risks to humans and the environment.
- Assists in the scoping ongoing site characterization.
- Identifies contaminants of potential concern and assumptions of exposure for developing risk-based preliminary remediation goals (PRGs).

As the remedial investigation/feasibility study proceeds, action levels will evolve from the PRGs which ultimately will become part of the final objectives for remedial action. These action levels will entail consideration of applicable or relevant and appropriate requirements (ARARs) for site-wide baseline risk assessments and, potentially, operable unit-specific risk assessments.

Although risk assessments generally include several receptors (e.g., future resident farmers, plant workers), the following discussion is targeted at pathways and receptors related to ground water.

Risk-based PRGs for ground water are frequently developed in accordance with the Human Health Evaluation Manual, Part B (EPA91). This approach is a first-tier type of analysis and typically is very conservative. The methodologies outlined in Appendix B for predicting radionuclide transport rates and concentrations are designed for conservative

analyses, yet they also are designed to be more realistic than the HHEM Part B approach.

In many cases, estimating flow and transport through the unsaturated zone is an integral component of the risk assessment, particularly if the compliance point is relatively near the contaminant source. In these instances, the release rates, concentrations and hold-up times within the unsaturated zone will influence receptor concentrations far more than flow and transport in the saturated zone.

Under these circumstances, a practical approach would be to use one of the many risk-based computer models that emphasize flow and transport in the unsaturated zone. However, if flow and transport processes in the saturated zone are deemed very important to the analysis, or if the receptor is located off the centerline of the plume or far from the source, it may be worthwhile to use a risk-based type code or calculations from Appendix B to give a transient source-type boundary. This can then be used in a more complex numerical model to simulate the flow and transport in the saturated zone more accurately.

One of the primary differences of the site modeling with risk-based codes is that the model is not

typically calibrated. In general, this is not a problem because the required data from the unsaturated zone rarely are collected during site characterization. Therefore, evaluation of the parameters during the sensitivity analysis is crucial.

The conceptual model sub-components of the risk-based codes related to ground-water flow and transport processes consist of the following:

- Infiltration
- Source Release Rate
- Source and Leach Strength
- Fate and Transport in the Unsaturated Zone
- Fate and Transport through the Saturated Zone

#### 4.5 Exposure Estimation—Ground Water

Appendix B describes methods for estimating ground-water concentration at the point of receptor exposure. With these estimated concentrations, the assessor can estimate exposure based on the equations and parameter values presented in the Exposure Factors Handbook (EPA 89).

## CHAPTER 5 - SUMMARY AND CONCLUSIONS

In this chapter, the modeling evaluation criteria and a checklist containing the major steps within these procedures are reviewed. With this checklist (Table 5-1), a person analyzing a specific project can identify potential problems in the model application.

### MODELING OBJECTIVES AND DATA REQUIREMENTS

- The purpose and scope of the modeling exercise should be clearly indicated.

The purpose of the modeling should be kept in mind when reviewing the modeling report. The reviewer should determine whether the analyses performed are consistent with the purpose of the project. Common problems are overkill (the modeling analyses are much too complex for the purpose of the project) and over-simplification (the modeling analyses are too simplistic to achieve the project objectives).

- The modeling objectives should be identified and related to the decision-making needs.

In the Summary and Conclusions of the model application report, each of these objectives should be discussed separately in the context of how the modeling was used to meet the objective and the degree to which the objective was met.

- The data required to construct a conceptual model should be described, and the relevance of the data to ground-water flow and contaminant transport should be discussed.

The data should be related to the processes being simulated, (e.g., groundwater flow, contaminant transport, variably-saturated flow and transport, etc.). It is important to ascertain that no important processes are overlooked and that all data types required to simulate a particular process have been identified. In addition to data related to the physical system, a detailed waste disposal history should be provided. The latter is a key element in determining the source term(s) for the contaminant transport modeling.

- The source of the data should be presented.

Data should be categorized based upon source type: (1) site-specific data collected in the field, (2) data obtained from the scientific literature, and (3) data values estimated through model calibration. Data obtained from literature should be thoroughly cited and should be representative of the same geologic and hydrologic conditions found at the site. Data values obtained through calibration should also be consistent with anticipated ranges of values (see the model calibration section).

- The uncertainties associated with the data should be discussed.

Are some field collection methods better than others? How reliable are literature values? A probable range and distribution in which the parameters will fall should be assigned, prior to the modeling analysis.

- The general sensitivity of the data to the determination of ground-water flow and contaminant transport calculations should be discussed.

This discussion should enable the field characterization program to be more focused. For example, bulk density is used for the transport calculations although the modeling results are typically insensitive to their values. Therefore, time and resources would be better spent obtaining site-specific distribution coefficients which may be critical to the analysis.

- Limitations and weaknesses in the data base should be presented as well as plans to enhance the data base.

Data gaps should be reviewed with the modeling objectives in mind. For example, scoping calculations may be performed with relatively little site-specific data. Detailed simulation of remedial measures, however, would require numerous field measurements of key hydraulic

and geochemical parameters (e.g., hydraulic conductivity, storage coefficient, distribution coefficients, etc.).

- Recommendations should be presented, detailing additional data needed to increase confidence in the modeling results.

#### CONCEPTUAL MODEL DEVELOPMENT

- The physical and hydrogeologic frameworks of the system should be described in detail.

The physical and hydrogeologic framework includes lithologic contacts, facies changes, discrete features such as fractures, and spatial variations of geologic units and their hydraulic properties. The thickness, top elevation, and bottom elevation should be described in detail for areally continuous hydrostratigraphic units (aquifers and aquitards). The rationale for the variability of the properties should be explained (e.g., depositional history).

The geometry of the system should be presented in three dimensions with a rationale for possible simplification. For example, the analysis of the unsaturated zone may be reduced to one or two dimensions. The saturated ground-water system may also be simplified to two-dimensions in plan view if vertical gradients are negligible.

- The boundaries of the system should be described in a water budget analysis.

The primary components of the water budget include recharge, evapotranspiration, runoff, pumping rates, and flow to other sources and sinks including rivers and lakes. The methodology for determining individual components of the water budget should also be included. Boundaries of the system should be identified based upon regional hydraulic features. Aquifer boundaries are seldom constrained to the immediate vicinity of the site and may extend far beyond the area of interest. It is important to characterize these regional features, however.

- The contaminant source term should be described in detail.

Source terms should be described in terms of geometry (in three dimensions), radionuclide concentrations leached from the source, timing of the release, and the release mechanism. The site waste disposal history described in the first section of the modeling report should be helpful in determining this information.

- The conceptual model should be consistent with the field data.

One of the fundamental problems in modeling is a poor conceptual model. Synthesizing the field data into a coherent picture of the relevant physical and chemical processes is critical to the subsequent modeling analyses. Errors in the conceptual model will propagate throughout the modeling. It is important to review the conceptual model and the raw data to determine whether there are significant errors at this early stage in the project.

- The rationale for any simplifications made to the conceptual model should be presented.

Examples of simplifications include (1) modeling ground-water flow at steady-state conditions, (2) simulating the unsaturated zone in one or two dimensions, and (3) approximating the source term at a constant concentration. Each simplification should be reviewed for consistency with the conceptual model of the site, the availability of data, and the potential impact on the accuracy of the modeling results.

- Uncertainties in the conceptual model should be presented and related to earlier discussions of data limitations and uncertainties.

Uncertainties can be related to the variability in field data or interpretations or simplifying assumptions required to evaluate the field data. Uncertainties can be evaluated through a sensitivity analysis in subsequent model phases, but should be discussed in the conceptual model portion of the report.

- Are sufficient data available to meet the modeling objectives?

Data in this context refer to site-specific data.

Data can always be obtained from the scientific literature; however, as the objectives of the modeling become more detailed, site-specific data requirements increase. It is important to relate the quantity and quality of site-specific parameter values to the types of analyses performed.

- Have database deficiencies been clearly identified and modeling implications discussed?

#### *Figures and Tables*

The following are illustrations and tables that should be included in the conceptual modeling report. Some figures may not be required; however, justification should be given if figures and tables are omitted.

- Map showing location of study area.
- Maps and cross sections showing the thickness of the unsaturated zone.
- Geologic map and cross sections indicating the areal and vertical extent of the system.
- Topographic map indicating surface water bodies.
- Contour maps showing the tops and/or bottoms of the aquifers and confining units.
- Isopach maps of hydrostratigraphic units.
- Maps showing extent and thicknesses of stream and lake sediments.
- Maps indicating any discrete features (e.g., faults).
- Maps and cross sections showing the unsaturated zone properties.
- Potentiometric surface maps of aquifer(s) showing hydraulic boundaries.
- Maps, cross sections, or tables showing storage properties of the aquifers and confining units.
- Maps, cross sections, or tables showing hydraulic conductivity of the aquifers, confining units, and stream and lake sediments.

- Maps, hydrographs, and/or tables of water-budget information, including evapotranspiration, runoff, ground-water recharge, ground-water pumping, and gains/losses between ground water and surface water.
- Maps, cross sections, or tables indicating transport parameters, including effective porosity, dispersion coefficients, and distribution coefficients.
- Areal and cross sectional isoconcentration maps of primary contaminants in soil and ground water.
- Time-series graphs of contaminant concentrations measured over time at monitoring wells or surface water locations.
- Relevant source-term inventory information.

## MODEL APPLICATION

### Scoping Analysis

- The results of any scoping analyses that are performed to support the modeling should be presented. These results should be able to support the approach taken for more complex modeling.

Even though scoping analyses represent simplified modeling approaches whereby model parameters are chosen to be conservative. Review of the scoping calculations should concentrate on whether the chosen parameter values and models (or equations) are conservative from a regulatory perspective.

### Code Selection

- Selection criteria should be clearly presented for the selected code(s).

Criteria used in selecting computer codes generally include (1) degree of code testing and documentation, (2) ease of use, (3) whether the code is proprietary or public, (4) physical and chemical processes to be solved, and (5) application history. Even if only one computer code is used in the project, a series of codes should be presented as possible candidates and rationale should be presented to justify the

selection of the chosen code.

- The general features of the code should be discussed.

Code features include whether the code is a proprietary version of a publicly available code, solution methodologies for the flow and transport equations, hardware requirements, degree of code testing, and availability of source code and documentation.

- The code assumptions and limitations should be described.

Of particular interest are those assumptions pertaining to the conceptual model. These would include code dimensionality, ability to simulate heterogeneities, and flow and transport through the unsaturated zone. The code should be capable of simulating all pertinent processes identified in the site conceptual model.

- The basis for regulatory acceptance should be discussed.

Regulatory acceptance criteria may include a history of use, particularly for applications in a similar regulatory context and degree of code testing. The code should also be well documented and the source code should be available for inspection. Code testing should ideally follow the three-level procedures advocated by the International Ground Water Modeling Center (IGWMC) or those used in the various international code testing studies (INTRACON, INTRAVAL, etc.).

- Documentation on the source code should be included, with an executable version of the code and data sets relevant to the problem. This allows the reviewer to independently verify the results presented in the modeling report and to review details from the individual model output files.

#### Layering and Gridding

- The rationale for the selection of the grid spacing, number of model layers, and the resulting number of nodes and elements should be given.
- The grid should be evaluated in terms of potential

inaccuracies or numerical problems.

Common features to evaluate include: (1) the model boundaries should not be too close to the area of active remediation (wells etc.), (2) model nodes should coincide with pumping centers otherwise the effects of these stresses will be offset, (3) the grid should be aligned with the principal axes of hydraulic conductivity, (4) in finite-difference models, the grid spacing between adjacent cells should not vary by more than a factor of 1.5, (5) in transport modeling, the Peclet number should not be greater than 2, (6) the maximum aspect ratio of the grid should not be greater than 100:1.

Other aspects of grid design are more subjective. For example, the degree of discretization (number of rows and columns) should be appropriate for the problem being solved. Areas of sharp contrast in hydraulic properties should be more finely discretized. Model layering should be consistent with the magnitude of vertical gradients and the degree of vertical heterogeneity. If matrix diffusion is important, confining units should be discretized into multiple layers.

#### *Figures and Tables*

- The grid should be presented as an overlay of a map of the area to be modeled.

A vertical cross section of the modeled area which displays the vertical layering of the model with respect to its hydrogeology should be included.

Horizontal and vertical grid coordinates and elevations should be identified clearly on all figures.

#### Boundary and Initial Conditions

- Selection of all boundaries and initial conditions should be justified.

The justification would involve a discussion of how a natural feature was simulated (e.g., a river or ground-water divide) including any assumptions related to the choice of boundary type and location. Of particular concern are boundaries that do not coincide with natural features but are somewhat

arbitrary. Careful scrutiny should be given to such artificial boundaries. Ideally, a sensitivity analysis would be performed on these arbitrary boundaries.

Descriptions of model boundaries should include whether the boundaries are transient or steady-state. For transient boundaries, the report should discuss how the boundary condition changes with time and how these changes were determined. In the natural system, boundaries may shift with time, and the effect that these positional changes may have on the results of modeling should be considered.

Boundaries should also be chosen to ensure that future simulations will not be adversely effected by pumping wells or other features that stress the system. Justification of the chosen boundaries should address this potential problem.

- Uncertainty surrounding boundaries and initial conditions should be discussed.

There is usually significant uncertainty in the selection of boundary conditions. These uncertainties include the type of boundary chosen to simulate a natural feature, the position of the boundary, the value of head or concentration at the boundary, the assignment of conductance properties to the boundary, and the transient response of the boundary. All of these factors should be addressed by the model report. A sensitivity analysis on boundary conditions should also be included.

- The following specific examples may be useful in reviewing the model boundary conditions:

Under steady-state conditions, the areal recharge should not exceed the saturated hydraulic conductivity of the surficial soil through which it must travel; otherwise ponding would occur.

Potentiometric lines on streams that are gaining water should point upstream, whereas the lines should point downstream along losing streams.

Contaminant source release rates should be discussed.

Ephemeral streams generally should not be modeled as constant head boundaries.

Streams are frequently modeled as ground-water divides, that is, all ground-water flowing towards the stream is assumed to be captured by the stream. The modeler should justify this assumption, as not all streams fully penetrate the aquifer.

Surface-water/ground-water interactions should be discussed.

Recharge and evapotranspiration are difficult to determine, and therefore, recharge as a flux boundary is often used as a calibration parameter. The method for determining recharge should be presented.

Interpretation and extrapolation methods (e.g., Kriging) should be described.

Boundaries between two types of porous media should always coincide with element boundaries.

#### *Figures and Tables*

- The report should clearly identify assigned boundaries and initial conditions in figures and tables. A typical figure would be a plot of the model grid for each layer clearly illustrating boundary cells. Each type of boundary (e.g., constant head, constant flux, and head-dependent flux) should be labeled using a different symbol or color. For transient boundaries, multiple figures representing different times may be used or tables of values may be more appropriate.
- The boundary condition sensitivity analysis should be illustrated using figures and tables.

#### Time Steps

- The Courant criterion outlined in Section 4.2.2.3 should be satisfied for transport simulations.
- Even for flow models, the time steps should be small at the start of the simulation and gradually increase. Time step size should be decreased when major changes in stresses are simulated.

#### Calibration

- The calibration process should be described in

detail, including any assumptions and limitations.

Proper justification should be given if the model was not calibrated. In some cases, such as a screening analysis, calibration may not be required. However, an uncalibrated model is not as reliable a decision-making tool as a well-calibrated model.

Documentation of the calibration process should include flow diagrams illustrating the approach that was taken to calibrate the model. The objectives or criteria used to calibrate heads, flows, and radionuclide concentrations should be presented. The method of calibration (inverse model, trial-and-error, or a combination of both) should be documented. If special calibration software is used (e.g. an inverse model), it should be documented and described under the code selection section.

If both steady-state and transient calibrations are performed, their similarities and differences within the results should be discussed. The rationale and selection of time steps for the transient calibration should be discussed.

- The sources and magnitudes of errors should be described.

All calibrated models have errors. These errors are often called residuals and represent the difference between a model-computed value and a value measured in the field (usually head or concentration). The errors should be described in detail in the report. The review should concentrate on potential effects on the predictive simulations which will be performed later (e.g., risk assessment).

- Modifications to the parameter values, boundary conditions, and imposed hydraulic stresses should be discussed in detail.

The calibration process is an exercise in parameter estimation where key model parameter and boundary values are adjusted within reasonable bounds to achieve the calibration objectives. The review should focus on the response of the modeled system to the altered values and the rationale for the parameter changes made during the calibration. The calibrated parameter values

should be compared with the initial range of these parameters. Particular emphasis should be placed on parameters that fall outside their originally estimated range. The final values should be compared to those identified in the conceptual model.

- The rationale for the convergence criterion for the heads and concentrations should be presented, in addition to a discussion of the overall mass balance results.

Problems that arose due to failure of the code to converge or numerical instabilities should be described. The mass-balance results should be discussed in relation to any convergence problems. Overall, the water balance should be in error by less than one percent.

The user-specified error or convergence criterion will result in a level of accuracy that is one to two orders of magnitude greater than the criterion. This difference should be evaluated with respect to the desired level of accuracy.

- The calibrated model should be a good match with the conceptual model, such as flow directions and parameter values.
- Specific examples to look for in reviewing the calibration include:

The calibrated parameters, especially hydraulic conductivity, should not appear patchworked. Unless there is evidence indicating that hydraulic conductivity values change substantially from one grid block to the next, it should be assumed that large percentages of the modeled area are relatively homogeneous.

Areal recharge should be uniform unless there is sufficient justification to vary the recharge rates locally.

Well logs and aquifer stress test data should be reviewed to ensure that the hydraulic conductivities assigned to that area are compatible.

The volume of water entering or exiting local streams, lakes, or rivers should be consistent with the field data.



It should be kept in mind that head and concentration values computed at a node are representative of an area rather than a point. Therefore, if drawdown values during aquifer tests are used as calibration points, even a well-calibrated model would not match the field data exactly because data collected from wells represent points in space.

Vertical gradients within an aquifer in which the well is not fully penetrating should be considered when the model is calibrated.

#### *Figures and Tables*

- Areal and cross-sectional diagrams of the error (residual) between computed and measured hydraulic head and radionuclide concentrations should be presented. The errors should not show significant spatial bias. For example, if all of the targets in the western half of the model are computed too high and those in the east are too low, there is a bias in the calibration. In this example, the gradients would be inaccurate.
- A list and a figure indicating the final calibrated values for parameters and boundary conditions should be included.
- The match to the calibration targets should be shown in figures as well as in tables. Sections within the model should be outlined and discussed according to their "goodness of fit" to the calibration targets.
- Particle tracks or calibrated plumes should be shown in planar and cross-sectional views.

#### Sensitivity Analysis

- The approach undertaken for the sensitivity analysis should be described in detail.

There are a variety of ways to perform a sensitivity analysis. According to ASTM, the sensitivity analysis should evaluate both the calibration and the predictions (if any). Sensitivity of predictions to model parameters and boundary conditions is important in evaluating the degree of uncertainty in the model. Both parameter values (e.g. hydraulic conductivity) and boundary conditions should be evaluated in the

sensitivity analysis.

The sensitivity of model calibration quality and model predictions to variations in parameter values, including grid spacing, time steps, and boundary conditions, should be discussed, emphasizing parameters in which there is a large degree of uncertainty and the results are very sensitive.

- The rationale for selecting parameters for the sensitivity analysis and for determining whether there were sufficient simulations investigating single or multiple parameters should be presented.
- The relevance of the overall uncertainty and sensitivity with respect to the objectives of the predictive simulations should be discussed.

#### *Figures and Tables*

- The results of the sensitivity analysis should be displayed in a graph or table.

A typical sensitivity graph plots a calibration statistic (sum of squared residuals for example) versus a range in parameter values for each parameter. Multiple parameters may be plotted on one graph. Model sensitivity coefficients may be computed as the change in a model-computed value (head or concentration) divided by the parameter change. These sensitivity coefficients may then be contoured to illustrate changes in model sensitivity through space. Where many parameters are involved, a table may be presented to identify the most sensitive parameters.

#### **Modeling to Support Baseline Risk Assessment**

- The objectives of the risk assessment should be stated.
- The modeling approach, in addition to any inherent limitations, should be clearly indicated.
- The conceptual model should be presented, in conjunction with the validity of and rationale for any simplifying assumptions.
- The method used to calculate infiltration rates and other relevant parameters should be included.

- A discussion of the source term should be presented, including its dimensions, strength, and composition.
- The means by which release rates and leachate concentrations are calculated should be described.
- The treatment of daughter-ingrowth in the source term in unsaturated and saturated zones should be described.
- The fate and transport processes active in the unsaturated and saturated zones should be presented.
- The processes by which the leachate becomes diluted along the transport path from the source term to the receptor should be discussed.
- If the output from the risk-based code is coupled to a more sophisticated code, this process should be described in detail.
- The process by which remedial action goals were determined from the results of the risk assessment should be discussed.
- The methods of calculation outlined in Appendix B can be used for independent verification of the results of the risk assessment.

#### *Figures and Tables*

- An areal and cross-sectional representation of the conceptual model should be shown, including the locations of the assumed receptor.
- Radionuclide breakthrough concentration plots should be included for each receptor and radionuclide of interest.
- Selected areal isoconcentration plots should be given.

#### **Preliminary Remedial Design**

- The report should follow the guidelines given earlier in this chapter and include discussions and similar presentations on developing the conceptual model, selecting the parameters, designing the grid, calibrating the model, and carrying out the sensitivity analyses.
- The assumptions and calculational procedures used to determine the specific assumptions associated with the remedial design should be presented, such as the locations of recovery wells and failure rates for barriers.
- In addition to the review of the grid design and time-stepping schemes previously presented, are there other relevant processes which may be important and should have been considered (e.g. matrix diffusion)?
- If a pump-and-treat scenario is modeled, does the model accurately simulate the rise and fall of the water table?
- If the model also was used for risk assessment, have conservative assumptions been removed and the model recalibrated? For instance, a conservatively low hydraulic conductivity would yield high well concentrations, which may be acceptable for the risk assessment, but would overestimate the capture zones and influent concentration of the remedial design.

#### *Figures and Tables*

- In addition to the figures and tables previously discussed that are relevant to the remedial design presentation, additional figures such as areal and cross sectional views of barrier walls, capture zones, and/or recovery wells should be included.

**Table 5-1. Major Steps in Modeling Evaluation Procedures**

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
<b>CHAPTER 2 OBJECTIVES AND DATA REQUIREMENTS</b>			
<i>Are the purpose and scope outlined?</i>			
<i>Are the objectives consistent with decision-making needs?</i>			
<i>Are the objectives satisfactory?</i>			
<i>Are a site description and waste disposal history provided?</i>			
<i>Are the data requirements for the proposed modeling outlined?</i>			
<i>Are the sources of data adequately presented?</i>			
<i>Are data uncertainties discussed?</i>			
<i>Is the probable sensitivity of the future modeling results presented for the data?</i>			
<i>Are the potential data limitations and weaknesses provided?</i>			
<i>Are the plans to resolve data limitations discussed?</i>			
<b>CHAPTER 3 CONCEPTUAL MODEL DEVELOPMENT</b>			
<i>Is the physical framework discussed in detail? Both regional and local?</i>			
<i>Is the hydrogeologic framework described in detail? Both regional and local?</i>			
<i>Is the nature of the contaminant source term described?</i>			
<i>Are the hydraulic boundaries described in detail?</i>			
<i>Are data base deficiencies clearly identified and modeling implications discussed?</i>			
<i>Is the conceptual model consistent with the field data?</i>			
<i>Are the uncertainties inherent in the conceptual model discussed?</i>			
<i>Are the simplifying assumptions outlined?</i>			
<i>Are the assumptions justified?</i>			
<i>Are the natural boundaries or the aquifer system described?</i>			
<i>Are the following figures and/or tables<sup>2</sup> included:</i>			
<ul style="list-style-type: none"> <li>• Map showing location of study area.</li> </ul>			

*In some instances tabular representation of the data may be appropriate.*

**Table 5-1 (Continued)**

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
• Geologic map and cross sections indicating the areal and vertical extent of the system.			
• Topographic map with the surface water bodies.			
• Contour maps showing the tops and/or bottoms of the aquifers and confining units.			
• Isopach maps of hydrostratigraphic units.			
• Maps showing extent and thicknesses of stream and lake sediments.			
• Maps indicating discrete features (e.g., faults), if present.			
• Maps and cross sections showing the unsaturated zone properties (e.g., thickness, $K_{sat}$ ).			
• Potentiometric surface maps of aquifer(s) and hydraulic boundaries.			
• Maps and cross sections showing storage properties of the aquifers and confining units. <sup>1</sup>			
• Maps and cross sections showing hydraulic conductivity of the aquifers, confining units and stream and lake sediments.			
• Maps and hydrographs of water-budget information.			
• Maps and cross sections indicating transport parameters (e.g., $K_d$ ). <sup>1</sup>			
• Areal and cross sectional isoconcentration maps of primary contaminants in soil and ground water.			
• Time-series graphs of contaminant concentrations.			
• Relevant source-term inventory information.			
<b>CHAPTER 4 MODEL APPLICATION</b>			
<b>Section</b>			
(4.1) SCOPING ANALYSIS			
<i>Are scoping analyses performed?</i>			
<i>Do scoping results lead to proposed modeling approach?</i>			
(4.2) SITE CHARACTERIZATION MODELING			
(4.2.1) Code Selection			
<i>Is the rationale for the selection clearly presented for proposed code(s)?</i>			
<i>Are the general features of the code(s) presented?</i>			
<i>Are the assumptions and limitations of the code(s) presented and compared to the conceptual model?</i>			

**Table 5-1 (Continued)**

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
<i>Is the basis for regulatory acceptance presented?</i>			
<i>Is the source documentation for the code included?</i>			
<i>Is an executable version of the code included?</i>			
<i>Is the source code readily available for inspection?</i>			
<i>Does the code have a history of use?</i>			
<i>Is the code well documented?</i>			
<i>Is the code adequately tested?</i>			
<i>Are the hardware requirements compatible with those available?</i>			
(4.2.2) Model Construction			
(4.2.2.1) Layering and Gridding:			
<i>Is the domain of the grid large enough so that the boundaries will not interfere with the results?</i>			
<i>Do the nodes fall near pumping centers on existing and potential future wells and along the boundaries?</i>			
<i>Is the grid oriented along the principal axes of hydraulic conductivity?</i>			
<i>Is the grid discretized at the scale appropriate for the problem?</i>			
<i>Are areas of sharp contrasts (e.g., hydraulic conductivity, concentration, gradient) more finely discretized?</i>			
<i>Is the Peclet number less than 2?</i>			
<i>Do adjacent elements vary in size by a distance less than a factor of 1.5?</i>			
<i>Are strong vertical gradients within a single aquifer accommodated by multiple planes or layers of nodes?</i>			
<i>If matrix diffusion is important, are the confining units adequately discretized in the relevant regions of the model?</i>			
<i>Is the grid more finely spaced along the longitudinal direction of simulated contaminant plumes?</i>			
<i>Is the aspect ratio less than 100:1?</i>			
<i>Are the following figures included:</i>			
<ul style="list-style-type: none"> <li>• Grid presented as an overlay of a map of the area to be modeled.</li> </ul>			
<ul style="list-style-type: none"> <li>• A vertical cross section(s) which displays the vertical layering of the model grid.</li> </ul>			
(4.2.2.2) Boundary and Initial Conditions			

**Table 5-1 (Continued)**

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
<i>Is justification provided for the selection of all boundary and initial conditions?</i>			
<i>Are model boundaries consistent with natural hydrologic features?</i>			
<i>Are the boundary and initial conditions consistent with the conceptual model?</i>			
<i>Are the uncertainties associated with the boundaries and initial conditions addressed?</i>			
<i>Are the boundaries far enough away from any pumping/injection centered to prevent "boundary effects"?</i>			
<i>Are transient boundaries discussed?</i>			
<i>Is the rationale given for simplifying the boundaries from the conceptual model discussed?</i>			
<i>Are the values for the assigned boundaries presented?</i>			
(4.2.2.3) Specification of Time Steps			
<i>Is the Courant criterion satisfied?</i>			
(4.2.2.4) Model Parameterization			
<i>Are data input requirements fully described?</i>			
<i>Is the discussion of the data well founded with respect to Objectives and Data Review Section?</i>			
<i>Are the interpretation and extrapolation methods (e.g., Kriging) adequately presented?</i>			
<i>Do the figures and tables completely describe the data input with respect to discrete components of the model?</i>			
<i>Are the model parameters within the range of reported or measured values?</i>			
(4.2.3) MODEL CALIBRATION			
<i>Has calibration been attempted?</i>			
<i>Is the rationale for model calibration approach presented?</i>			
<i>Are the calibration procedures described in detail?</i>			
<i>Are the calibration criteria presented?</i>			
<i>Does the calibration satisfactorily meet specified criteria?</i>			
<i>Is the rationale presented for selecting convergence criteria?</i>			
<i>Are code convergences and numerical instabilities discussed?</i>			
<i>Do the calibrated parameters fall within their expected ranges?</i>			

**Table 5-1 (Continued)**

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
<i>Are discrepancies explained?</i>			
<i>Has the calibration been tested against actual field data?</i>			
<i>Are the differences between steady-state and transient calibrations presented?</i>			
<i>Could other sets or parameters have calibrated the code just as well? Is this discussed?</i>			
<i>Are areal and cross-sectional representations of the final calibrated results included for both hydraulic heads and radionuclide plume(s)?</i>			
<i>Does calibration of the model take into account the inconsistency between point measurements at wells and areal averages of model output?</i>			
<i>Is the match between the calibration targets and final parameters shown diagrammatically?</i>			
<i>Were calibrating errors presented quantitatively through the use of descriptive statistics?</i>			
<i>If particle-tracking was performed, are these results shown?</i>			
<i>Is the calibrated model consistent with the conceptual model?</i>			
<i>Are any changes to the conceptual model discussed and justified?</i>			
<i>Is non-uniform areal recharge applied? Is this approach justified?</i>			
<i>Does the calibration properly account for vertical gradients?</i>			
<i>Is the calibrated hydraulic conductivity field consistent with the geologic logs and aquifer stress tests?</i>			
<i>Are the convergence criteria appropriate?</i>			
<i>Was a mass balance performed?</i>			
<i>Is the water-balance error less than 1%?</i>			
<i>Are the mass balance results for the calibrated model discussed?</i>			
<i>Is the model's water balance consistent with known flows of rivers and levels of lakes?</i>			

**Table 5-1 (Continued)**

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
<b>(4.2.4) SENSITIVITY ANALYSES</b>			
<i>Was a sensitivity analysis performed?</i>			
<i>Is the approach to the sensitivity analysis detailed?</i>			
<i>Were all input parameters selected for investigation? If not, was rationale presented for excluding parameters?</i>			
<i>Was a sensitivity analysis performed on the boundary conditions?</i>			
<i>Are the ranges of parameters appropriate?</i>			
<i>Were sufficient simulations performed? Was justification provided?</i>			
<i>Was the relevance of the sensitivity analysis results to the overall project objectives discussed?</i>			
<i>Are the results presented so that they are easy to interpret?</i>			
<i>Were sensitivity analyses performed for both the calibration and the predictive simulations?</i>			



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## **APPENDIX A**

### **FATE AND TRANSPORT OF RADIONUCLIDES**

**Contents - Appendix A**

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## APPENDIX A. FATE AND TRANSPORT OF RADIONUCLIDES

The following discussion is intended to explicate the potential effects that simplifying assumptions (e.g.,  $K_d$ ) may have on the modeling results.

The nature of the ground water environment restricts the number of processes that control the fate of radionuclides as they are transported from their source to the accessible environment. These processes fall into two categories: radioactive decay and those processes related to transport. Transport-related processes (e.g., sorption, ion exchange, and precipitation) can facilitate or retard the movement of ground-water contaminants, but radioactive decay always results in a loss of activity of the original radionuclide. Radioactive decay, however, can result in an increase in radioactive or chemically toxic daughter products as the original radionuclide disintegrates.

Various mechanical and geochemical processes will affect the transport of contaminants by flow through either a porous matrix or a fracture system in a porous matrix. The mechanical processes considered are advection, dispersive effects (hydrodynamic dispersion, channeling), and diffusion. Among the chemical processes considered in this paper are adsorption on mineral surfaces, including the kinetics of adsorption, and processes leading to precipitation. Although vapor transport is not always directly associated with ground-water flow, the two processes are closely related; therefore, gaseous transport is also briefly discussed. Furthermore, some radionuclides can occur and migrate in the gaseous phase. Gas phase migration can therefore be an important mechanism for some radionuclides to migrate from the repository to the accessible environment. For example, radioactive carbon-14 can be in the form of carbon dioxide gas, and tritium (radioactive hydrogen) can be in the form of hydrogen gas or tritiated water vapor.

### A.1 Physical Transport and Retardation Processes

In both saturated and partially saturated conditions, ground water can carry material along in solution or as suspended solids. The rate at which the transported material moves is affected by a variety of factors, the most important being the velocity of the flowing water and the partitioning of the material between liquid (i.e., water) and solid (i.e., rock) phases. The dominant physical processes are advection, dispersive effects, and diffusion.

**(a) Advection and hydrodynamic dispersion.** The process by which solutes are

transported by the bulk motion of water is known as advection. There is a tendency, however, for the solute to spread out from the path that it would be expected to follow according to the advective hydraulics of the flow system. This spreading phenomenon is called hydrodynamic dispersion. It causes dilution of the solute and occurs because of spatial variations in ground-water flow velocities and mechanical mixing during fluid advection; molecular diffusion, due to the thermal-kinetic energy of the solute particles, also contributes to the dispersion process.

Dispersion can result from diffusion, channeling, and turbulent flow, but dispersion by itself does not affect the average rate at which the transported material moves. It can, however, cause some of the contaminant (in a diluted state) to move faster than the average ground-water flow velocity. This may be significant for radionuclides with relatively short decay half-lives; if some of the radionuclide arrives relatively quickly at the accessible environment due to dispersion, it will have higher radioactivity because of the shorter decay time.

Dispersion is generally responsible for the shape of the tracer-test breakthrough curves. The low concentrations of the radionuclides that mark the first arrival at the withdrawal well have been dispersed ahead of the bulk or average ground-water velocity. The peak of the breakthrough curve represents the average velocity of the contaminant (advection dominated), and the tail of the breakthrough curve is formed by radionuclides that have been dispersed along longer flow paths and at slower velocities than the average rate of ground water.

Dispersion is the primary mechanism responsible for dilution (mixing) processes in ground water but is generally less significant than in air and in surface water. In both air and surface water, dispersive dilution is often a major phenomenon because the flow can be turbulent. Turbulent flow means that all the flow paths are not essentially parallel to the gross direction of motion. Flow components that are perpendicular to the bulk fluid motion cause the plume to spread laterally not longitudinally, thus reducing the concentration in the plume, as the volume of contaminated air or surface water increases. In ground water, however, the magnitude of dilution is usually much smaller, partly because turbulent flow rarely exists. The slow speed of ground water, coupled with the effects of small channels in the intergranular pore space, tends to keep the flow smooth and laminar. In an idealized conceptual model, the interconnecting pore spaces can be thought of as forming flow channels or tubes; any tendency for the flow to eddy is resisted by the sides of the flow channel. However, since the interconnecting pore spaces do not make a continuous flow channel in real materials, there is some lateral mixing due to branching of flow channels and spatial variation in flow velocity.

Dispersion (neglecting molecular diffusion) is not significantly affected by laminar eddy currents. If molecular diffusion is momentarily disregarded, dispersion in porous or fractured media is caused by five principal phenomena: anisotropic permeability, varying pore sizes, varying path length, variation in the velocity gradient across pore space, and flow splitting around soil particles with mixing within the pore space. These five phenomena all contribute to longitudinal dispersion; anisotropic permeability and flow splitting around the soil particles can cause lateral dispersion. In nearly all ground-water systems, longitudinal dispersion effects are much larger than lateral dispersion effects. Researchers have reported longitudinal dispersivity values ranging from about 1 to 25 times higher than transverse dispersivity values (GEL85). In fractured systems, the longitudinal dispersivity would likely be much greater than the transverse.

**(b) Molecular diffusion.** Diffusion in solutions is the process whereby ionic or molecular constituents move under the influence of their kinetic activity in the direction of their concentration gradient. Molecular diffusion is a relatively slow process but also contributes to the overall dispersion process, primarily through micro-scale mixing within individual pore or fracture channels which leads to large-scale bulk dilution and spreading in very slow moving ground water.

The diffusion of radionuclides from water moving within fractures, or coarse-grained material, into the finer-grained rock matrix (i.e., matrix diffusion) can be an important means of slowing the transport of the dissolved radionuclides, particularly for non-sorbing or low-sorbing soluble species. The apparent diffusion coefficient for a given radionuclide depends on properties that are intrinsic to the chemical species (e.g., ion mobility), as well as properties of the rocks (such as porosity, tortuosity, and sorption ratios).

A radionuclide introduced into a fractured porous medium will migrate through the fracture openings by means of advection as well as hydrodynamic dispersion. The radionuclide may also diffuse slowly into the porous matrix. If molecular diffusion is occurring, it will dominate flow and transport within the porous matrix because the fluid velocity in the porous matrix is usually very low. When introduced into a fractured aquifer, the radionuclide moves rapidly within the fracture network. As time passes, the zone of contamination will diffuse farther into the porous matrix. Since the porous matrix has a very large capacity to store the contaminant, it plays a significant role in retarding the advance of the concentration front in the fractures. If the source of contamination is discontinued and the water-bearing unit is flushed by non-contaminated water, the contaminant mass in the fractures will be removed relatively quickly, whereas the



contaminant in the porous matrix will be removed very slowly via diffusion back into the fracture openings.

**(c) Gaseous transport.** A limited number of radionuclides can form volatile species capable of being transported in a moving vapor or gas. Among these are tritium, carbon-14, and iodine-129. On a macroscopic scale, factors that affect transport in flowing ground water also affect transport in flowing gas (i.e., the velocity of the gas determines the potential for advective transport). In the absence of flow, diffusion is the only mechanism for transport in the gaseous state. The processes of partitioning of the volatile species between the gaseous, liquid, and solid state and isotopic exchange must also be considered when assessing the impact of gaseous transport.

## A.2 Chemical Transport and Retardation Processes

In addition to the physical processes, the transport of radionuclides is affected by a wide range of chemical processes. Many of these reactions are poorly understood and are the subject of ongoing research. From a practical view, the important aspect is the removal of solute from solution irrespective of the process. For this reason, most computer codes simply lump all of the cumulative effects of the geochemical processes into a single term (i.e., distribution coefficient- $K_d$ ) which describes the degree to which the radionuclide is retarded relative to the ground water. Thus, the distribution coefficient relates the radionuclide concentration in solution to concentrations adsorbed on the rocks. The following paragraphs summarize the primary geochemical processes that can play a role in the transport of radionuclides.

**(a) Sorption.** An important mechanism in retarding the migration of radionuclides in ground water is sorption, which is defined to include all solute-rock interactions that cause the radionuclides to migrate at a slower rate than the ground water itself. The amount of sorption is dependent on both the chemistry of the water and of the rocks; because some of the chemical reactions are relatively slow, it can be a function of time as well.

Sorption coefficients are usually obtained using a standard batch test where rocks or soils are put in contact with ground water in which small amounts of dissolved radionuclides have been mixed. A problem with this technique is that more detailed geochemical data are necessary to support the validity of applying the sorption measurement to the real-world physical and chemical conditions and expected travel time of the radionuclides (which may be of the order of

hundreds to thousands of years). Such mechanisms as dissolution/ precipitation, complexing, adsorption/desorption, phase transformations, and solubility should be understood for radionuclides of interest in the geochemical environment.

The tendency of a radionuclide dissolved in ground water to be sorbed by the aquifer's solid phase can be expressed in terms of the soil/solution partition coefficient,  $K_d$ , also referred to as a distribution coefficient.  $K_d$  is the simplest mathematical approach to adsorption and may be derived from the Freundlich isotherm equation

$$x/m = K_d C^{1/n} \quad (1)$$

where  $x/m$  is the amount adsorbed (Ci chemical per gram of soil), and  $C$  is the concentration of chemical Ci/ml in the aqueous phase. The value of  $1/n$  depends on the sorbate and sorbent being studied and is usually close to 1 (LYM82).

Sorption of radionuclides in the saturated zone will be due primarily to the high surface area (per unit mass) of minerals such as clays. Lipophilic substances tend to form films at water/solid interfaces just as they do at the air/water interface. Thus, if the saturated zone contains clays or other high surface area minerals, the ground water is presented with a large water/solid interface on which some types of contaminants can form a surface film. Adsorption isotherms in which sorption can be correlated with the surface area of the adsorbent are called Langmuir isotherms. Adsorption phenomena of this type are not linear and can reach a saturation limit after which further adsorption will not occur, even from water with greater concentrations of radionuclides.

Several variations of the adsorption isotherm equation are available for the fitting of empirical data from experimental sorption studies (KIN86). The means for calculating sorption retardation of dissolved inorganic radionuclides is similar to the method used for computing retardation of organic contaminants by soil carbon content and octanol/water partition coefficients. The distribution coefficient for a specific radionuclide depends in part on chemical composition of aqueous solutions. Thus, for a given geologic material, a radionuclide can have a wide range of distribution coefficients, depending on the total chemical characteristics of the water.

Limitations of the distribution-coefficient approach to geologic investigations include:

- The assumption of a linear sorption isotherm. The terms "sorption isotherm," "Freundlich isotherm," or "Langmuir isotherm" are generally used to define the relationships between

sorption and the concentration of the element being sorbed at a constant temperature.

- Total reversibility in the sorption/desorption reaction is assumed. However, the distribution between the solid phase and the aqueous phase may include precipitation or irreversible reactions or both.
- Sorption/desorption reactions are generally assumed to be instantaneous. However, in some cases the reaction rate may be too slow to justify that assumption.
- The aqueous-phase speciation is not well known for many of the radionuclides.

These limitations do not necessarily apply to all of the radionuclides. For example, the solution chemistry of the alkaline earths (Cs, Ra, and Sr) is well known, and the aqueous-phase species can be predicted with relatively high certainty provided that the nature of the soil and rocks is known. When measured sorption values are very high or very low, the range of individual measurements may be quite large. A very high or very low  $K_d$  indicates that one phase, either the solution or the solid, has very little of the radionuclide present; therefore, very few detectible radioactive disintegrations occur, giving rise to relative high potential counting errors compared to those obtained where sorption ratios are close to unity.

**(b) Ion exchange phenomena.** Ion exchange is one of several possible sorption processes. It is a particularly important process for many common cationic radionuclides and therefore deserves separate focus. The primary retardation mechanisms for both organic and inorganic ionic contaminants in ground-water systems are ion exchange and precipitation. Ion exchange is primarily effective on cations (positively charged ions), although in certain hydrogeochemical environments anions are also retarded by ion exchange. Ion exchange capacity within a geologic material is almost exclusively limited to colloidal clay and silica particles (diameters in the range  $10^{-3}$  to  $10^{-6}$  mm), because these particles have a large ionic charge relative to their surface areas. This charge is the result of (1) cationic substitutions within the crystal lattice and (2) ionic dissociation at the surface. To neutralize this charge, an adsorbed layer of cations and anions forms a zone adjacent to the hydroxylated layer (PAR67). The net charge of this zone can be negative or positive, depending on the pH of the immediate environment. At low pH, a positively charged surface prevails; at neutral to high pH, a negatively charged surface develops (FRE79). The tendency for sorption of either cations or anions therefore depends on the pH. Most natural ground-water systems have a pH in the neutral to positive range. Therefore, most systems tend to have a stronger tendency for cation exchange than for anion exchange.

Neutralized colloidal particles may be transported in the ground water with organic and inorganic contaminants on their surfaces. Additionally, humic substances can exist as colloidal particles and also serve as ion exchangers. Some radionuclide species such as plutonium and other transuranic elements have been reported to exist as suspended colloids (CLE81). Some contaminants that might otherwise be sorbed to stationary material in the aquifer could be transported in the sorbed layers of these mobile colloids. Sorption in this case has facilitated transport. The cation exchange capacity (CEC) of soils and other geological materials is usually expressed as the number of milliequivalents of cations that can be exchanged in a sample with dry mass of 100 grams.

**(c) Speciation.** The solubility of the waste elements can influence their transport by limiting the maximum concentration of the elements dissolved in the aqueous phase. Speciation, defined as the formation of various complexes and oxidation states in the aqueous phase, in turn affects the solubility and mobility. Speciation and solubility of individual waste elements depend on the chemical properties of the waste element, on the state of the local water (composition, pH, oxidation state, and temperature), and, if nonequilibrium processes are important, on factors such as precipitation and dissolution kinetics, oxidation-reduction kinetics, the identity of the solids present, water-flow conditions, and colloid formation.

Elements dissolved in water can exist as various chemical species such as different oxidation states or complexes with other ions in water (STU81). Solubility generally increases as the variety and concentration of complexes of an element increase; thus, the solubility is influenced by the tendency of a given element to form complexes and the concentrations of species with which it can complex. Sorptive behavior depends on the size and charge of the sorbing species; both of these quantities vary among the complexes of a given element. Thus, speciation can influence sorption. Plutonium, for example, can exist at several different oxidation states in either a cationic or anionic form. It can also be complexed with various other ionic species such as carbonate. Each of the various species may have different solubility and mobility characteristics.

Aqueous species of most elements can be experimentally detected in solution by a number of techniques; spectroscopy is most commonly used. However, concentrations of aqueous species are normally calculated from a knowledge of the overall composition of the solution (total concentrations of the elements in solution) and the formation constants of possible aqueous species using equilibrium thermodynamic methods. Equilibrium thermodynamic methods work

well (given the proper data) for the various complexes of a particular oxidation state, but may yield inaccurate results for the distribution of the element among possible oxidation states (LIN84).

**(d) Precipitation (phase separation from ground water).** After a radionuclide has entered the ground water, changes in the temperature, pH, and other chemical constituents may bring about precipitation (i.e., phase separation) of the intruding radionuclide. The solubility of most radionuclides varies directly with the temperature, and the groundwater's level of acidity can also affect the solubility (SPO81). If an element can also exist in various oxidation states, variables that control oxidation-reduction behavior also influence solubility. Unlike complex formation, which is essentially always an equilibrium process, precipitation processes are often not in equilibrium or in metastable equilibrium (STU81). If dissolution and precipitation kinetics are relatively rapid, over the time frame of interest, equilibrium behavior can be assumed. If kinetics are very slow, a metastable equilibrium may exist where the aqueous phase is in metastable equilibrium with some solid other than the most stable (least soluble) one. In some intermediate cases, the dissolution or precipitation rates may be comparable to the time scale of interest; for these cases, kinetic data are required to describe aqueous concentrations accurately.

Coprecipitation refers to a group of processes whereby more than one compound precipitates at one time (SPO81). Three examples are mixed-solid formation, adsorption during precipitation, and inclusion during precipitation.

**(e) Natural colloid formation.** A number of actinides, plutonium in particular, can form natural colloids under conditions of near neutral solutions of low ionic strength (AVO84). These colloids are optically clear in solution, show a characteristic adsorption spectrum, and do not settle out of solution. Colloidal plutonium shows x-ray diffraction patterns similar to crystalline plutonium dioxide; higher order lines are missing, indicating small crystalline size (20 to 30 angstroms). There is also some indication that americium may form colloids under similar conditions (OLO84).

A possible mode of radionuclide transport involves the movement of radioactive particles suspended in the ground water. Colloidal particles (up to 0.5 micrometers in diameter) remain suspended for long periods and hence may migrate with the ground water. As the solid waste form is leached, particles containing radionuclides may form by the sorption of dissolved radionuclides on nonradioactive particles.

To estimate the amount of radionuclides that can be transported by colloidal suspension, it is first necessary to determine whether colloidal-sized particles exist in the ground water. Then, the sorption ratios for waste elements on these particles must be measured or estimated from the composition of the particles. In addition, the conditions under which colloids can form from the waste elements or from the waste and their stability after formation must be determined. Finally, the conditions necessary for the filtration or sorption of the particles by the rock matrix itself must be defined.

Matter in the colloidal state has a relatively large surface area; thus the most important properties of colloids are those that depend on surface interactions, such as adsorption. Drever (DRE82) discusses the nature and geochemistry of colloids, with emphasis on the charge surrounding colloids and its effect on suspension stability.

Olofsson *et. al.* (OLO81) classify radiocolloids (colloids containing radionuclides) as true colloids or pseudocolloids depending on their formation process. True colloids are formed by condensation of molecules or ions as a result of hydrolytic or precipitation processes. Colloids consist mostly of hydroxides or polymers formed by hydrolysis, and they have a very rapid formation rate. Pseudocolloids, on the other hand, are formed as a result of adsorption on impurities in the solution and tend to be much larger than true colloids. Pseudocolloids can be of two types, reversible and irreversible. The formation rate of pseudocolloids is basically determined by the sorption rate on colloidal impurities (OLO82).

Radiocolloids are believed to be a significant factor for the transport of radionuclides in some environments and might facilitate their transport away from the source area (AVO82).

Radiocolloids may arise from a variety of sources. The corrosion of metal containers can lead to the formation of absorbent colloids. Degradation of engineered backfills may also lead to colloidal formation. If the waste form is leached by ground water, naturally occurring colloids derived from smectites, vermiculites, illites, kaolinite, and chlorite present in groundwater may also adsorb radionuclides. Champ *et. al.* (CHA82) have demonstrated experimentally the existence of rapid transport of plutonium colloids using core samples and ground water.

Transport of particulates in geologic media will depend on aqueous flow rate, on pore and fracture size in the rock, on ions carried in the water, and on the nature of the particulate matter. Several mechanisms may remove colloidal particulates from ground water such as mechanical filtration by the rock matrix, sorption on the surface of the rock pores (van der Waals forces), and

neutralization of the repulsive charges on the colloids, thus allowing them to coagulate. In addition, colloids will be subject to gravitational settling for particles larger than about 0.1 micrometer (TRA87).

**(f) Radiolysis.** Radiation can affect the solubility of waste elements by altering the composition of the water or by influencing the crystallinity of the solids that form (AUS69). The primary effect of gamma radiation will be a reduction in water pH and a trend toward more oxidizing conditions as long as air is present; secondary effects will be the production of nitrate (or nitrite) anions if nitrogen is present. Gamma-emitting radionuclides tend to be relatively short-lived and will be most important early in the life of a repository and, if ground water travel rates are slow, will have the greatest effect on the water near the waste.

Alpha radiation can affect water compositions in ways that are similar to the effects of gamma radiation. The primary effects of alpha radiation are a decrease in pH and a trend toward more oxidizing conditions in the water. Solids composed of alpha-emitters tend to show self-irradiation damage to their crystal structure; the solubilities of solids like the actinide oxides and hydroxides are affected in that amorphous solids, which are generally more soluble than crystalline solids, are more likely to be the natural precipitation products (NIT85). Some alpha-emitters are relatively long-lived and may be of concern for hundreds or thousands of years. Neutron radiation can have effects on other elements through neutron capture reactions. However, these effects are generally only significant near the source of strong neutron-emitters and would not be expected to affect ground-water chemistry or the migration of radionuclides downgradient, away from the waste source. Beta radiation is relatively weak and similarly would not be expected to have significant effects on ground-water chemistry or radionuclide migration away from the immediate vicinity of the source.

**(g) Biofixation.** A mechanism that appears to affect the transport of radionuclides under some conditions is microbial fixation (WES84). Radionuclides may be immobilized and/or mobilized by organisms in the repository environment. Immobilization may occur if radionuclides are incorporated into the cell structure of microorganisms or plants that are relatively stationary. On the other hand, radionuclides may be mobilized by forming biocolloids with bacteria, spores, and viruses.

**(h) Natural organic matter interactions.** Organic matter, in some instances, plays a significant role in the transport of radionuclides (LEV79). Wastes in the repository will contain a

significant quantity of organic matter. The most important transport-related interactions between organic matter and radionuclides are:

- Mobilization - Decomposition of organic material raises the partial pressure of carbon dioxide (CO<sub>2</sub>) in ground water and soil and adds organic CO<sub>2</sub> and organic acids which leach and mobilize certain radionuclides (e.g., uranium).
- Transportation - Uranium can then be transported as bicarbonate anion or as soluble organic complex in ground water.
- Concentration - The humic acid can precipitate in ground water when pH becomes more acidic or where increased salt content is encountered. The humic acids can exchange or chelate uranium. Concentration factors greater than 10,000 times that of the ground water have been observed on the organic material.

**(i) Anion exclusion.** The negative charge present on many mineral surfaces can repel the approach of anions. The exclusion may limit the diffusion of anions into the matrix, thereby allowing the anions to move at the higher velocity of the water moving in the center of the fractures or intergranular pore space, away from the surface film. The same phenomenon can restrict the entry of anions into the smaller pores. This process is significant to the transport of radionuclides because negatively charged radiocolloids could potentially move faster than the average rate of the ground water. Under some geochemical conditions (i.e., very low pH), mineral surfaces may assume a more positive charge and thus repel cations rather than anions and cause the cations to move faster than the average ground- water rate.

**(j) Organic complexation.** Natural and anthropogenic organic colloids occurring in the subsurface can act as a sorbent for radionuclides in adsorption-desorption and cation exchange processes. This association of radionuclides with organic matter is a relationship that has been well documented in both the field and laboratory. Due to the large surface area per unit mass and anionic surface functional groups associated with some organic colloidal material, radionuclides have a significant potential to be adsorbed. If the radionuclide is adsorbed onto mobil colloidal matter, the radionuclide may be transported as a colloid.

The chemical and/or physical reaction which influences the radionuclide complexation with organic colloids will vary considerably with a number of experimental variables. Complexation increases at higher pH's and high humic substance concentrations and decreases at high ionic strengths.



The chemical and/or physical reaction which influences the radionuclide complexation with organic colloids is a reversible process. Parameters that influence reversibility include: pH, ionic strength, and radionuclide and organic compound concentrations. Complexation reversibility may be an important factor when ground water from various flow regions mix together in common hydrogeological units. When complexation reactions are reversed, the fate and transport mechanisms associated with the complexation may change accordingly.

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## **APPENDIX B**

### **SCOPING ANALYSIS PROCEDURES**

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## APPENDIX B - SCOPING ANALYSIS PROCEDURES

Prior to scoping calculations, the appropriate release mechanisms for the movement of radionuclides to the ground water need to be determined. If it is relatively certain that one or more transport mechanisms (e.g., unsaturated zone) is unimportant, than it may be neglected. The physical and chemical processes that may affect the fate and transport of radionuclides at the site (e.g., fracture flow, vapor transport) also need to be determined. A previous report issued as part of this interagency agreement outlines how to determine what site related characteristics may be important (EPA94).

Having made these determinations, it must then be decided how accurate the results need to be and what level analysis is appropriate to obtain the desired results. If the physical and chemical processes at the site are complex and will not be satisfactorily predicted with simplistic data analysis, then it may be necessary to consult with experts in the field regarding how to proceed. It is not practical to perform complex analyses without the use of computer programs and considerable expert help.

The calculational methods presented in this appendix have been divided into two parts: the release analysis and the fate analysis. The equations in the release analysis section are used to estimate contaminant release concentrations and volumetric release rates. The fate analysis deals with the processes influencing radionuclide transport and how to estimate radionuclide concentration in ground water.

### B.1 Release Analysis - Ground Water

- (1) Estimating contaminant release concentration. The release concentration of a radionuclide depends upon characteristics of both the waste and the site. For lagoons or impoundments, the concentration of the radionuclide in the lagoon or impoundment is considered to be the concentration of the leachate. For solid-waste disposal sites, the equilibrium solubility of the solid waste is generally used as the initial concentration, with the assumption that the waste will have equilibrated with the percolating rainwater. This may not be the case, however, for all radionuclides. Therefore, it may be necessary to estimate radionuclide concentrations as a function of the equilibrium partitioning between the solid and solution, i.e., the distribution coefficient,  $K_d$ . The following formulae provide a means to estimate leachate concentration under equilibrium partitioning conditions.

$$C_{wat} = \frac{M_{Ci}}{A \cdot \theta \cdot T + \rho K_d} \quad (\text{B-1})$$

$C_{wat}$	=	concentration in the leachate (Ci/m <sup>3</sup> -H <sub>2</sub> O)
$M_{Ci}$	=	amount of nuclide in source (Ci)
$A$	=	area of the source (m <sup>2</sup> )
$T$	=	thickness of the source (m)
$K_d$	=	distribution coefficient (cm <sup>2</sup> /gr)
$\rho$	=	bulk density (gr/cm <sup>3</sup> )
$\theta$	=	volumetric water content

where

$$\theta = \theta_{sat} * R_{sat} \quad (\text{B-2})$$

$\theta_{sat}$	=	total porosity
$R_{sat}$	=	saturation ratio

Under saturated conditions  $R_{sat} = 1$ . Under unsaturated conditions, the saturation ratio is a function of the infiltration rate, the saturated hydraulic conductivity, and the texture of the soil. The saturation ratio can be estimated using the following equation (CLA78):

$$R_{sat} = \left( \frac{I}{K_{sat}} \right)^{\frac{1}{2b+3}}$$

where

$I$	=	infiltration rate (m/yr)
$K_{sat}$	=	saturated hydraulic conductivity (m/yr), and
$b$	=	soil-specific exponential parameter (dimensionless)

Representative values of  $K_{sat}$ ,  $\theta_{sat}$  and  $b$  for various soil textures are listed in Table C.2-C.4 (Appendix C).

- (2) Estimating volumetric release rate. The volume of leachate is calculated in two ways, one for solid wastes and one for liquid wastes. For solid wastes, percolating water (from direct precipitation and/or stormwater runoff onto the site) is frequently the primary source of liquid. In some cases the waste may be buried below the water table so that

direct contact with groundwater is the principal leaching mechanism. The release rate to groundwater for radionuclides leaching from percolating precipitation through a buried source, can thus be calculated using the following equation:

$$L_c = C_{wat} \cdot A \cdot I \quad (B-3)$$

where

$$\begin{aligned} L_c &= \text{contaminant release rate (Ci/day)} \\ I &= \text{infiltration rate (M/day)} \\ A &= \text{area of contributing source (M}^2\text{)} \end{aligned}$$

The release rate to ground water for leaching of wastes that are disposed of below the water table can be calculated using the following equation:

$$L_c = K i A \cdot C_{wat} \quad (B-4)$$

where

$$\begin{aligned} K &= \text{hydraulic conductivity (M/day)} \\ i &= \text{hydraulic gradient (M/M)} \end{aligned}$$

For liquid wastes (i.e., lagoons or surface impoundments), precipitation has a minimal effect, since the liquid wastes will percolate to ground water under the influence of gravity. In this case, the rate of percolation depends on the permeability of the liner or the underlying or surrounding soil at the disposal site. The volumetric release rate for liquid wastes can be estimated using the following equation (BOW79):

$$Q = K_s i A \quad (B-5)$$

where

$$\begin{aligned} Q &= \text{volumetric flow rate (m}^3\text{/sec)} \\ K_s &= \text{Darcy's coefficient; for unlined lagoons use native soil hydraulic conductivity (m/sec)} \\ A &= \text{area of lagoon (m}^2\text{)}. \end{aligned}$$

The hydraulic gradient,  $i$ , is determined as follows:

$$i = \frac{\text{Hydraulic head}}{\text{liner thickness or underlying soil}} \quad (B-6)$$

The hydraulic head is the sum of the pressure and gravitational heads. In this case, it is



approximately equal to the depth from the top of the free liquid in the lagoon to the base of the liner or soil layer from which the parameter  $K_s$  in Equation B-5 is obtained; the liner thickness in Equation B-6 refers to the thickness of a liner when present, or for an unlined system, the depth of the soil to the water table. When the depth to the water table is large relative to the depth of free liquid in the lagoon, the hydraulic gradient will be approximately equal to 1.0. Alternatively, for systems with a thin liner and an appreciable depth of free liquid, the hydraulic gradient can be much greater.

The  $Q$ , in Equation B-5, is then used to estimate activity release with the following equation:

$$L_c = M_c Q \quad (\text{B-7})$$

where

$$\begin{aligned} L_c &= \text{contaminant release rate (Ci/day)} \\ M_c &= \text{contaminant concentration in lagoon fluid (Ci/m}^3\text{)} \\ Q &= \text{volume release rate (m}^3\text{/day)}. \end{aligned}$$

Equations B-5 and B-7 model the release rate from a lagoon regardless of whether the flow is saturated or unsaturated. For unlined active lagoons, the flow is typically saturated all the way to the water table. For clay-lined lagoons, the flow is saturated through the liner and unsaturated between the liner and the water table. Equations

B-5 and B-7 are appropriate when lagoon releases are analyzed but should not be used for spills or other conditions where there is no ponding of the radionuclides on the surface for a long period of time. Under these conditions, the assumption of saturated flow (through the liner or soil) may be violated.

Equations B-4 and B-6 apply to liquids that are mostly water. The hydraulic conductivity is defined in terms of the fluid properties density and viscosity. For liquids with a density or viscosity that differs from water,  $K_s$  can be corrected for this viscosity and density by calculating the term  $K_c$ , using the following:

$$K_c = K_w (\rho_c / \rho_w) (\mu_w / \mu_c) \quad (\text{B-8})$$

where

$$K_c = \text{corrected } K_s \text{ term} = \text{hydraulic conductivity of liquid contaminant (m/sec)}$$

$K_w$	=	hydraulic conductivity for water (m/sec)
$\rho$	=	density of liquids; c = non-aqueous; w = water (mg/liter)
$\mu$	=	dynamic viscosity of liquids; c = non-aqueous; w = water; (mg/m/sec).

and then substituting  $K_c$  for  $K_s$  in Equation B-5. For waste sites that are lined with flexible membrane liners (FML), the release rate depends on the characteristics of the contaminant as well as the liner (STE78). Liners that have been in place for long periods of time or otherwise subjected to significant chemical, radiological, physical, or geological degradation processes may have significantly greater permeation properties than in their original undergraded state.

## B.2 Fate Analysis - Ground Water

The nature of the ground-water environment restricts the number of processes that control the fate of radionuclides as they are transported from their source to the receptor area. These processes fall into two categories: radioactive decay and transport processes. Transport-related processes (i.e., sorption, ion exchange, and precipitation of solids) can facilitate or retard the movement of ground-water contaminants, but radioactive decay always results in a loss of activity (disintegrations or decays per second) of the original radionuclide. However, radioactive decay can result in an increase in radioactive or chemically toxic daughter products as the parent radionuclide disintegrates.

### B.2.1 Estimations of Ground-water Concentration

There are several different approaches to estimating the concentration of a radionuclide at the receptor if radioactive decay is the only process affecting concentrations (i.e., no dilution). One approach is based on the proportionality of volume and concentration of the waste versus those of ground water.

If limited ground-water monitoring data at the release point are available and sufficient environmental fate data are available to calculate an overall dilution rate (see Section B.3), the concentration at the receptor well can be calculated.

The concentration of a decaying substance at the selected point downgradient from the release point is given by the following equation:

$$C_{well} = C_{wat} \cdot e^{-\lambda \cdot \frac{x}{V_c}} \quad (B-9)$$

where

$C_{well}$	=	concentration at downgradient distance x (Ci/m <sup>3</sup> )
$C_{wat}$	=	leachate concentration (Ci/m <sup>3</sup> -H <sub>2</sub> O)
$e$	=	2.71828
$x$	=	distance downgradient from point of introduction (m)
$V_c$	=	contaminant velocity (m/yr)
$\lambda$	=	the radioactive decay constant which is equal to $\ln 2$ /half-life of the isotope (yr <sup>-1</sup> for $\lambda$ ).

In the absence of ground-water monitoring data, mathematical models are often used to estimate concentrations of contaminants in ground water at receptor wells or discharge points. Two general classes of models can be used for this purpose: numerical and analytical. Numerical models use various numerical analysis methods to solve the partial differential equations of flow and transport. Analytical models generally consist of algebraic equations which approximate the true solution of the differential equations. Both approaches have advantages, disadvantages, and limitations. For the purpose of scoping calculations, only analytical models will be considered (Section B.4).

### B.3 Quantitative Fate Estimation

Radioactive releases may travel in the unsaturated zone before entering the zone of saturation. However, the release can also be directly into the zone of saturation. The predominant direction of the unsaturated zone flow is downward until the flow reaches the zone of saturation. Within the zone of saturation, the flow is predominantly lateral. Ground-water velocity can be determined for both the vadose (unsaturated) and saturated zones and is examined in the next section.

- (1) Equations for ground-water flow and radioactivity transport. The movement of radionuclides in ground water can be described by two equations: one for the movement of the carrier fluid (water) and one for the mass transport of the dissolved constituents (radionuclides). In using these equations, the movement of the water in the region under consideration must be known before the transport equation can be solved.

- (a) **Unsaturated flow.** The most significant nongaseous contaminant movement in soils is a function of liquid movement. Vapor phase movement can be significant for certain volatile contaminants (e.g., tritium and carbon-14). Soluble solid radionuclides dissolved in rainwater, surface run-off onto the site, or water applied through human activity will percolate into the soil. After rainwater infiltrates the surface of the ground, it generally travels vertically downward through the unsaturated zone (vadose zone) under the influence of gravity and capillary forces until it reaches the water table.

The movement of water through partially saturated soil is described by Richards equation, which can be written for an incompressible soil medium as

$$\frac{\partial \theta}{\partial t} = \nabla \cdot (\bar{K} k_r(\theta)) \underline{\nabla} h + \underline{\nabla} z \quad (\text{B-10})$$

where

$\theta$	=	volumetric water content
$h$	=	pressure head (length)
$z$	=	elevation above datum (length)
$\bar{K}$	=	saturated hydraulic conductivity tensor (length/time)
$k_r$	=	relative permeability
$t$	=	time (time)
$\nabla$	=	divergence operator.

Solving Equation B-10 to predict rates of water flow and changes in water content in a soil, is best accomplished by using a numerical computer model. A variety of such models exist for simulating one, two, and three dimensional unsaturated flow problems.

While computer modeling is often an integral part of exposure assessment analysis, utilization of complex computer models can require a very skilled and experienced modeler. Another consideration is that the prediction accuracy of models is often compromised since key parameters (e.g., soil hydraulic characteristics, heterogeneity), are imperfectly known, and values may have to be estimated from literature references in the absence of actual site-specific

measurements.

For these reasons, reliance on relatively simple approaches for determining travel times through the unsaturated (vadose) zone may be justified. The interstitial pore water velocity for transport through the unsaturated zone can be calculated from the average percolation or recharge rate as follows (ENF82):

$$V_{pw} = \frac{I}{\theta} \quad (\text{B-11})$$

where

- $V_{pw}$  = interstitial ground-water (pore water) velocity (length per unit time)
- $I$  = average infiltration or recharge rate which is the volumetric flow rate per unit area per unit time
- $\theta$  = average volumetric water content of the unsaturated zone (decimal fraction, representing volume of water per volume of soil).

In general, the flow rate  $q$  varies with time, for instance, in response to atmospheric conditions (rainfall) or man-induced hydraulic loadings. The soil water content  $\theta$  will vary with time and also with depth. However, for the purposes of estimating travel times, the use of time-averaged flow rates and water contents may be justified. Under steady-state flow conditions, the volumetric water content,  $\theta$ , of the soil will approach a constant and spatially uniform value, that the soil can support the imposed flow rate,  $I$ ; i.e., the hydraulic conductivity of the soil under the unsaturated conditions will be equal to the flow rate,  $I$ :

$$I = K_s k_r \quad (\text{B-12})$$

where

- $K_s$  = vertical hydraulic conductivity of soil under saturated conductivity (length/time)

The relative hydraulic conductivity,  $k_r$ , is generally obtained from an equation that describes the dependence of hydraulic conductivity or soil water content. One commonly used expression is the Brooks-Corey relation:

$$k_r = \left( \frac{\theta}{\theta_s} \right)^{2b+3} \quad (\text{B-13})$$

where

$$\begin{aligned}\theta_s &= \text{volumetric water content of soil under saturated conditions} \\ &\quad \text{(porosity) (volume/volume)} \\ b &= \text{pore size index (dimensionless)}\end{aligned}$$

Equations B-12 and B-13 can be combined to yield the following equation for the average soil water content (CLA78):

$$\theta = \theta_s \frac{I}{K_s}^{1/(2b+3)} \quad (\text{B-14})$$

Representative values of  $\theta$ ,  $b$ , and the term  $1/(2b+3)$  are listed in Tables C-1 - C-4 (Appendix C).

The saturated volumetric water content,  $\theta_s$ , saturated hydraulic conductivity,  $K_s$ , and the exponential coefficient,  $b$ , are all related to soil properties and are usually different in different soil types. The most reliable values for these parameters are empirical values (if available) measured at the site. Where empirical values are unavailable, the values in Tables C-1 and C-2 provide guides for the rough estimation of  $\theta_s$  and the term  $1/(2b+3)$ . Representative values of  $K_s$  from two different sources are presented in Tables C-3 and C-4. These tables demonstrate the variability in estimates for these values.

Theoretically, the value of  $\theta$  cannot exceed  $\theta_s$ , which is the saturated soil moisture content. Note also that the percolation rate,  $I$ , cannot exceed the saturated hydraulic conductivity,  $K_s$ , for the site soil. Whenever  $I \geq K_s$  (and therefore  $\theta$  as calculated by Equation B-14  $\geq \theta_s$ ) for the duration of the study period, it must be assumed that saturated conditions exist and that saturated flow prevails.

Equations B-17 and B-18 in the next subsection provide a means of estimating saturated flow velocities. Records of estimated percolation rates,  $I$ , for the site locality during the time period in question (or annual average recharge rate estimates) are often available from local hydrology, climate, or soil authorities, including regional U.S. Geological Survey (USGS) and U.S. Soil Conservation Service offices. The following equation can be used to estimate the term  $I$  (ENF82):

$$I = HL + P_r - ET - Q_r \quad (\text{B-15})$$

where

$I$	=	average infiltration or recharge rate
$HL$	=	hydraulic loading from manmade sources (length per unit time), which is the flow rate divided by the contaminant source area.
$P_r$	=	precipitation (length per unit time)
$ET$	=	evapotranspiration (length per unit time)
$Q_r$	=	runoff (length per unit time).

This estimation procedure can be used to evaluate infiltration rates,  $I$ , at sites where the information sources listed above cannot provide them directly. This estimation procedure requires data for precipitation, evapotranspiration, and runoff rates. In addition to the above sources, the National Weather Service, Forest Service offices, National Oceanic and Atmospheric Administration (NOAA) gauging stations, or other first order weather stations (e.g., at local airports) are possible sources for these three types of data. The average precipitation rate per unit time,  $P_r$ , for the study period can be obtained from various local weather authorities such as those listed.

A value of  $ET$  for substitution into Equation B-15 can be estimated by using measured Class A pan evaporation rates (a measure of local evaporation rates under standardized conditions, available from the nearest NOAA gauging station) in the equation:

$$ET = EVAP \times C_{et} \times C_{veg} \quad (B-16)$$

where:

$EVAP$	=	region-specific or site-specific measured evaporation rates (length per unit time)
$C_{et}$	=	correction factor for converting measured pan evaporation rates to evapotranspiration rates from turf grass (unitless)
$C_{veg}$	=	correction factor for converting evapotranspiration from turf grass to evapotranspiration from other vegetative cover types (unitless).

Values for  $C_{et}$  are taken from Table C-7, which requires climatological and pan descriptive information.

The term  $C_{veg}$  is used mainly for agricultural crops (Table C-8) and varies with the thickness, depth, and characteristics of vegetative cover. Typical values are 0.87 for shorter broadleaf plants (alfalfa) to 0.6 for taller broadleaf plants (potatoes, sugar beets) and 0.6 for taller grains and grasses. Where crop-specific data are unavailable, a conservative default value for this term is the smallest reasonable value, or 0.6.  $ET$  rates can vary significantly, of course, if vegetative cover varies.

A value of  $Q_r$ , or the average runoff over the study period, for input into Equation B-15, however, can generally be obtained from local USGS gauging stations. For relatively level sites, a reasonable conservative default value is  $Q_r = 0$ , where site-specific data are unavailable or cannot be estimated.

The above method for predicting the average velocity of water migrating through the unsaturated zone will in many cases yield reasonable approximations; however, heterogeneities, such as root holes and macropores, can result in faster velocities than predicted. The analyst is not expected to correct for this, yet it is important to be aware of the limitations of the method.

- (b) **Saturated flow.** Darcy's law may be used to describe the volumetric flow of water through a porous medium under saturated conditions. The volumetric flow (or discharge) is proportional to the product of the driving force, the soil's ability to transmit water, and the cross-sectional area perpendicular to the flow direction. The driving force is the difference in the energy (hydraulic head) between two points in the aquifer divided by the distance between the two points. This driving force is called the hydraulic gradient. The ability of soil or rock to transmit water is represented by an empirically determined coefficient of hydraulic conductivity. The hydraulic conductivity is determined by the properties of the liquid (water or contaminant) and the permeability of the porous medium. Typical examples of hydraulic conductivity for different porous materials are presented in Table C-6. The soil has an intrinsic permeability, which is determined by the size, orientation, and connectedness of the pore spaces.

Estimating radionuclide transport velocity is based on estimating the velocity of water. For those contaminants that flow with the water, contaminant velocity equals water velocity (vertical and/or horizontal). For those that flow at rates that differ from water, the estimated water velocity must be multiplied by a factor to



approximate the contaminant velocity.

Ground-water flux per unit cross-sectional area in the saturated zone is calculated using Darcy's law, which is as follows (BOU78):

$$V = K_s i \quad (\text{B-17})$$

where

$$\begin{aligned} V &= \text{Darcy flux of water, also termed the specific discharge} \\ &\quad \text{(length/time)} \\ K_s &= \text{hydraulic conductivity of soil or aquifer material} \\ &\quad \text{(length/time)} \\ i &= \text{hydraulic gradient (length/length)}. \end{aligned}$$

Although  $V$  has the units of velocity (length per time), it is a specific discharge rate or flux (volume of water flowing per unit cross-sectional area of geologic material per unit time). However,  $V$ , is the Darcy flux, rather than the macroscopic velocity of the water. The actual ground-water velocity is calculated from the Darcy flux, by dividing it by soil porosity, or, for precise modeling, by effective porosity. (This approach takes into account the fact that the entire cross-section of the pore is not flowing because of boundary layer effects, dead end pores, and unconnected pores.) For clay soils, the effective porosity also corrects for the effect of electro-osmotic counterflow and the development of electrokinetic streaming potentials (BOU78). The equation for calculating ground-water velocity from Darcy velocity using effective porosity is as follows (BOU78):

$$V_{pw} = V/n_e \quad (\text{B-18})$$

where

$$\begin{aligned} V_{pw} &= \text{ground-water (pore water) velocity (length/time)} \\ V &= \text{Darcy velocity (superficial velocity, specific discharge} \\ &\quad \text{(length/time)} \\ n_e &= \text{effective porosity (dimensionless fraction)}. \end{aligned}$$

The above terms should be determined for the site being studied. If this is not possible for all parameters, then literature values can be used when site-specific data are not available (Tables C-9 and C-10).

The hydraulic gradient (the change in the hydraulic head or elevation of the water

table over a measured distance) should also be taken from field data obtained during the site investigation. Water levels in existing nearby wells screened at appropriate intervals can indicate hydraulic gradient.

Effective porosity,  $n_e$ , can be approximated by the difference between the moisture content at saturation and the "wilting point" (-15 bar)<sup>3</sup>. The equation is as follows (RAW86):

$$n_e = n_{sat} - n_{(-15)} \quad (B-19)$$

where

$n_e$	=	effective porosity (fraction, dimensionless)
$n_{sat}$	=	water content when the pores are fully saturated (fraction, dimensionless)
$n_{(-15)}$	=	wilting point moisture content (fraction, dimensionless).

This estimation procedure addresses the fraction of the pore spaces that contributes to flow, but does not address the effect of electro-osmotic counterflow and the development of electrokinetic streaming potentials. For clays, this can be a significant difference. Literature values listed in Table C-10 should be used for clay solids (these values incorporate the effects of the clay's ionic double layer (RAW82); either technique Equation B-19 or the tables, can be used for sand or loam soil.

The above method for predicting the average velocity of groundwater is the most widely accepted approximation; however, it is only an approximation, and further refinement can be made to this approach to improve its accuracy. Corrections for the path length difference between the straight line distance versus the tortuous path that groundwater flows through can improve the precision (FRE79). However, this correction factor is difficult to estimate.

**Example B.1.** For saturated ground-water flow, calculate the pore or seepage velocity in an "average" sandstone under a gradient of 0.01 cm/cm. Use arithmetic mean values in tables (Appendix C).

Equation B-18 applies. The arithmetic mean hydraulic conductivity,  $K$ , is  $3.31 \times 10^{-4}$  cm/s from

---

<sup>3</sup> The wilting point is determined by drawing a suction of -15 bar to draw water out of the soil in a manner similar to the section of a plant root; the bar is a measure of pressure (dynes/cm<sup>2</sup>).

Table C-6. The arithmetic mean effective porosity,  $n_e$ , is 0.21 from Table C-10. Therefore,

$$\begin{aligned} V_{pw} &= V/n_e = -Ki/n_e = 3.31 \times 10^{-4} \text{ cm/s} \times 0.01/0.21 \\ &= 1.58 \times 10^{-5} \text{ cm/s.} \end{aligned}$$

[End of Example B.1]

- (c) **Mass transport.** Cationic radionuclides that are migrating as a dilute solute may be subject to retardation effects. Concentrated plumes are not as susceptible to this phenomenon. Algorithms describing retardation are based on the assumption that adsorption of radionuclides is primary due to sorption on mineral surfaces. The mass transport equation uses the retardation coefficient to estimate the rate of movement of the radionuclide. The most general form of the mass transport equation is for transport in saturated-unsaturated media. If local equilibrium of mass transfer and first-order chemical reactions are assumed, sorption can be represented as a linear relationship, and the general mass transport equation can be written as:

$$R_F \theta \frac{\partial c}{\partial t} - \nabla \cdot (\theta \bar{D} \cdot \nabla c) + \nabla \cdot (\bar{V}c) + \left[ \frac{\partial c}{\partial t} (\theta R_F) + \lambda \theta_e R_F \right] c = 0, \quad (\text{B-20})$$

where

$$\begin{aligned} c &= \text{the concentration of dissolved constituent (Ci/M}^3\text{)} \\ \bar{D} &= \text{the dispersion tensor (M}^2\text{/day)} \\ \bar{V} &= \text{the flux (M/day)} \\ \lambda &= \text{the radioactive decay constant equal to } \ln 2/\text{half-life of the} \\ &\quad \text{isotope (1/day).} \end{aligned}$$

The term  $R_F$  is the retardation factor, which for saturated flow (i.e.,  $\theta = \eta$ ) becomes:

$$R_F = \frac{n}{n_e} + \frac{\rho_b}{n_e} K_d, \quad (\text{B-21})$$

where

$$n = \text{the total porosity,}$$

$n_e$  = the effective porosity,  
 $\rho_b$  = the bulk density (g/cm<sup>3</sup>),  
 $K_d$  = the distribution coefficient (mL/g).

By assuming  $n = n_e$ ,  $R_F$  can be more conservatively estimated as

$$R_F = 1 + \frac{\rho_b}{n_e} K_d \quad (\text{B-22})$$

An equivalent retardation factor may be defined for fracture flow where the exposed area of the fracture is used rather than the porosity (FRE79).

**Example B.2.** Calculate the retardation factor,  $R_F$ , for strontium in an "average" fine sandstone with a bulk density,  $\rho_b$ , of 2.8 g/cm<sup>3</sup> and a distribution coefficient of 20 mL/g.

The arithmetic mean values of  $n$ ,  $n_e$  are found from Tables C-11 and C-12 to be 0.34 and 0.21, respectively. The retardation coefficient,  $R_d$ , calculated from Equation B-21 is therefore

$$R_F = \frac{0.34}{0.21} + \frac{2.8}{0.21} \times 20 = 268.3.$$

Equation B-22 gives

$$R_F = 1 + \frac{2.8}{0.21} \times 20 = 267.7.$$

[End of Example B.2]

The approximate rate of movement of the radionuclide is  $V_{pw}/R_F$  ( $V_{pw}$  is equal to the pore velocity which is defined in Equation B-18), which may be used to estimate travel time.

- (2) Chain decay of radionuclides. Radionuclides decay to stable products or to other radioactive species called daughters. In some species, several daughter products may be produced before the parent species decays to a stable element. For some radionuclides, the daughter(s) may present a potentially greater adverse health risk than the parent.

Accounting for the chain-decay process is particularly important for predicting potential impacts of actinide and transuranic migration. In considering this process over the transport path of radionuclides, one transport equation must be written for each original species and each daughter product to yield the concentration of each radionuclide (original species and daughter products) at points of interest along the flow path in order to estimate total radiological exposures. In a constant one-dimensional velocity field, the general equations can be written as (BUR80):

$$\begin{aligned}
 R_{F1} \frac{\partial c_1}{\partial t} + V_{pw} \frac{\partial c_1}{\partial x} &= D_x \frac{\partial^2 c_1}{\partial x^2} - R_{F1} \lambda_1 c_1, \\
 R_{F2} \frac{\partial c_2}{\partial t} + V_{pw} \frac{\partial c_2}{\partial x} &= D_x \frac{\partial^2 c_2}{\partial x^2} - R_{F2} \lambda_2 c_2 + R_{F1} \lambda_1 c_1, \\
 R_{Fi} \frac{\partial c_i}{\partial t} + V_{pw} \frac{\partial c_i}{\partial x} &= D_x \frac{\partial^2 c_i}{\partial x^2} - R_{Fi} \lambda_i c_i + R_{F,i-1} \lambda_{i-1} c_{i-1},
 \end{aligned} \tag{B-23}$$

where

$$\begin{aligned}
 R_{Fi} &= \text{the retardation factor for species } i \\
 V_{pw} &= \text{the pore velocity} = V/n_e \\
 C_i &= \text{the concentration of species } i \\
 D_x &= \text{the dispersion coefficient} \\
 \lambda_i &= \text{the decay coefficient for species } i.
 \end{aligned}$$

Equation B-23 describes the material balances of the *i*th member of a decay chain and all preceding chain members.

- (3) Net Dilution. Dilution (mixing) processes in ground water are generally less significant than dilution processes in air and in surface water. In both air and surface water, dispersive dilution is often a major phenomenon because the flow can be turbulent. Turbulent flow means that all the flow paths are not essentially parallel to the gross direction of motion. Flow components that are perpendicular to the bulk fluid motion cause the plume to spread laterally not longitudinally, thus reducing the concentration in the plume, while the volume of contaminated air or surface water increases.

However, in ground water, the magnitude of dilution is usually much smaller, partly because turbulent flow rarely exists. The slow speed of ground water, coupled with the

effects of small channels in the intergranular pore space, tends to keep the flow smooth and laminar. In an idealized conceptual model, the interconnecting pore spaces can be thought of as forming flow channels or tubes; any tendency for the flow to eddy is resisted by the sides of the flow channel. However, since the interconnecting pore spaces do not make a continuous flow channel, in real soil there is some lateral mixing due to branching of flow channels and spatial variation in flow velocity. Dispersion (neglecting molecular diffusion) is not significantly affected by laminar eddy currents. If molecular diffusion is momentarily disregarded, dispersion in porous or fractured media is caused by six principal phenomena: (1) varying permeability, (2) varying pore sizes, (3) varying path length, (4) variation in the velocity gradient across pore space, (5) anisotropic permeability and (6) flow splitting around soil particles with mixing within the pore space. These six phenomena contribute to longitudinal dispersion; the first and last two phenomena can cause lateral dispersion. In nearly all ground-water systems, longitudinal dispersion effects are much larger than lateral dispersion effects. Researchers have reported longitudinal dispersivity values ranging from about 1 to 25 times higher than transverse dispersivity values (GEL85).

Molecular diffusion is a relatively slow process but also contributes to the overall dispersion process in two ways: micro-scale mixing within an individual pore or fracture channels that lead to large-scale bulk dilution and spreading in a slow-moving ground-water system. For short-term releases (i.e., spills), longitudinal mixing and resulting dilution of plume concentrations can be significant. In this case, the plume can effectively mix with the uncontaminated water in front of and behind the slug of contamination, whereas continuous-release sources can result in plumes of sufficient length that the middle section cannot effectively mix with clean water in front or behind it.

A very simplistic approximation of the net dilution may be made by using a form of Darcy's law in conjunction with Equation B-9. The results of Equation B-9 were used in Section B.3 to estimate the concentration of a radionuclide reaching a receptor if radioactive decay were the only means by which the concentration was diminished. That is, there were no dilution effects along the radionuclides' travel path to the receptor. In an actual system, leachate concentrations would be diluted by mixing with the ambient water along the travel path. As a first approximation, the degree of mixing may be estimated by the following:

$$Vol = KiT_e W\theta_T \quad (B-24)$$

where

$Vol$	=	aquifer volumetric flow rate (m <sup>3</sup> /y)
$K$	=	hydraulic conductivity of the aquifer (m/y)
$i$	=	hydraulic gradient (m/m)
$W$	=	width of the Source Area (m)
$T_e$	=	effective mixing thickness (m)
$\theta_T$	=	total porosity of aquifer (dimensionless)

The effective mixing thickness ( $T_e$ ) of the aquifer may be estimated from the following formula:

$$T_e = \left( \frac{I}{V} \right) \ell \quad (B-25)$$

where

$I$	=	infiltration rate (m/y)
$V$	=	specific aquifer (m/y) discharge (B-17)
$\ell$	=	distance from the contaminant source to the receptor.

Equation B-25 represents the vertical distance traveled by the contaminant over length  $\ell$ , assuming the vertical velocity is  $I$ , and the horizontal velocity is the aquifer flow rate.

The maximum value for the effective mixing thickness would be the thickness of the aquifer. The concentration of a radionuclide in a downgradient receptor may subsequently be adjusted for dilution using the  $C_{well}$  concentration obtained from formula B-10, in conjunction with Equation B-26.

$$M_{well} = C_{wat} \cdot e^{\frac{\lambda}{v_c}} \cdot I \cdot A \quad (B-26)$$

where

$C_{wat}$	=	leachate concentration (Ci/m <sup>3</sup> )
$I$	=	infiltration rate (m/yr)
$A$	=	source area

$$D_{well} = \frac{M_{well}}{Vol}$$

where

$D_{well}$  = concentration of radionuclide in downgradient well corrected for dilution

(Ci/m<sup>3</sup>)

$M_{well}$  = Mass of radionuclide corrected only for radioactive decay (Ci)

#### B.4 Analytical Methods for Aquifer Flow and Transport

An excellent discussion of simple mathematical methods to compute radionuclide travel times and dilution rates is included as Chapter 4 in NUREG/CR-3332 (COD83). The relevant portions of that discussion, as well as the example problems, figures, and tables, have been excerpted to form the basis of Sections B.4 and B.5.

Analytical ground-water transport models can be used for certain types of analyses where available data do not warrant a more complicated numerical analysis. Such models are useful for scoping the transport problem and may frequently be adequate for regulatory needs if model and corresponding input data are chosen conservatively.

In this section and Section B.5, a series of simple analytical models used at the U.S. Nuclear Regulatory Commission (NRC) is presented. Many of these models have been computerized and are available from the NRC (COD82). In their simplest forms, however, most can be used with the aid of only a calculator.

The models are developed for the limiting case of unidirectional saturated advective transport of a single dissolved substance with three-dimensional dispersion in an isotropic homogeneous aquifer as discussed in Section B.2.1. Equation B-27 is the governing differential equation of solute transport for that set of conditions.

$$\frac{\partial c}{\partial t} + \frac{V_{pw}}{R_d} \frac{\partial c}{\partial x} = \frac{D_x}{R_d} \frac{\partial^2 c}{\partial x^2} + \frac{D_y}{R_d} \frac{\partial^2 c}{\partial y^2} + \frac{D_z}{R_d} \frac{\partial^2 c}{\partial z^2} - \lambda c, \quad (\text{B-27})$$

where

$c$  = the concentration in the liquid phase (Ci/cm<sup>3</sup>)  
 $D_x, D_y, D_z$  = the dispersion coefficients in the x, y, and z directions respectively (cm<sup>2</sup>/s)  
 $\lambda$  = the decay coefficient, (1/s)  
 $V_{pw}$  = the x component ground-water pore velocity (cm/s)  
 $R_F$  = the retardation factor (dimensionless).

The dispersion coefficient can be approximated from Equation B-28. For unidirectional



flow,  $V_2 = V_3 = 0$ ,  $V_1 = V$ , and  $\theta$  can be approximated for saturated flow by the effective porosity,  $n_e$ . Also, since  $V_{pw} = V/n_e$ ,

$$D_x = \alpha_L V_{pw} \quad (\text{B-27a})$$

$$D_y = \alpha_T V_{pw} \quad (\text{B-27b})$$

$$D_z = \alpha_T V_{pw} \quad (\text{B-27c})$$

where  $\alpha_L$  and  $\alpha_T$  are the longitudinal and transverse dispersivities respectively.

$$\theta D_{ij} = \alpha_T V \delta_{ij} + (\alpha_L - \alpha_T) V_i V_j / V \quad (\text{B-28})$$

where

$\delta_{ij}$	=	1 for $i=j$ , $\delta_{ij} = 0$ for $i \neq j$ (Kronecker delta function)
$\theta$	=	the volumetric water content
$\alpha_T$	=	the transverse dispersivity (cm)
$\alpha_L$	=	the longitudinal dispersivity (cm)
$V$	=	the magnitude of the flux (cm/s)
$V_i V_j$	=	the components of the flux (cm/s).

#### B.4.1 Point Concentration Model

The first model presented can be used for calculating the concentration in the aquifer at some point downgradient of a release (e.g., water supply well).

Equation B-27 is solved in terms of Green's functions:

$$C_i = \frac{1}{n_e R_F} X(x, t) Y(y, t) Z(z, t) \quad (\text{B-29})$$

where  $C_i$  is the concentration at any point in space for an instantaneous one-curie release,  $n_e$  is the effective porosity of the medium, and  $X, Y, Z$  are the Green's functions in the  $x, y, z$  coordinate directions, respectively. Equation B-29 has been developed for a variety of boundary and source configurations:

- (1) For the case of a point source at  $(0, 0, z_s)$  in an aquifer of infinite lateral  $(x, y)$  extent and depth  $b$ , as illustrated in Figure B.1,

$$e c_i = \frac{1}{n_e R_F} X_1 Y_1 Z_1, \quad (\text{B-30})$$

where

$$X_1 = \frac{1}{\sqrt{4\pi D_x t/R_F}} \exp\left[-\frac{(x - V_{pw} t/R_F)^2}{4 D_x t/R_F} - \lambda t\right] \quad (\text{B-31})$$

$$Y_1 = \frac{1}{\sqrt{4\pi D_y t/R_F}} \exp\left(-\frac{y^2}{4 D_y t/R_F}\right) \quad (\text{B-32})$$

$$Z_1 = \frac{1}{b} \left\{ 1 + 2 \sum_{m=1}^{\infty} \exp\left(-\frac{m^2 \pi^2 D_z t}{b^2 R_d}\right) \cos m \pi \frac{z_s}{b} \cos m \pi \frac{z}{b} \right\}. \quad (\text{B-33})$$

- (2) For the vertically averaged concentration in case 1 above (equivalent to a vertical line source of length  $b$ ),

$$c_i = \frac{1}{n_e R_F} X_1 Y_1 Z_2, \quad (\text{B-34})$$

where

$$Z_2 = \frac{1}{b}. \quad (\text{B-35})$$

- (3) For a horizontal line source of length  $w$  centered at  $(0, 0, z_s)$ , as illustrated in Figure B.2,

$$c_i = \frac{1}{n_e R_F} X_1 Y_2 Z_1, \quad (\text{B-36})$$

where

$$Y_2 = \frac{1}{2w} \left\{ \operatorname{erf} \frac{(w/2 + y)}{\sqrt{4D_y t/R_F}} + \operatorname{erf} \frac{(w/2 - y)}{\sqrt{4D_y t/R_F}} \right\} \quad (\text{B-37})$$

and erf is the error function. Tables of the error function are available in standard mathematical texts (ABR70).

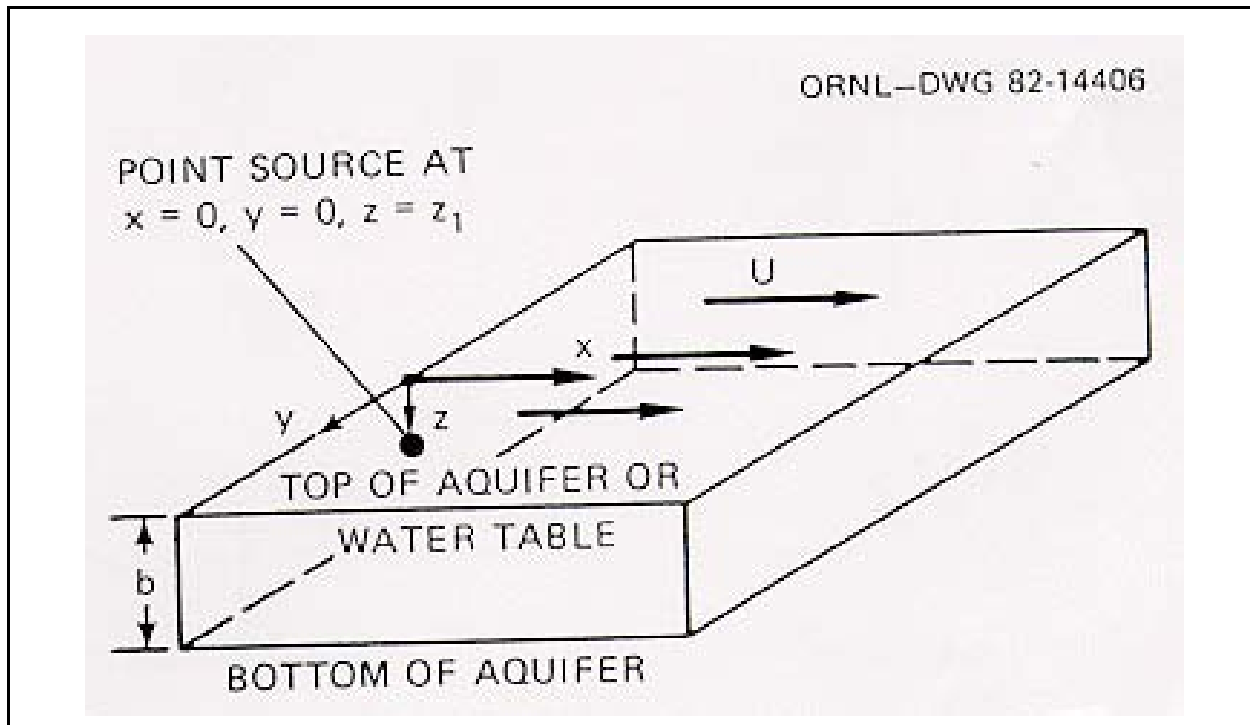


Figure B.1. Idealized ground-water system for point concentration model, point source (Codell and Duguid, 1983).

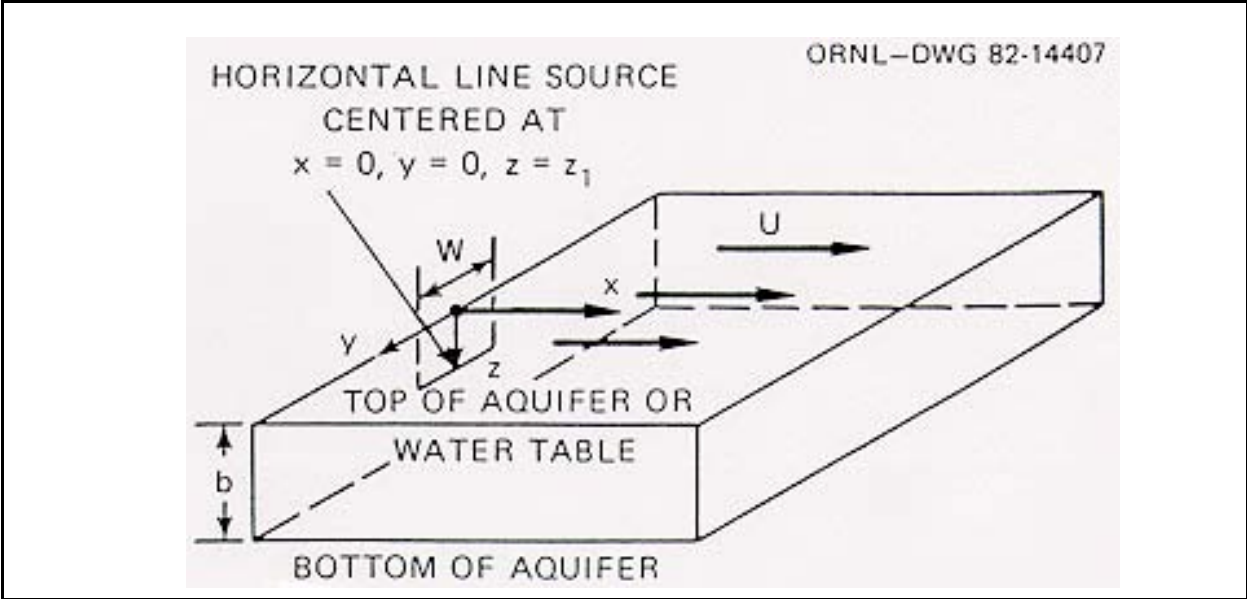


Figure B.2. Idealized ground-water system for point concentration model, horizontal line source (Codell and Duguid, 1983).

- (4) For the vertically averaged concentration in case 3 above (equivalent to an area source of width  $w$  and depth  $b$ ),

$$C_i = \frac{1}{n_e R_F} X_1 Y_2 Z_2 ; \quad (\text{B-38})$$

- (5) For a point source at  $(0, 0, z_s)$  in an aquifer of infinite lateral extent and depth,

$$C_i = \frac{1}{n_e R_F} X_1 Y_1 Z_3 \quad (\text{B-39})$$

$$Z_3 = \frac{1}{\sqrt{4\pi D_z t/R_F}} \left\{ \exp\left(\frac{-(z - z_s)^2}{4 D_z t/R_F}\right) + \exp\left(\frac{-(z + z_s)^2}{4 D_z t/R_F}\right) \right\}. \quad (\text{B-40})$$

where

- (6) For a horizontal line source of width  $w$  centered at  $(0, 0, z_s)$  in an aquifer of infinite lateral extent and depth,

$$C_i = \frac{1}{n_e R_F} X_1 Y_2 Z_3 . \quad (\text{B-41})$$

- (7) For a horizontal area source of length  $l$  and width  $w$  centered at  $(0, 0, 0)$  in an aquifer of constant depth  $b$ , as illustrated in Figure B.3, the solution to Equation B-29 becomes:

$$C_i = \frac{1}{n_e R_F} X_2 Y_2 Z_2 , \quad (\text{B-42})$$

where

$$X_2 = \frac{1}{2l} \left\{ \operatorname{erf} \frac{\left(x + \frac{l}{2}\right) - \frac{V_{pw} t}{R_F}}{\sqrt{4 D_x t/R_F}} - \operatorname{erf} \frac{\left(x - \frac{l}{2}\right) - \frac{V_{pw} t}{R_F}}{\sqrt{4 D_x t/R_F}} \right\} \exp(-\lambda t) . \quad (\text{B-43})$$

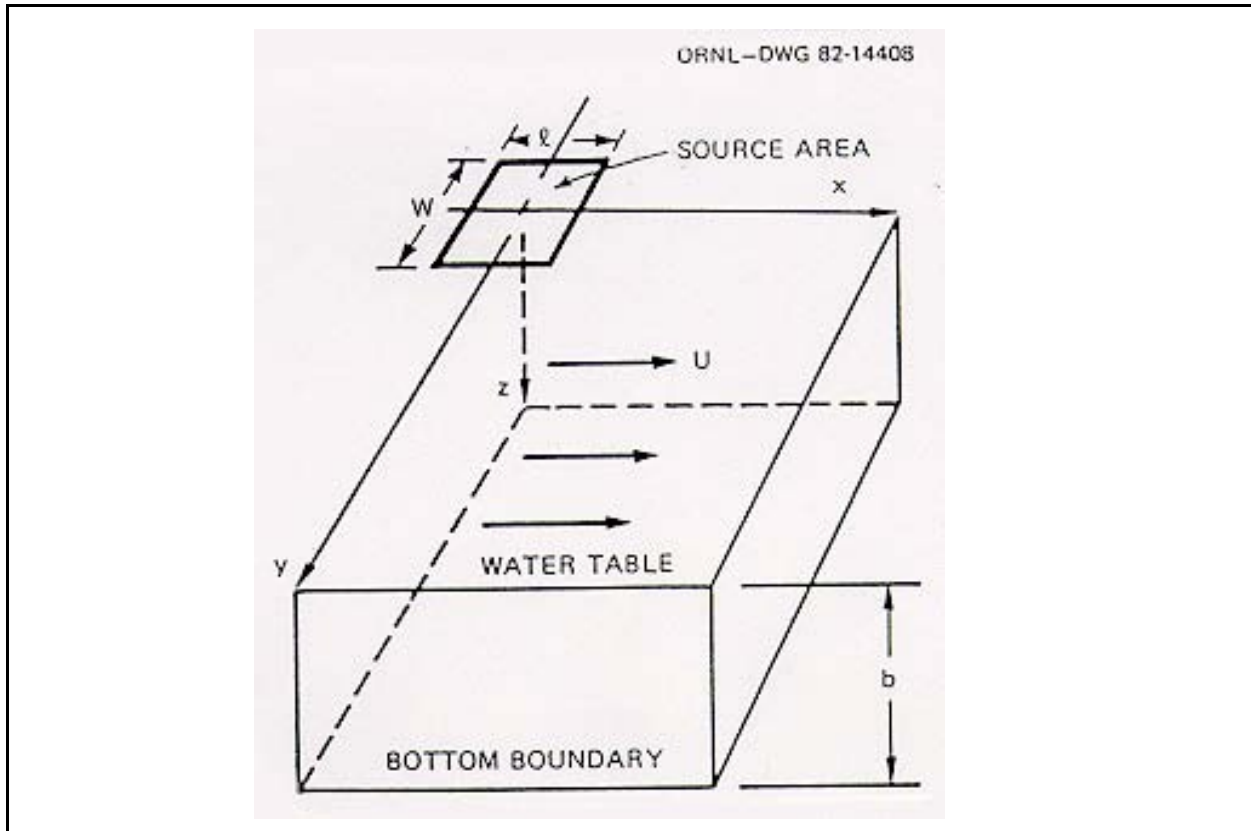


Figure B.3 Vertically averaged ground-water dispersion model (Codell and Duguid, 1983).

**Example B.3.** Concentration in an aquifer of limited thickness.

One curie of a radioactive pollutant leaks quickly into a water table aquifer through a highly permeable ground cover over a square surface area 50 m on each side. The pollutant has a half-life of 30 y. A well tracer test indicates that the ground water is moving in the direction of two wells at a speed,  $V_{pw}$ , of 1.5 m/d and that the longitudinal and transverse dispersivities,  $\alpha_L$  and  $\alpha_T$ , are 20 to 10 m, respectively.

The saturated thickness of the water table aquifer,  $b$ , is 50 m and has an effective porosity,  $n_e$ , of 0.2. The pollutant has been determined to have a retardation factor,  $R_F$ , of 20 in the aquifer.

Calculate the concentration of the pollutant in wells whose downgradient coordinates with respect to the center of the source area are

(a)  $x = 200 \text{ m}, y = 0 \text{ m}$

$$(b) \ x = 400 \text{ m}, y = 50 \text{ m}$$

The wells are open to the entire depth of the aquifer.

Case 7 in the preceding section applies to this example, since the source is a horizontal area type and the wells are screened over the total depth, which would vertically average the concentration (Figure B.4).

Equation B-42 is therefore evaluated with Green's function:

$$\begin{aligned} X_2 & \text{ determined by Eq. B-43,} \\ Y_2 & \text{ determined by Eq. B-37, and} \\ Z_2 & \text{ determined by Eq. B-35.} \end{aligned}$$

The dispersion coefficients are calculated by Equations B-27a and B-27b.

$$\begin{aligned} D_x & = \alpha_L V_{pw} = 20 \times 1.5 = 30 \text{ m}^2 \\ D_y & = \alpha_T V_{pw} = 10 \times 1.5 = 15 \text{ m}^2 \end{aligned}$$

Figure B.4 shows the concentration as a function of time calculated for the two wells.

[End of Example B.3]

#### B.4.2 Flux Models

The flux model is used to calculate the discharge rate of a radionuclide entering a surface water body that has intercepted the aquifer containing the transported material as depicted in Figure B.5. It is assumed that all material entering the aquifer eventually enters the surface water except for that which has been lost through radioactive decay. The assumptions that apply to the point concentration model also apply to this model. The model provides only the rate of input to the surface water at an average distance  $x$  downgradient from the surface. Actually, the contaminant would enter the surface water as a diffuse patch, but the model described here gives no information about the spatial distribution of this patch.

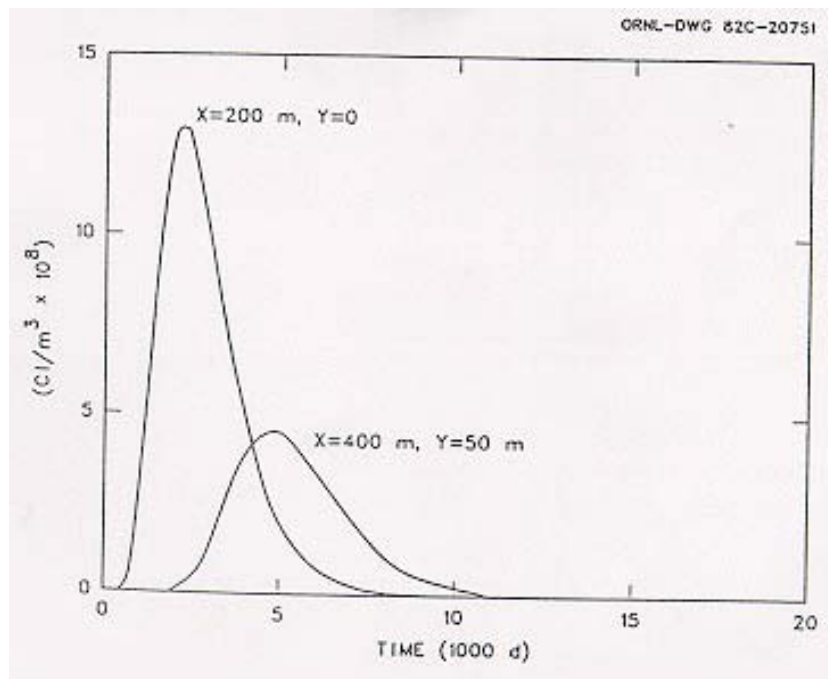


Figure B.4 Concentration in downgradient wells for Example B.3.

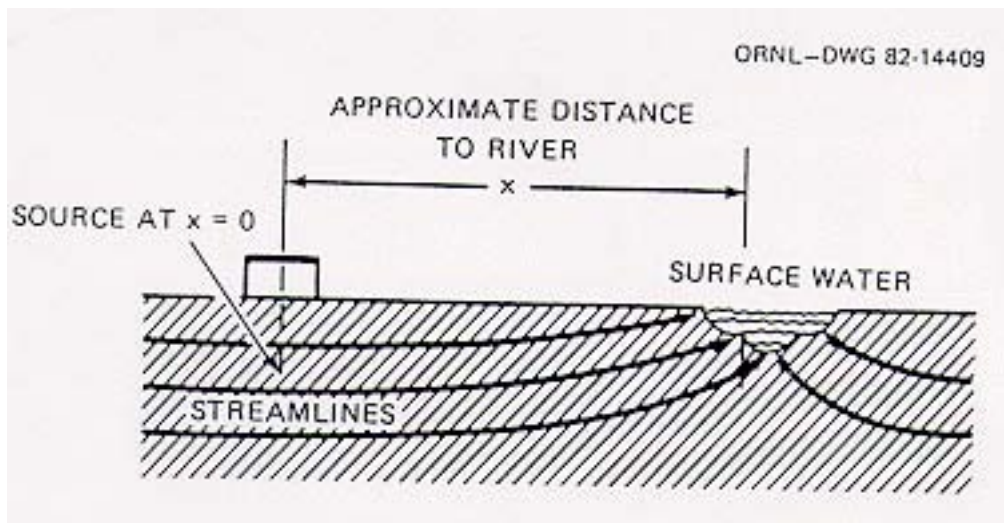


Figure B.5. Ground-water/surface-water interface, flux model.



In the unidirectional flow field assumed, the flux  $F$  (Ci/s) of material crossing an area  $dA = dy dz$  perpendicular to the  $x$  axis is described by the equation

$$\frac{dF}{dA} = \left( V_{pw} c - D_x \frac{\partial c}{\partial x} \right) n_e, \quad (\text{B-44})$$

where  $c$  is the concentration in the dissolved phase. The total flux across the plane would be

$$F = n_e \int_0^b \int_{-\infty}^{\infty} \left( V_{pw} c - D_x \frac{\partial c}{\partial x} \right) dy dz. \quad (\text{B-45})$$

#### B.4.3 Source Released from a Vertical Plane ( $x = 0$ )

If  $C_i$  is the concentration from an instantaneous release of 1 Ci at  $x = 0$  and time  $t = 0$ , as described by Equation B-29, then the resulting flux at distance  $x$  downgradient would be

$$F_i = \frac{\left( x + V_{pw} \frac{t}{R_F} \right)}{4 \sqrt{D_x \pi t^3 / R_F}} \exp \left[ - \frac{\left( x - V_{pw} \frac{t}{R_F} \right)^2}{4 D_x t / R_F} - \lambda t \right]. \quad (\text{B-46})$$

#### B.4.4 Horizontal Area Source

For conditions expressed by Equation B-43, the corresponding flux would be

$$F_i = \frac{1}{2\ell \sqrt{\pi D_x t / R_d}} \left[ \frac{V_{pw}}{R_d} \sqrt{\pi D_x t / R_F} [erf(z_1) - erf(z_2)] - \frac{D_x}{R_F} [\exp(-z_1^2) - \exp(-z_2^2)] \right] \cdot \exp(-\lambda t), \quad (\text{B-47})$$

where

$$z_1 = \frac{x - \frac{V_{pw}}{R_F} t + \frac{\ell}{2}}{\sqrt{4 D_x t / R_F}}, \quad \text{and} \quad z_2 = \frac{x - \frac{V_{pw}}{R_F} t - \frac{\ell}{2}}{\sqrt{4 D_x t / R_F}}.$$

**Example B.4.** For the same conditions in the previous example, calculate the flux of the pollutant into a river intercepting the ground-water flow, which is a distance  $x$  of 2000 m downgradient from the center of the source.

Equation B-47 applies in this case. Figure B.6 shows the flux into the river as a function of time.

[End of Example B.4]

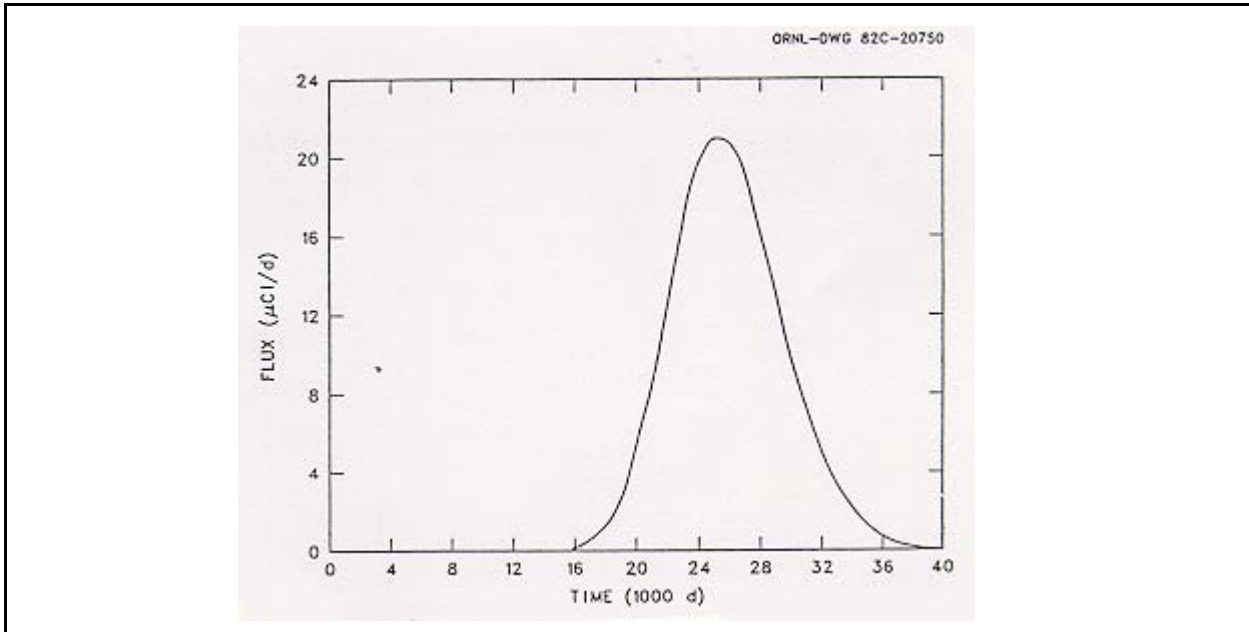


Figure B.6. Flux of pollutant into river for Example B.4.

#### B.4.5 Generalization of Instantaneous Models

Equations B-5 and B-27 are formulated only in terms of instantaneous releases. They can be generalized for arbitrary releases by use of the convolution integral:

$$\theta = \int_0^t f(\tau) \theta_i(t - \tau) d\tau, \quad (\text{B-48})$$

where  $\theta$  is the solution at time  $t$  for the arbitrary release,  $\theta_i(t - \tau)$  is the solution at time  $(t - \tau)$  for an instantaneous release at  $(t - \tau) = 0$ , and  $f(\tau)$  is the source release rate at  $\tau$  in curies/s.

Certain analytical solutions can be found to Equation B-48 for simple source release rate functions. For example, Wilson and Miller (WIL78) develop the solution to Equation B-48 for a continuous release in terms of the "well function." Most useful solutions to Equation B-48 use numerical integration, generally involving a digital computer.

Several special precautions must be taken, however, to preserve computational accuracy, because the terms within the integral of Equation B-48 can be very nearly zero over part of the integration range. Computer programs for solving the equations in this section are described by Codell *et al.* (COD82). Program listings in BASIC and FORTRAN are given in this reference. An alternative method for simulating a continuous source function is to present the continuous source as a series of instantaneous ones. The analytical solutions are then linearly summed. Complicated areal source terms can also be solved in an analogous fashion by representing the source area by a series of point sources and linearly summing the solutions.

## B.5 Simplified Analytical Methods for Minimum Dilutions

Simplified forms of the equations of Section B.4 have been developed for calculating the minimum dilutions (i.e., maximum concentration) of volume  $V_r$  of a substance instantaneously released from a point source into an aquifer.

### B.5.1 Dilution at Downgradient Wells in Confined Aquifers for an Instantaneous Point Source at the Surface

At some distance downgradient from a release at the surface of a confined aquifer, the concentration can be considered to be mixed in the vertical direction. Close to the point of release, or in an unconfined aquifer, the vertical dispersion will not be influenced by the vertical boundaries of the aquifer. Between these regions, there is a region where the concentration cannot be considered mixed, but the boundaries (top and bottom) affect the dispersion. The degree of vertical mixing can be characterized in a confined aquifer of constant thickness and uniform transport properties by the factor

$$\phi = \frac{b^2}{\alpha_T x} \quad , \quad (B-49)$$

where

$\alpha_T$  = the vertical (transverse) dispersivity (ft)  
 $b$  = the thickness of the aquifer (ft)

$x$  = the distance downgradient of the release (ft).

The factor  $\phi$  can be used to characterize the aquifer in three approximate regions:

- (a) If  $\phi < 3.3$ , the release may be considered to be within 10% of being vertically mixed in the aquifer;
- (b) If  $\phi > 12$ , the release may be considered to be within 10% of the aquifer;
- (c) If  $3.3 < \phi < 12$ , the release is neither completely mixed nor unaffected by the boundaries.

Different methods apply to each of the three regions.

**Vertically Mixed Region ( $\phi < 3.3$ ).** For an instantaneous release at  $x = 0$ , the minimum dilution corrected for decay directly downgradient of a source would be

$$D_L = R_F 4 \pi n_e x b \frac{\sqrt{\alpha_L \alpha_T}}{V_T} \exp(\lambda t) , \quad (\text{B-50})$$

where

$D_L$	=	minimum dilution = $c_0/c$
$R_f$	=	retardation factor
$n_e$	=	effective porosity
$V_T$	=	volume of liquid source term ( $\text{cm}^3$ )
$\alpha_L, \alpha_T$	=	dispersivities (cm) in the indicated direction
$x$	=	distance downgradient (cm)
$b$	=	aquifer thickness (cm)
$t$	=	travel time (y)
$\lambda$	=	decay constant = $\ln 2/t_{1/2}(1/y)$ .

The travel time,  $t$ , can be approximated as

$$t = \frac{x}{V_{pw}} R_F , \quad (\text{B-51})$$

where  $V_{pw}$  is the pore velocity defined by Equation B-18.

**Unmixed Region ( $\phi > 12$ ).** For an instantaneous release at  $x = 0$  on the surface of the aquifer, the minimum dilution of the surface of the aquifer directly downgradient from the source would be determined from Equation B-52,

$$D_L = \frac{n_e R_F (4\Pi x)^{3/2} \sqrt{\alpha_L \alpha_T^2}}{2V_T} \exp(\lambda t) , \quad (\text{B-52})$$

where  $\alpha_L, \alpha_T$  are dispersivities in the indicated direction and the other terms are as previously defined.

**Intermediate Region ( $3.3 < \phi < 12$ ).** For an instantaneous release at  $x = 0$  on the surface of an aquifer, the minimum dilution on the surface of the aquifer directly downgradient from the source would be

$$D_L = \frac{R_F 4\Pi n_e x b \sqrt{\alpha_L \alpha_T} \exp(\lambda t)}{V_T F(\phi)} \quad (\text{B-53})$$

where

$$F(\phi) = 1 + 2 \sum_{n=1}^{\infty} \exp\left(\frac{-n^2 \Pi^2}{\phi}\right) \quad (\text{B-54})$$

and the other terms are as previously defined.

The function  $F(\phi)$  is conveniently plotted in Figure B.7. It can be easily seen that for small values of  $\phi$ ,  $F$  approaches the value of 1.0, which yields the vertically mixed case. For large values of  $\phi$ , the slope of  $F$  is 1/2, and the unmixed case prevails. This method may be used for any value of  $\phi$  that can be read on Figure B.5.

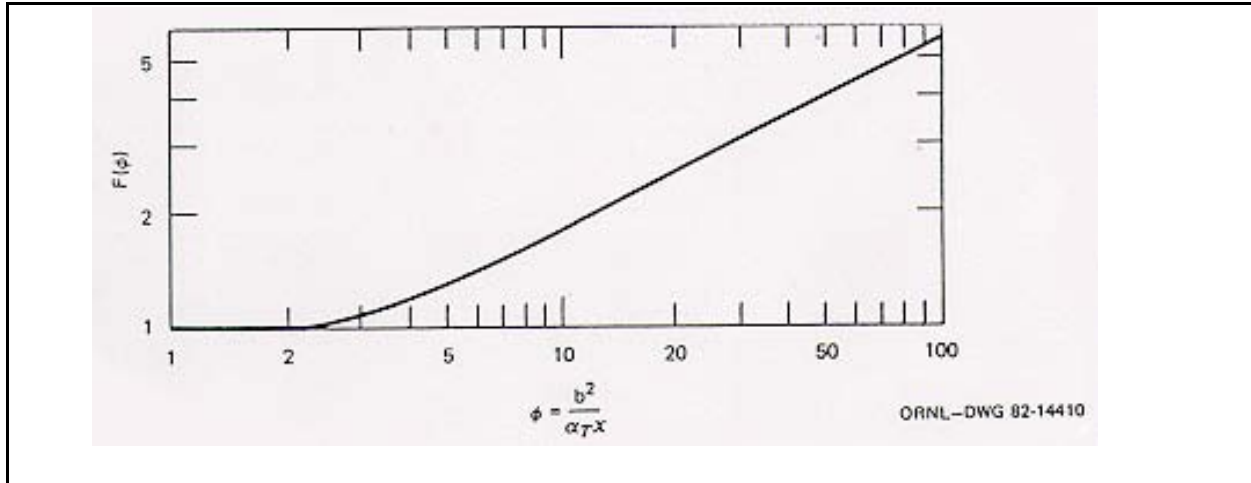


Figure B.7. Mixing factor for confined aquifers.

### B.5.2 Ground-Water/Surface Water Interface-Instantaneous Source

For an instantaneous release to the ground-water at  $x = 0$ , the minimum dilution in an intercepting river, corrected for decay, can be determined from:

$$D_L = \frac{2 R_F Q \sqrt{\pi \alpha_L x}}{V_{pw} V_T} \exp(\lambda t) , \quad (\text{B-55})$$

where

- $Q$  = flow rate of river ( $\text{cm}^3/\text{s}$ )
- $\alpha_L$  = the longitudinal dispersivity of the aquifer (cm)
- $V_T$  = the volume of release (e.g., tank volume) ( $\text{cm}^3$ )
- $V_{pw}$  = pore velocity of ground water (cm/s).

Relatively simple equations can be used for estimating average concentration in ground water or in surface water supplies contaminated by ground water (Equations B.56 and B.57).

### B.5.3 Quantity of Released Radioactivity Crossing a Vertical Plane

In the case of ground-water flow to an intercepting river, the total quantity  $M$  (curies) of the dissolved substance entering the river would be

$$M = \int_0^{\infty} F dt , \quad (\text{B-56})$$

where  $F$  is the flux defined for either an instantaneous point or vertical plane source by Equation B-45 or a horizontal area source by Equation B-47. Equation B-56 can be integrated graphically or numerically and in some cases may have an analytical solution.

If dispersion is relatively small (e.g.,  $\alpha_x \ll l$ ), the following approximation may be used:

$$M = M_0 e^{-\lambda t} \text{ curies} , \quad (\text{B-57})$$

where  $M_0$  is the quantity of radioactivity released instantaneously from the source (curies),  $t$  is the travel time (y), and  $\lambda$  is the decay coefficient (1/y).

If the substance is being released from the source at a rate proportional to the quantity remaining (e.g., an exponentially decaying source term),

$$M = M_0 \frac{\lambda'}{\lambda' + \lambda} e^{-\lambda t} , \quad (\text{B-58})$$

where  $\lambda'$  is the release rate from the source (1/y), and  $M_0$  is the initial quantity of material in the source term (curies).

#### B.5.4 Direct Ground-Water Usage

The U.S. Nuclear Regulatory Commission developed a model for calculating the quantity of a radionuclide ingested by a population using the contaminated ground water (NRC78). Ground-water usage was considered to be spatially continuous instead of being from discrete well points.

The total amount of the released radionuclide ingested by the population is

$$I = \int_0^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c Q_g dx dy dt ,$$

where

- $I$  = the ultimate number of curies ingested from the release  
 $c$  = the ground-water concentration (Ci/L)  
 $Q_g$  = the ground-water withdrawal rate for drinking water purposes (m<sup>3</sup>/d / m<sup>2</sup>).

If all usage is restricted to a downgradient distance  $\ell$  and beyond from the release point, Equation B-59 may be integrated in closed form to give

$$I = \frac{\frac{M_0 Q_g}{2n_e R_F b} \exp \left[ \frac{\ell V_{pw}}{2D_x} - \left( \frac{R_F \ell^2 (\lambda + \gamma)}{D_x} \right)^{1/2} \right]}{\sqrt{\lambda + \gamma} (\sqrt{\lambda + \gamma} - \sqrt{\gamma})} \quad , \quad (B-60)$$

where

$$\gamma = \frac{(V_{pw})^2}{4R_F D_x}$$

$M_0$  is the total quantity of the radionuclide discharged to the point source, and the other terms are as previously defined.

If usage of the ground water is restricted between two downgradient distances,  $\ell_1$  and  $\ell_2$ , the curies ingested would be defined as:

$$I = I(\ell_1) - I(\ell_2)$$

where  $I(\ell_1)$  and  $I(\ell_2)$  are evaluations of Equation B-60 for  $\ell_1$  and  $\ell_2$  respectively.

**Example B.5.** The use of several of the simpler analytical models in Section B.4 will be demonstrated by way of a hypothetical example:

Leakage into the ground water rapidly empties a 1000-ft<sup>3</sup> tank containing 4000  $\mu$ Ci/mL of <sup>3</sup>H, 2000  $\mu$ Ci/mL of <sup>90</sup>Sr, and 3000  $\mu$ Ci/mL of <sup>137</sup>Cs at a radioactive waste site. The site is 50 ft above the mean level and 3000 ft upgradient from a river that has representative low flow of 5000 ft<sup>3</sup>/s and is the sink for all surficial ground water in the area. Two shallow wells are located 400 and 2500 ft directly downgradient from the site of the spill. Ground water exists in a homogeneous alluvial sand layer 100 ft thick under water table



conditions. Dispersivities for the sand have been determined in the near field from single-well tracer tests to be 0.5 ft for  $\alpha_T$  and 1.0 ft for  $\alpha_L$ . The bulk density  $\rho_b$  of the sand is  $2.6 \text{ g/cm}^3$ . Its total porosity  $n$  and effective porosity  $n_e$  are 0.4 and 0.25, respectively. The permeability  $K$  is 0.02 cm/s. Distribution coefficients  $K_d$  for the sand have been determined to be 0, 2.0, and 20.0 mL/g for dilute solutions of  $^3\text{H}$ ,  $^{90}\text{Sr}$  and  $^{137}\text{Cs}$ , respectively. Using this information, calculate the following:

- the maximum concentrations of the radioactive components in the river,
- the maximum concentrations of the components in the near well,
- the maximum concentrations of the components in the far well, and
- the total quantity of each radionuclide escaping to the river.

**Solution**

- If it is assumed that the source is released over a short period, Equation B-55 for instantaneous releases may be used to calculate the maximum river concentrations of  $^3\text{H}$ ,  $^{90}\text{Sr}$ , and  $^{137}\text{Cs}$ . First determine the pore velocity  $V_{pw}$  from Equation B-18 and the effective porosity  $n_e$ :

$$V_{pw} = \frac{V}{n_e} = - \frac{K \frac{\Delta H}{\Delta x}}{n_e} .$$

The gradient

$$\frac{\Delta H}{\Delta x} = \frac{- 50 \text{ ft}}{3000 \text{ ft}} = - 0.0167 ;$$

therefore,

$$V_{pw} = \frac{- 2 \times 10^{-2} \text{ cm/s} \times - 0.0167}{0.25} \times \frac{86,000 \text{ s/d}}{30.48 \text{ cm/ft}} = 3.78 \text{ ft/d} .$$

The retardation factors for  $^3\text{H}$ ,  $^{90}\text{Sr}$  and  $^{137}\text{Cs}$  can be determined from Equation B-22:

$${}^3\text{H} \quad R_F = 1 + \frac{2.6}{0.4} \times 0.0 = 1 ,$$

$${}^{90}\text{Sr} \quad R_F = 1 + \frac{2.6}{0.4} \times 2.0 = 14 ,$$

$${}^{137}\text{Cs} \quad R_F = 1 + \frac{2.6}{0.4} \times 20 = 131 .$$

The travel times for the three components are calculated by Equation B-47:

$${}^3\text{H} \quad t = \frac{xR_F}{V_\rho} = \frac{3000 \text{ ft} \times 1}{3.78 \text{ ft/d}} \times \frac{y}{365 \text{ d}} = 2.17 \text{ y} ,$$

$${}^{90}\text{Sr} \quad t = \frac{3000 \text{ ft} \times 14}{3.78 \text{ ft/d}} \times \frac{y}{365 \text{ d}} = 30.4 \text{ y} ,$$

$${}^{137}\text{Cs} \quad t = \frac{3000 \text{ ft} \times 131}{3.78 \text{ ft/d}} \times \frac{y}{365 \text{ d}} = 284.8 \text{ y} .$$

The half-lives of  ${}^3\text{H}$ ,  ${}^{90}\text{Sr}$ , and  ${}^{137}\text{Cs}$  are 12.3 y, 29 y, and 30.1 y, respectively. The decay-corrected minimum dilutions in the river are found by applying Equation B-55:

$$\begin{aligned} {}^3\text{H} \quad D_L &= \frac{2 \times 1.0 \times \frac{5000 \text{ ft}^3}{s} \times \sqrt{\pi \times 1.0 \text{ ft} \times 3000 \text{ ft}}}{3.78 \text{ ft/d} \times 1000 \text{ ft}^3 \times \frac{d}{86,400 \text{ s}}} \\ &\quad \times \exp\left(\frac{\ln 2}{12.3 \text{ y}} \times 2.17 \text{ y}\right) \\ &= 2.51 \times 10^7 , \end{aligned}$$

$$\begin{aligned}
{}^{90}\text{Sr} \quad D_L &= \frac{2 \times 14 \times \frac{5000 \text{ ft}^3}{s} \times \sqrt{\pi \times 1.0 \text{ ft} \times 3000 \text{ ft}}}{3.78 \text{ ft/d} \times 1000 \text{ ft}^3 \times \frac{d}{86,400s}} \\
&\times \exp\left(\frac{\ln 2}{29 \text{ y}} \times 30.4 \text{ y}\right) \\
&= 6.42 \times 10^8 ,
\end{aligned}$$

$$\begin{aligned}
{}^{137}\text{Cs} \quad D_L &= \frac{2 \times 131 \times \frac{5000 \text{ ft}^3}{s} \times \sqrt{\pi \times 1.0 \text{ ft} \times 3000 \text{ ft}}}{3.78 \text{ ft/d} \times 1000 \text{ ft}^3 \times \frac{d}{86,400s}} \\
&\times \exp\left(\frac{\ln 2}{30.1 \text{ y}} \times 284.8 \text{ y}\right) \\
&= 2.05 \times 10^{12} .
\end{aligned}$$

The peak concentrations in the river are determined by dividing the tank concentrations by the dilution factors:

$$c({}^3\text{H}) = 4000 \mu\text{Ci/mL} / 2.51 \times 10^7 = 1.59 \times 10^{-4} \mu\text{Ci/mL} ,$$

$$c({}^{90}\text{Sr}) = 2000 \mu\text{Ci/mL} / 6.42 \times 10^8 = 3.12 \times 10^{-5} \mu\text{Ci/mL} ,$$

$$c({}^{137}\text{Cs}) = 3000 \mu\text{Ci/mL} / 2.05 \times 10^{12} = 1.46 \times 10^{-9} \mu\text{Ci/mL} .$$

(b) Minimum dilution in well (400 ft downgradient).

First determine whether or not the thickness of the aquifer would affect the results by calculating the factor  $\phi$  from Equation B-50:

$$\phi = \frac{b^2}{\alpha_r x} = \frac{(100 \text{ ft})^2}{0.5 \text{ ft} \times 400 \text{ ft}} = 50 .$$

Therefore, in this region the release will be relatively unaffected by the thickness of the aquifer, and Equation B-53 applies.

The travel times are estimated using the retardation factors and pore velocity calculated above:

$${}^3\text{H} \quad t = \frac{400 \text{ ft} \times 1}{3.78 \text{ ft/d}} \times \frac{\text{y}}{365 \text{ d}} = 0.29 \text{ y} ,$$

$${}^{90}\text{Sr} \quad t = \frac{400 \text{ ft} \times 14}{3.78 \text{ ft/d}} \times \frac{\text{y}}{365 \text{ d}} = 4.06 \text{ y} ,$$

$${}^{137}\text{Cs} \quad t = \frac{400 \text{ ft} \times 131}{3.78 \text{ ft/d}} \times \frac{\text{y}}{365 \text{ d}} = 38 \text{ y} .$$

Applying equation B.52:

$$\begin{aligned}
 {}^3\text{H} \quad D_L &= \frac{0.25 \times 1 \times (4\pi \times 400 \text{ ft})^{3/2} \sqrt{1 \text{ ft} \times 0.5 \text{ ft} \times 0.5 \text{ ft}}}{2 \times 1000 \text{ ft}^3} \\
 &\quad \times \exp\left(\frac{\ln 2}{12.3 \text{ y}} \times 0.29 \text{ y}\right) \\
 &= 22.6 ,
 \end{aligned}$$

$$\begin{aligned}
 {}^{90}\text{Sr} \quad D_L &= \frac{0.25 \times 14 \times (4\pi \times 400 \text{ ft})^{3/2} \sqrt{1 \text{ ft} \times 0.5 \text{ ft} \times 0.5 \text{ ft}}}{2 \times 1000 \text{ ft}^3} \\
 &\quad \times \exp\left(\frac{\ln 2}{29 \text{ y}} \times 4.06 \text{ y}\right) \\
 &= 343.6 ,
 \end{aligned}$$

$$\begin{aligned}
 {}^{137}\text{Cs} \quad D_L &= \frac{0.25 \times 131 \times (4\pi \times 400 \text{ ft})^{3/2} \sqrt{1 \text{ ft} \times 0.5 \text{ ft} \times 0.5 \text{ ft}}}{2 \times 1000 \text{ ft}^3} \\
 &\quad \times \exp\left(\frac{\ln 2}{30.1 \text{ y}} \times 38 \text{ y}\right) \\
 &= 6999.9 .
 \end{aligned}$$

The peak well concentrations are therefore 177  $\mu\text{Ci/mL}$  for  $^3\text{H}$ , 5.8  $\mu\text{Ci/mL}$  for  $^{90}\text{Sr}$ , and 0.43  $\mu\text{Ci/mL}$  for  $^{137}\text{Cs}$ .

(c) Well 2500 ft downgradient. Calculate  $\phi$  for this region from Equation B-49:

$$\phi = \frac{(100 \text{ ft})^2}{0.5 \text{ ft} \times 2000 \text{ ft}} = 8.0 .$$

Therefore, this well is in the intermediate region, and Equation B-53 applies. The factor  $F(\phi)$  can be read from Figure B.6 to be 1.6. Travel times for each component calculated from Equation B-46 are

$$^3\text{H} \quad t = \frac{2500 \text{ ft} \times 1}{3.78 \text{ ft/d}} \times \frac{\text{y}}{365 \text{ d}} = 1.81 \text{ y} ,$$

$$^{90}\text{Sr} \quad t = \frac{2500 \text{ ft} \times 14}{3.78 \text{ ft/d}} \times \frac{\text{y}}{365 \text{ d}} = 25.4 \text{ y} ,$$

$$^{137}\text{Cs} \quad t = \frac{2500 \text{ ft} \times 131}{3.78 \text{ ft/d}} \times \frac{\text{y}}{365 \text{ d}} = 237.4 \text{ y} .$$

Applying Equation B-53:

$$\begin{aligned} ^3\text{H} \quad D_L &= \frac{1 \times 4\pi \times 0.25 \sqrt{0.5 \text{ ft} \times 1.0 \text{ ft}} \times 2500 \text{ ft} \times 100 \text{ ft}}{1000 \text{ ft}^3 \times 1.6} \\ &\quad \times \exp\left(\frac{\ln 2}{12.3 \text{ y}} \times 1.81 \text{ y}\right) \\ &= 271.8 , \end{aligned}$$

$$\begin{aligned}
 D_L &= \frac{14 \times 4\pi \times 0.25 \sqrt{0.5 \text{ ft} \times 1.0 \text{ ft}} \times 2500 \text{ ft} \times 100 \text{ ft}}{1000 \text{ ft}^3 \times 1.6} \\
 {}^{90}\text{Sr} &\quad \times \exp\left(\frac{\ln 2}{29 \text{ y}} \times 25.2 \text{ y}\right) \\
 &= 8874 ,
 \end{aligned}$$

${}^{137}\text{Cs}$

$$\begin{aligned}
 D_L &= \frac{131 \times 4\pi \times 0.25 \sqrt{0.5 \text{ ft} \times 1.0 \text{ ft}} \times 2500 \text{ ft} \times 100 \text{ ft}}{1000 \text{ ft}^3 \times 1.6} \\
 &\quad \times \exp\left(\frac{\ln 2}{30.1 \text{ y}} \times 237.4 \text{ y}\right) \\
 &= 1.07 \times 10^7 .
 \end{aligned}$$

The peak well concentrations are therefore 14.7  $\mu\text{Ci/mL}$  for  ${}^3\text{H}$ , 0.32  $\mu\text{Ci/mL}$  for  ${}^{90}\text{Sr}$ , and  $2.8 \times 10^{-4}$   $\mu\text{Ci/mL}$  for  ${}^{137}\text{Cs}$ .

(d) Quantity  $M$  of each radionuclide eventually reaching river.

Equation B-57 applies to this case because  $\alpha_L \ll \ell$  (i.e., 1 ft vs 1000 ft). Travel times are estimated in part (a) above. The quantity of each radionuclide initially in the tank is the concentration multiplied by the volume. Therefore,

$$\begin{aligned}
 {}^3\text{H} \quad M &= 4000 \mu\text{Ci/mL} \times 1000 \text{ ft}^3 \times 28,300 \text{ mL/ft}^3 \\
 &\quad \times \exp\left(\frac{-\ln 2}{12.3 \text{ y}} \times 2.17 \text{ y}\right) \times 10^{-6} \text{ Ci}/\mu\text{Ci} \\
 &= 1.002 \times 10^5 \text{ Ci} ,
 \end{aligned}$$

$$\begin{aligned}
^{90}\text{Sr} \quad M &= 2000 \mu\text{Ci}/\text{mL} \times 1000 \text{ ft}^3 \times 28,300 \text{ mL}/\text{ft}^3 \\
&\quad \times \exp\left(\frac{-\ln 2}{29 \text{ y}} \times 30.4 \text{ y}\right) \times 10^{-6} \text{ Ci}/\mu\text{Ci} \\
&= 27,370 \text{ Ci} ,
\end{aligned}$$

$$\begin{aligned}
^{137}\text{Cs} \quad M &= 3000 \mu\text{Ci}/\text{mL} \times 1000 \text{ ft}^3 \times 28,300 \text{ mL}/\text{ft}^3 \\
&\quad \times \exp\left(\frac{-\ln 2}{30.1 \text{ y}} \times 284.7 \text{ y}\right) \times 10^{-6} \text{ Ci}/\mu\text{Ci} \\
&= 120.7 \text{ Ci} .
\end{aligned}$$



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## **APPENDIX C**

### **DEFAULT PARAMETER VALUES**

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Table C-1. Representative Values for Saturated Moisture Contents and Field Capacities of Various Soil Types

	Number of soils	Saturated moisture content ( $\theta_s$ ) <sup>a</sup>	
		Mean	$\pm 1$ standard deviation
Sand	762	0.437	0.347 - 0.500
Loamy sand	338	0.437	0.368 - 0.506
Sandy loam	666	0.453	0.351 - 0.555
Loam	383	0.463	0.375 - 0.551
Silt loam	1,206	0.501	0.420 - 0.582
Sandy clay loam	498	0.398	0.332 - 0.464
Clay loam	366	0.464	0.409 - 0.519
Silty clay loam	689	0.471	0.418 - 0.524
Sandy clay	45	0.430	0.370 - 0.490
Silty clay	127	0.479	0.425 - 0.533
Clay	291	0.475	0.427 - 0.523

<sup>a</sup> From total soil porosity measurements compiled by Rawls et al. (1982) from numerous sources.

Source: Rawls, W.J., D.L. Brakensiek, K.E. Saxton, 1982. Estimation of soil water properties. *Trans. Am. Soc. Agri. Eng.* 25(5):1316-1320 and 1328. As cited in EPA88b.

Table C-2. Representative Values of Hydraulic Parameters

Soil texture	No. of soils <sup>a</sup>	b <sup>b</sup>	$\frac{1}{2b+3}$	$\theta_s^c$
Sand	13	4.05 (1.78) <sup>d</sup>	0.090	0.395 (0.056)
Loamy sand	30	4.38 (1.47)	0.085	0.410 (0.068)
Sandy loam	204	4.90 (1.75)	0.080	0.435 (0.086)
Silt loam	384	5.30 (1.87)	0.074	0.485 (0.059)
Loam	125	5.39 (1.87)	0.073	0.451 (0.078)
Sandy clay loam	80	7.12 (2.43)	0.058	0.420 (0.059)
Silt clay loam	147	7.75 (2.77)	0.054	0.477 (0.057)
Clay loam	262	8.52 (3.44)	0.050	0.476 (0.053)
Sandy clay	19	10.40 (1.64)	0.042	0.426 (0.057)
Silt clay	441	10.40 (4.45)	0.042	0.492 (0.064)
Clay	140	11.40 (3.70)	0.039	0.482 (0.050)

<sup>a</sup> Number of individual soil samples included in data compiled by Clapp and Hornberger (1978).

<sup>b</sup> Empirical parameter relating soil matrix potential and moisture content; shown to be strongly dependent on soil texture.

<sup>c</sup> Volumetric soil moisture content (volume of water per volume of soil).

<sup>d</sup> Standard deviation in parentheses.

Source: Adapted from: Clapp, R.B., and G.M. Hornberger. 1978. "Empirical Equations for Some Soil Hydraulic Properties." Water Resour. Res. 14(4): 601-604.

Table C-3. Representative Values of Saturated Hydraulic Conductivity

Soil texture	Number of soils <sup>a</sup>	Hydraulic conductivity (K <sub>s</sub> ; cm/sec) <sup>b</sup>
Sand	762	$5.8 \times 10^{-3}$
Loamy sand	338	$1.7 \times 10^{-3}$
Sandy loam	666	$7.2 \times 10^{-4}$
Loam	383	$3.7 \times 10^{-4}$
Silt loam	1,206	$1.9 \times 10^{-4}$
Sandy clay loam	498	$1.2 \times 10^{-4}$
Silt clay loam	366	$4.2 \times 10^{-5}$
Clay loam	689	$6.4 \times 10^{-5}$
Sandy clay	45	$3.3 \times 10^{-5}$
Silt clay	127	$2.5 \times 10^{-5}$
Clay	291	$1.7 \times 10^{-5}$

<sup>a</sup> Number of individual soil samples included in data compiled by Rawls et al. (1982).

<sup>b</sup> Predicted values based on compiled soil properties.

Source: Adapted from: Rawls, W.J., 1986. Computer printouts from the soils data base, dated August 28, 1986. From WJ Rawls, Beltsville, MD: Beltsville Agricultural Research Center. As cited in EPA88b.

Table C-4. Saturated Hydraulic Conductivity Ranges for Selected Rock and Soil Types

	Saturated hydraulic conductivity (cm/sec)	
<u>Soils</u>		
Unweathered marine clay	$5 \times 10^{-11}$ $10^{-7}$	-
Glacial till	$10^{-10}$	- $10^{-4}$
Silt, loess	$10^{-7}$	- $10^{-3}$
Silty sand	$10^{-5}$	- $10^{-1}$
Clean sand	$10^{-4}$	- 1
Gravel	$10^{-1}$	- $10^2$
<u>Rocks</u>		
Unfractured metamorphic and igneous rock	$10^{-8}$	- $10^{-2}$
Shale	$5 \times 10^{-12}$	- $10^{-7}$
Sandstone	$10^{-8}$	- $5 \times 10^{-4}$
Limestone and dolomite	$5 \times 10^{-8}$	- $5 \times 10^{-4}$
Fractured igneous and metamorphic rock	$10^{-6}$	- $10^{-2}$
Permeable basalt	$10^{-5}$	- 1
Karst limestone	$10^{-4}$	- 1

Source: Adapted from: Freeze, R.A. and J. Cherry, 1979. Groundwater, Prentice-Hall, Englewood Cliffs, N.J.



Table C-5. Distribution Coefficient ( $K_d$ ) of Selected Radionuclides Sorbed by Clays and Cation Exchange Capacity for Selected Clay Minerals

Material	Average Percent Activity Sorbed <sup>(a)</sup>				Average $K_d$ <sup>(b)</sup>			
	Cesium	Cobalt	Strontium-85	Zirconium-Niobium-85	Cesium	Cobalt	Strontium-85	Zirconium-Niobium-85
Illite	98	86	27	94	180,000	6,400	370	47,500
Kaolinite	68	61	66	94	2,200	3,100	4,000	56,000
Montmorillonite	50	62	67	35	1,000	1,700	2,100	540
Vermiculite	100	99	97		12,000	4,700	1,800	

<sup>(a)</sup> Average percent and average  $K_d$  of radionuclides sorbed by clays in distilled water at pH 6 over a period of 7 days (vermiculite, 8 days).

<sup>(b)</sup> Reported in millequivalents per 100g of soil [Source: GRI68].

Source: Derived from:

Webster, G.B. et al., 1976. "Radionuclide Migration from Low-Level Wastes: A Generic Overview," in M.W. Carter et al. (editors), Management of Low-Level Radioactive Waste, Pergamon Press, New York, NY, pp. 1041-1072.

Grim, 1968.

Table C-6. Typical Values of Hydraulic Conductivity of Porous Materials

Material	Number of analyses	Arithmetic Range (cm/s)	mean (cm/s)
<b>Igneous rocks</b>			
Weathered granite	7	$(3.3-52) \times 10^{-4}$	$1.65 \times 10^{-3}$
Weathered gabbro	4	$(0.5-3.8) \times 10^{-4}$	$1.89 \times 10^{-4}$
Basalt	93	$(0.2-4250) \times 10^{-8}$	$9.45 \times 10^{-6}$
<b>Sedimentary materials</b>			
Sandstone (fine)	20	$(0.5-2270) \times 10^{-6}$	$3.31 \times 10^{-4}$
Siltstone	8	$(0.1-142) \times 10^{-8}$	$1.9 \times 10^{-7}$
Sand (fine)	159	$(0.2-189) \times 10^{-4}$	$2.88 \times 10^{-3}$
Sand (medium)	255	$(0.9-567) \times 10^{-4}$	$1.42 \times 10^{-2}$
Sand (coarse)	158	$(0.3-6610) \times 10^{-4}$	$5.20 \times 10^{-2}$
Gravel	40	$(0.3-31.2) \times 10^{-1}$	$4.03 \times 10^{-1}$
Silt	39	$(0.09-7090) \times 10^{-7}$	$2.83 \times 10^{-5}$
Clay	19	$(0.1-47) \times 10^{-8}$	$9 \times 10^{-8}$
<b>Metamorphic rocks</b>			
Schist	17	$(0.002-1130) \times 10^{-6}$	$1.9 \times 10^{-4}$

Source: McWhorter, D.B., and D.K. Sunada, 1977. Ground-Water Hydrology and Hydraulics, Water Resources Publications, Fort Collins, Colo.

Table C-7. Suggested Value for  $C_{et}$  Relating Evaporation from a U.S. Class A Pan to Evapotranspiration from 8 to 15-cm Tall, Well-Watered Grass Turf

short green crop		Pan surrounded by a dry surface ground					Pan surrounded by a		
		Average regional relative humidity, %*			Upwind fetch of dry fallow (m from pan)		Average regional relative humidity, %*		
Wind	Upwind fetch of crop (m from pan)	20-40	40-70	>70		20-40	40-70	>70	
							0	0.55	0.65
Light <170 km/day	0.75	0	0.7	0.8	0.85				
	10	0.65	0.75	0.85	10	0.6	0.7	0.8	
	100	0.7	0.8	0.85	100	0.55	0.65	0.75	
	1000	0.7	0.85	0.85	1000	0.5	0.6	0.7	
Moderate 170-425 km/day	0	0.5	0.6	0.65	0	0.65	0.75	0.8	
	10	0.6	0.7	0.75	10	0.55	0.65	0.7	
	100	0.65	0.75	0.8	100	0.5	0.6	0.65	
	1000	0.7	0.8	0.8	1000	0.45	0.55	0.6	
Strong 425-700 km/day	0	0.45	0.5	0.6	0	0.6	0.65	0.7	
	10	0.55	0.6	0.65	10	0.5	0.55	0.65	
	100	0.6	0.65	0.7	100	0.45	0.5	0.6	
	1000	0.65	0.7	0.75	1000	0.4	0.45	0.55	
Very strong >700 km/day	0	0.4	0.45	0.5	0	0.5	0.6	0.65	
	10	0.45	0.55	0.6	10	0.45	0.5	0.55	
	100	0.5	0.6	0.65	100	0.4	0.45	0.5	
	1000	0.55	0.6	0.65	1000	0.3	0.4	0.45	

\* Mean of maximum and minimum relative humidities.

Source: Jenson, M.E., ed., 1973. Consumptive use of water and irrigation water requirements. New York, NY: American Society of Civil Engineers. As presented by Enfield et al. 1982. Approximating pollutant transport to ground water. Ground Water 20(6): 711-722. As cited in EPA88b.

Enfield, C.G., R.F. Carsel, S.Z. Cohen, T. Phan, D.M. Walters, 1982. Approximating pollutant transport to ground water. Ground Water 20(6): 711-722. As cited in EPA88b.

Table C-8. Crop Coefficients for Estimating Evapotranspiration

Crop	Period	Coefficient ( $C_{veg}$ )
Alfalfa	April 1 - October 10	0.87
Potatoes	May 10 - September 15	0.65
Small grains	April 1 - July 20	0.6
Sugar beets	April 10 - October 15	0.6

Source: Jenson, M.E., ed., 1973. Consumptive use of water and irrigation water requirements. New York, NY: American Society of Civil Engineers. As presented by Enfield et al. 1982. Approximating pollutant transport to ground water. Ground Water 20(6): 711-722. As cited in EPA88b.

Enfield, C.G., R.F. Carsel, S.Z. Cohen, T. Phan, D.M. Walters, 1982. Approximating pollutant transport to ground water. Ground Water 20(6): 711-722. As cited in EPA88b.

Table C-9. Typical Values of Porosity of Aquifer Materials

Aquifer material	Number of analyses	Range	Arithmetic mean
Igneous Rocks			0.45
Weathered granite	8	0.34-0.57	0.43
Weathered gabbro	4	0.42-0.45	0.43
Basalt	94	0.03-0.35	0.17
Sedimentary Materials			
Sandstone	65	0.14-0.49	0.34
Siltstone	7	0.21-0.41	0.35
Sand (fine)	245	0.25-0.53	0.43
Sand (coarse)	26	0.31-0.46	0.39
Gravel (fine)	0.2580.38		0.34
Gravel (coarse)	15	0.24-0.36	0.28
Silt	281	0.34-0.51	0.45
Clay	74	0.34-0.57	0.42
Limestone	74	0.07-0.56	0.30
Metamorphic Rocks			
Schist	18	0.04-0.49	0.38

Source: McWhorter, D.B., and D.K. Sunada, 1977. Ground-Water Hydrology and Hydraulics, Water Resources Publications, Fort Collins, Colo. Reprinted with permission.

Table C-10. Typical Values of Effective Porosity (or Specific Yield) of Aquifer Materials

Aquifer material	Number of analyses	Range	Arithmetic mean
<b>Sedimentary Materials</b>			
Sandstone (fine)	47	0.02-0.40	0.21
Sandstone (medium)	10	0.12-0.41	0.27
Siltstone	13	0.01-0.33	0.12
Sand (fine)	287	0.01-0.46	0.33
Sand (medium)	297	0.16-0.46	0.32
Sand (coarse)	143	0.18-0.43	0.30
Gravel (fine)	33	0.13-0.40	0.28
Gravel (medium)	13	0.17-0.44	0.24
Gravel (coarse)	9	0.13-0.25	0.21
Silt	299	0.01-0.39	0.20
Clay	27	0.01-0.18	0.06
Limestone	32	0-0.36	0.14
<b>Wind-Laid Materials</b>			
Loess	5	0.14-0.22	0.18
Eolian Sand	14	0.32-0.47	0.38
Tuff	90	0.02-0.47	0.21
<b>Metamorphic Rock</b>			
Schist	11	0.22-0.33	0.26

Source: McWhorter, D.B., and D.K. Sunada, 1977. Ground-Water Hydrology and Hydraulics, Water Resources Publications, Fort Collins, Colo. Reprinted with permission.

Table C-11. Dispersivity Values  $\alpha_L$  and  $\alpha_T$  Obtained Directly through Measurements of Tracer Breakthrough Curves in Groundwater Solute Transport

Setting	$\alpha_L$ (m)	$\alpha_T$ (m)	$\Delta x^a$ (m)	$\bar{U}^b$ (m/d)	Method
Chalk River, Ontario alluvial aquifer	0.034				Single-well tracer test
Chalk River, strata of high velocity Alluvial aquifer	0.034-0.1				Single-well
Alluvial, strata of high velocity	0.5				Two-well
Lyons, France alluvial aquifer	0.1				Two-well
Lyons (full aquifer)	0.1-0.5				Single-well
Lyons (full aquifer)	5				Single-well
Lyons (full aquifer)	12.0	31.1-14		7.2	Single-well test with resistivity
Lyons (full aquifer)	8	0.015-1		9.6	Single-well test with resistivity
Lyons (full aquifer)	5	0.145-14.5		13	Single-well test with resistivity
Lyons (full aquifer)	7	0.009-1		9	Single-well test with resistivity
Alsace, France alluvial sediments	12	4			Environmental tracer
Carlsbad, N. Mex. fractured dolomite	38.1		38.1	0.15	Two-well tracer
Savannah River, S.C. fractured schistgneiss	134.1		538	0.4	Two-well

Table C-11 (Continued)

Setting	$\alpha_L$ (m)	$\alpha_T$ (m)	$\Delta x^a$ (m)	$\bar{U}^b$ (m/d)	Method
Barstow, Calif. alluvial sediments	15.2		6.4		Two-well
Dorset, England chalk (fractured)	3.1		8		Two-well
(intact)	1.0		8		Two-well
Berkeley, Calif. sand/gravel	2-3		8	311-1382	Multiwell trace test
Mississippi limestone	11.6				Single-well
NTS, carbonate aquifer	15				Two-well tracer
Pensacola, Fla. limestone	10		312	0.6	Two-well

<sup>a</sup> $\Delta x$  = distance between wells in two-well test.

<sup>b</sup> $\bar{U}$  = groundwater seepage velocity.

Source: Evenson, D.E., and M.D. Dettinger, 1980. *Dispersive Processes in Models of Regional Radionuclide Migration*, University of California, Lawrence Livermore Laboratory, Livermore.