A TECHNICAL GUIDE TO GROUND-WATER MODEL SELECTION AT SITES CONTAMINATED WITH RADIOACTIVE SUBSTANCES

A Cooperative Effort By

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PREFACE

A joint program is underway between the EPA Offices of Radiation and Indoor Air (ORIA) and Solid Waste and Emergency Response (OSWER), the DOE Office of Environmental Restoration and Waste Management (EM), and the NRC Office of Nuclear Material Safety and Safeguards (NMSS). The purpose of the program is to promote the appropriate and consistent use of mathematical models in the remediation and restoration process at sites containing, or contaminated with, radioactive materials. This report is one of a series of reports designed to accomplish this objective. Other reports completed under this program have identified the models in actual use at NPL sites and facilities licensed under RCRA, and at DOE sites and NRC sites undergoing decontamination and decommissioning (D&D), as well as the role of modeling and modeling needs in each phase of the remedial investigation. This report specifically addresses the selection of ground-water flow and contaminant transport models and is intended to be used by hydrogeologists and geoscientists responsibile for identifying and selecting ground-water flow and contaminant transport models for use at sites containing radioactive materials.

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S.1 INTRODUCTION

A joint program is underway between the Environmental Protection Agency (EPA) Offices of Radiation and Indoor Air (ORIA) and Solid Waste and Emergency Response (OSWER), the Department of Energy (DOE) Office of Environmental Restoration and Waste Management (EM), and the Nuclear Regulatory Commission (NRC) Office of Nuclear Material Safety and Safeguards (NMSS). The purpose of the program is to promote the appropriate and consistent use of mathematical models in the remediation and restoration process at sites containing, or contaminated with, radioactive materials. This report, which is one of a series of reports designed to accomplish this objective, specifically addresses the selection of ground-water flow and contaminant transport models. It is intended to be used by hydrogeologists and geoscientists responsible for identifying and selecting ground-water flow and contaminant transport models for use at sites containing or contaminated with radioactive materials.

Previous reports in this series have determined that the types of models and the processes that require modeling during the remedial process depend on a combination of the following five factors:

1. reasons for modeling,
2. contaminant/waste characteristics,
3. site environmental characteristics,
4. site land use and demography, and
5. phase of the remedial process.

This report describes and provides a rationale for the methods for selecting ground-water flow and contaminant transport models and computer codes that meet the modeling needs at sites containing, or contaminated with, radioactive materials. The selection process is described in terms of the various site characteristics and processes requiring modeling and the availability, reliability, and useability of the computer codes that meet the modeling needs.

Though this report is limited to a discussion of the model selection process, the proper application of the selected codes is as important, if not more important, than code selection. A code, no matter how well suited to a particular application, could give erroneous and highly misleading results if used improperly or with incomplete or erroneous input data. Conversely, even a code with very limited capabilities, or a code used at a site which has not been well characterized, can give very useful results if used intelligently and with a full appreciation of the limitations of the code and the input data.

It was not possible, within the scope of this report, to address computer code applications, quality control, and the presentation and interpretation of modeling results. Future reports to be prepared under this program will address these important topics.

The report is divided into five sections. Following this introduction, Section 2 presents an overview of the types of ground-water modeling decisions facing the site remediation manager. This section is designed to help the site manager and/or earth scientists to determine the role of, and need for, modeling in support of remedial decision making.

Section 3 addresses the construction of a conceptual model of a site and how it is used in the initial planning and scoping phases of a site remediation, especially as it pertains to the selection and use of ground-water flow and contaminant transport codes.

Section 4 describes the various site characteristics and ground-water flow and contaminant transport processes that may need to be explicitly modeled. The purpose of this section is to help the earth scientists recognize the conditions under which specific code features and capabilities are needed to support remedial decision making during each phase in the site remediation process.

Section 5 describes the computer code review and evaluation process for screening and selecting the computer codes that are best suited to meet site-specific modeling needs.

S.2 MODELING QUESTIONS FACING THE SITE REMEDIATION MANAGER

A review of current regulations and guidelines pertaining to the remediation of sites on the National Priorities List (NPL) and in the NRC's Sites Decommissioning Management Program (SDMP) reveals that fate and effects modeling is not explicitly required. However, in order to make informed and defensible remedial decisions, ground-water flow and contaminant transport modeling can be useful and is often necessary.

S.2.1 When is Ground-Water Modeling Needed?

The first questions that a site remediation manager will need to answer regarding ground-water modeling include: Is ground-water modeling needed, and how will modeling aid in the remedial decision making process?

The ground-water pathway may be considered a potentially significant exposure pathway if (1) the radionuclide concentrations in the ground water exceed the levels acceptable to the cognizant regulatory authorities or (2) the contamination at the site could eventually cause the radionuclide concentrations in ground water to exceed the applicable criteria. On this basis, if the measured concentrations of radionuclides in ground water downgradient from the site, or in leachate at the site, exceed the applicable criteria, and the ground water in the vicinity of the site is being used, or has the potential to be used, as a source of drinking water, it is likely that ground-water modeling will be useful, if not necessary, in support of remedial decision making at the site.

The "applicable criteria" are ill-defined at this time because both NRC and EPA are engaged in rulemaking activities intended to define the criteria. However, in the interim, the drinking-water standards set forth in 40 CFR 141 should guide remedial decision making. For example, 40 CFR 141 has been cited as an applicable or relevant and appropriate regulation (ARAR) in establishing the remediation goals at most of the approximately 50 sites contaminated with radioactive material that are currently on the National Priorities List.

At some sites, information may not be available regarding the levels of radionuclide contamination in ground water or leachate. Alternatively, radionuclide measurements may have been made, but yield inconclusive results. Under these conditions, the radionuclide concentrations in leachate and ground water can be <u>estimated</u> based on knowledge of the radionuclide concentrations in the soil or the waste at the site and empirically determined partition factors. Partition factors relate a given concentration of a contaminant in the waste or the soil to that in the leachate or ground water.

If the product of the radionuclide concentrations in the waste or contaminated soil with the appropriate partition factors results in radionuclide concentrations in leachate or ground water in excess of the applicable criteria, it may be concluded that the radionuclide concentrations in ground water in the vicinity of the site could exceed the applicable criteria. Though it is not necessarily always the case, if the measured or derived concentrations of radionuclides in ground water exceed the applicable criteria, it is likely that ground-water modeling will serve a useful role in support of remedial decision making at the site.

S.2.2 When is Modeling Not Needed or Inappropriate?

It is important to be able to recognize the circumstances under which modeling would be ineffective and should probably not be performed. There are three general scenarios in which modeling would be of limited value. These are:

1. Presumptive remedies can be readily identified,

2. Decision making is based on highly conservative assumptions, and/or

3. The site is too complex to model realistically.

The first case arises in situations where a presumptive remedy is apparent; that is, where the remedy is obvious based on regulatory requirements or previous experience, and there is a high level of assurance that the site is well understood and the presumptive remedy will be effective. An example would be conditions that obviously require excavation or removal of the contaminant source.

The second case is based on the assumption that decision making can proceed based on conservative estimates of the behavior and impacts of contaminants at the site rather than detailed modeling. This strategy

could be used in the initial scoping, site characterization, or remedial phase of the investigation. For example, a conservative approach to the risk assessment would be to assume that the contaminant concentrations at the receptor(s) are identical to the higher concentrations detected at the contaminant source. Thus, the need for modeling to determine the effects of dilution and attenuation on contaminant concentrations is removed.

The third case involves sites where modeling would be helpful in supporting remedial decision making, but the complexity of the site precludes reliable modeling. These complexities could be associated with the contaminant source, flow and transport processes, or characteristics of the wastes and contaminants. For example, the contaminant source may be so poorly defined in terms of areal extent, release history, and composition that it cannot be reliably defined and little would be gained from flow and transport modeling.

Complex flow and contaminant transport processes present another difficulty in that user-friendly computer codes currently do not exist that accommodate a number of these processes, which include: turbulent ground-water flow, facilitated transport (e.g., due to the formation of colloids), and flow and transport through a fractured unsaturated zone.

The availability of computer codes is also an issue when characteristics of the contaminants are typified by complex geochemical reactions, such as phase transformations and non-linear sorption processes. Currently, ground-water flow and contaminant transport codes that provide credible mathematical descriptions of the more complex geochemical processes have not been developed. If modeling is not possible because of the overall complexity of the site characteristics, it is common for a greater emphasis to be placed on empirical rather than predicted data. This may involve establishing long-

term monitoring programs, which, in effect, have objectives similar to those of ground-water modeling.

S.2.3   What Role Will Ground-Water Modeling Play in Support of Remedial Decision Making?

Once it is determined that the ground-water exposure pathway is potentially important, ground-water flow and transport modeling can have a wide range of uses in support of remedial decision making. The following are the principal reasons for modeling on a remedial project. These applications can surface during any phase of the remedial process. However, some of these reasons are more likely to occur during specific phases of a remedial project.

1. When it is not feasible to perform field measurements; i.e.,

    !   Cannot get access to sampling locations
    !   Budget is limited
    !   Time is limited

2. When there is concern that downgradient locations may become contaminated at some time in the future; i.e.,

    !   When transport times from the source of the contamination to potential receptor locations are long relative to the period of time the source of the contaminant has been present.
    !   When planning to store or dispose of waste at a specific location and impacts can be assessed only through the use of models.

3. When field data alone are not sufficient to characterize fully the nature and extent of the contamination; i.e.,

    !   When field sampling is limited in space and time, and
    !   When field sampling results are ambiguous or suspect.

4. When there is concern that conditions at a site may change, thereby changing the fate and transport of the contaminants; i.e.,

    !   seasonal changes in environmental conditions
    !   severe weather (e.g., floods)
    !   accidents (e.g., fires)

5. When there is concern that institutional control at the site may be lost at some time in the future

resulting in new exposure scenarios, or a change in the fate and transport of the contaminants; i.e.,

! trespassers
! inadvertent intruder (construction/ agriculture)
! human intervention (drilling, excavations, mining)

6. When remedial actions are planned and there is a need to predict the effectiveness of alternative remedies.

7. When there is a need to predict the time when the concentration of specific contaminants at specific locations will decline to acceptable levels (e.g., natural flushing).

8. When there is concern that at some time in the past individuals were exposed to elevated levels of contamination and it is desirable to reconstruct the doses.

9. When there is concern that contaminants may be present but below the lower limits of detection.

10. When field measurements reveal the presence of some contaminants, and it is desirable to determine if and when other contaminants associated with the source may arrive, and at what levels.

11. When field measurements reveal the presence of contaminants and it is desirable to identify the source or sources of the contamination.

12. When there is a need to determine the timing of the remedy; i.e., if the remedy is delayed, is there a potential for environmental or public health impacts in the future?

13. When there is a need to determine remedial action priorities.

14. When demonstrating compliance with regulatory requirements.

15. When estimating the benefit in a cost-benefit analysis of alternative remedies.

16. When performing a quantitative dose or risk assessment pertaining to the protection of

remediation workers, the public, and the environment prior to, during, and following remedial activities.

17. When designing the site characterization program (e.g., placement of monitor wells, determining data needs) and identifying exposure pathways of potential significance.

18. When there is a need to compute or predict the concentration distribution in space and time of daughter products from the original source of radionuclides.

19. When there is a need to quantify the degree of uncertainty in the anticipated behavior of the radionuclides in the environment and the associated doses and risks.

20. When communicating with the public on the potential impacts of the site and the benefits of the selected remedy.

S.2.4 What Will the Results of a Modeling Exercise Yield?

Once the need for, and role of, modeling is identified, it is appropriate to determine or define the form of the results or output of the modeling exercise. In general, the results are expressed as a concentration, such as pCi/L in ground water at a specific location. The derived radionuclide concentrations could also be expressed as a function of time or as a time-averaged value.

Some computer codes have the ability to convert the derived radionuclide concentrations in ground water to doses or risks to individuals exposed to the contaminated ground water. These results are generally expressed in units of mrem/yr or lifetime risk of cancer for the exposed individuals.

Some computer codes can present the results in terms of cumulative population impacts. These results are generally expressed in terms of person-rems/yr or total number of cancers induced per year in the exposed population.

The specific regulatory requirements that apply to the remedial program determine which of these "end products" are needed. In general, these modeling results are used to assess impacts or compliance with

applicable regulations; however, information regarding radionuclide flux and plume arrival times and distributions is also used to support a broad range of remedial decisions.

These modeling endpoints must be clearly defined, since the type of endpoint will help to determine the type of ground-water flow and contaminant transport model that will support the endpoint of interest. For example, a baseline risk assessment at a site contaminated with radioactive material is used in determining the annual radiation dose to an individual drinking water obtained from a potentially contaminated well. The endpoint in this case is the dose to an individual expressed in units of mrem/yr. In order to estimate this dose, it is necessary to estimate the average concentration of radionuclides in the well water over the course of a year. The models, input parameters, and assumptions needed to predict the annual average radionuclide concentration are different than those needed to predict the time varying concentration at a given location. The latter usually requires much more input data and models capable of simulating dynamic processes.

S.3 CONSTRUCTING A CONCEPTUAL MODEL OF A SITE - THE FIRST STEP IN THE MODEL SELECTION PROCESS

The first step in the model selection process is the construction of a conceptual model of the site. The conceptual model depicts the types of waste and contaminants, where they are located (e.g., are they currently only in the surficial soil or have they migrated to the underlying aquifer?), and how they are being transported offsite (e.g., 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 help visualize the direction and path followed by the contaminants, the controlling factors that affect the contaminant migration through the subsurface (i.e., hydrogeology, system boundary conditions), 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 regarding a site accumulates, the conceptual model is continually revised and refined.

A mathematical model translates the conceptual model into a series of equations which simulate the fate and effects of the contaminants as depicted in the conceptual model at a level of accuracy that can support remedial decision making. A computer code is simply a tool that is used to solve the equations which constitute the mathematical model of the site and display the results in a manner convenient to support remedial decision making. Accordingly, code selection must begin with the construction of a conceptual model of the site.

The components that make up the initial conceptual model of the site include:

1. the waste/contaminant characteristics,
2. the site characteristics, including hydrogeology, land use, and demography, and
3. the exposure scenarios and pathways.

S.3.1 Waste/Contaminant Characteristics

To the extent feasible, the site conceptual model should address the following characteristics of the waste/contaminants:

! Types and chemical composition of the radionuclides

! Waste form and containment

! Source geometry (e.g., volume, area, depth, homogeneity)

Within the context of ground-water modeling, these characteristics are pertinent to modeling the source term, i.e., the rate at which radionuclides are mobilized from the source and enter the unsaturated and saturated zones of a site.

S.3.2 Site Characteristics

The conceptual model of the site should begin to address the complexity of the environmental and hydrogeological setting. A complex setting, such as complex lithology, a thick unsaturated zone, and/or streams or other bodies of water on site, generally indicates that the direction and velocity of ground-water flow and radionuclide transport at the site cannot be reliably simulated using simple models.

However, even at complex sites, complex models may not be needed. For example, if a conservative approach is taken, where transport through the unsaturated zone is assumed to be instantaneous, then the complex processes associated with flow and transport through the unsaturated zone would not need to be modeled. Such an approach would be appropriate at sites where the remedy is likely to be removal of the contaminated surface and near-surface material.

The site conceptual model will also need to identify the locations where ground water is currently being used, or may be used in the future, as a private or municipal water supply. At sites with multiple user locations, an understanding of ground-water flow in two or three dimensions is needed in order to predict realistically the likelihood that the contaminated plume will be captured by the wells located at different directions, distances, and depths relative to the sources of contamination.

Simple ground-water flow and transport models typically are limited to estimating the radionuclide concentration in the plume centerline down-gradient from the source. Accordingly, if it is assumed that the receptors are located at the plume centerline, a simple model may be appropriate. Such an assumption is often appropriate even if a receptor is not currently present at the centerline location because the results are generally conservative. In addition, risk assessments often postulate that a receptor could be located directly down-gradient of the source at some time in the future.

The need for complex models increases if there are a number of water supplies in the vicinity of the source. Under these circumstances, it may be necessary to calculate the cumulative population doses and risks, which require modeling the radionuclide concentrations at a number of specific receptor locations. Accordingly, off-centerline modeling which includes dispersion may be needed.

S.3.3   Exposure Scenarios and Pathways

The conceptual model of the site will also need to define the exposure scenarios and pathways at the site. An exposure scenario pertains to the assumed initial conditions or initiating events responsible for the transport of the radionuclides and exposure of the nearby population. Depending on the regulatory requirements and the phase in the remedial process, the exposure scenarios that will need to be modeled can include any one or combination of the following:

! The no action alternative - Under this scenario, the radiation doses and risks to members of the public, now and in the future, are derived assuming no action is taken to remedy the site or protect the public from gaining access to the site.

! Trespassers - This scenario postulates that an individual trespasses on the site.

! Inadvertent intruder - This scenario postulates that an individual establishes residence at the site.

! Routine emissions - This scenario simply assesses offsite doses and risks associated with the normally anticipated releases from the site. (This concept is similar to the "No Action Alternatives," but is used within the context of NRC licensed facilities.)

! Accidents - This scenario assesses doses and risks associated with postulated accidental releases from the site.

! Alternative remedies - This set of scenarios assesses the doses and risks to workers and the public associated with the implementation of specific remedies and the reduction in public doses and risks following implementation of the remedy.

The number of scenarios that may be postulated is virtually unlimited. Accordingly, it is necessary to determine which scenarios reasonably bound what may in fact occur at the site. The types of scenarios selected for consideration influence modeling needs because they define the receptor locations and exposure pathways that need to be modeled.

For each scenario, an individual or group of individuals may be exposed by a wide variety of pathways. The principal pathways include:

! External exposure to deposited radionuclides

- External exposures to airborne, suspended, and resuspended radionuclides

- Inhalation exposures to airborne, suspended, and resuspended radionuclides

- Ingestion of radionuclides in food items and drinking water

- Ingestion of contaminated soil and sediment

- External exposures from immersion in contaminated water

S.4 CODE SELECTION - RECOGNIZING IMPORTANT MODEL CAPABILITIES

The greatest difficulty facing the investigator during the code selection process is not determining which codes have specific capabilities, but rather which capabilities are actually required to support remedial decision making during each remedial phase at a specific site. This section is designed to help the remedial manager recognize the conditions under which specific model features and capabilities are needed to support remedial decision making.

S.4.1 Code Selection During the Different Phases of a Remedial Program

Successful ground-water modeling requires the selection of a computer code that is not only consistent with the site characteristics but also with the modeling objectives, which are strongly dependent on the phase of the remedial process; i.e., scoping versus site characterization versus the selection and implementation of a remedy. Table S-1 presents an overview of how the overall approach to modeling a site differs as a function of the phase of the remedial process.

The most common code selection mistakes are selecting codes that are more sophisticated than are appropriate for the available data or the level of the result desired, and the application of a less sophisticated code that does not account for the flow and transport processes that dominate the system.

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

Attributes	Scoping	Characterization	Remediation
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	One Dimensional	1,2-Dimensional/Quasi-3-dimensional	Fully 3-Dimensional/Quasi-3-dimensional
Boundary and Initial Conditions	Uncomplicated Boundary and Uniform Initial Conditions	Non-Transient 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

For example, a typical question that often arises is: should three-dimensional codes be used as opposed to two- or one-dimensional codes? Inclusion of the third dimension requires substantially more data than one- and two- dimensional codes. Similar questions need to be considered which involve the underlying assumptions in the selection of an approach and the physical processes which are to be addressed. If the modeler is not practical, sophisticated codes are 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 appropriate to the problem and progress toward the more sophisticated codes until the modeling objectives are achieved.

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 phases of the remedial process may limit the modeling to one or two dimensions. In certain cases, this may be sufficient to support remedial decision making. If the modeling objectives cannot be met in this manner, additional data will be needed to support the use of more complex models.

It is generally in the later phases of the investigation that sufficient data have been obtained 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 equations.

Modeling objectives at each stage of the remedial investigation must be very specific and well defined early in the project. All too often, modeling is performed without developing a clear rationale to meet the objectives, and only after the modeling is completed are the weaknesses in the approach discovered.

The modeling objectives must consider the available data and the remedial decisions that the model results are intended to support. The selected modeling approach should not be driven by the data availability, but the modeling objectives should be defined in terms of what can be accomplished with the available data. If the modeling objectives demand more sophisticated models and input data, the necessary data should be obtained.

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

S.4.2   The Effects of Waste/Contaminant and Site Characteristics on Code Selection

After the conceptual model is formulated and the modeling objectives are clearly defined, the investigator should have a relatively good idea of the level of sophistication that the anticipated modeling will require. It now becomes necessary to select one or more computer code(s) that have the attributes necessary to mathematically describe the conceptual model at the desired level of detail. This step in the code selection process requires detailed analysis of the conceptual model to determine the degree to which specific waste/contaminant and site characteristics need to be explicitly modeled.

The code selection process consists primarily of determining which waste/contaminant and site charac-teristics and flow and transport processes need to be explicitly modeled in order to achieve the modeling objectives. Once these are determined, the code selection process becomes simply a matter of identi-fying the codes that meet the defined modeling needs.

Table S-2 lists code attributes related to various waste/contaminant and site characteristics. This table illustrates the site-related criteria generally considered in the identification of candidate computer codes.

The general components of the conceptual model that need to be considered when selecting an appropriate computer code are the following:

!   Source Characteristics

!   Aquifer and Soil/Rock Characteristics

Table S-2. Site-Related Features of Ground-Water Flow and Transport Codes

Section 4.3.1.1   Source Characteristics
> Point Source
> Line Source
> Areally Distributed Source
> Multiple Sources
> Specified Concentration
> Specified Source Rate
> Time-Dependent Release

Section 4.3.1.2   Aquifer and Soil/Rock Characteristics
> Confined Aquifers
> Confining Unit(s)
> Water-Table Aquifers
> Convertible Aquifers
> Multiple Aquifers
> Homogeneous
> Heterogeneous
> Isotropic
> Anisotropic
> Fractures
> Macropores
> Layered Soils

Section 4.3.1.3   Fate and Transport Processes
> Dispersion
> Advection
> Matrix Diffusion
> Density-Dependent Flow and Transport
> Retardation
> Non-linear Sorption
> Chemical Reactions/Speciation
> Single Species First Order Decay
> Multi-Species Transport with Chained Decay Reactions

Section 4.3.1.4   Multiphase Fluid Conditions
> Two-Phase Water/NAPL
> Two-Phase Water/Air
> Three-Phase Water/NAPL/Air

Section 4.3.1.5   Flow Conditions
> Fully Saturated
> Convertible Aquifers
> Variably Saturated/Non-Hysteretic
> Variably Saturated/Hysteretic

Section 4.3.1.6   Time Dependence
> Steady-State
> Transient

! Fate and Transport Processes   ! Multiphase Fluid Conditions

Each of these topics is presented as a major heading in Table S-2. These broad subjects are further broken down into their individual components both in Table S-2 and in the discussion that follows.

Source Characteristics

Computer codes can accommodate the spatial distribution of the contaminant source in a number of ways. The most common are:

- Point source, such as a waste drum or tank,

- Line source, such as a trench, and

- Area source, such as ponds, lagoons, or landfills.

The determination of how the spatial distribution of the source term should be modeled (i.e., point, line, or area) is dependent on a number of factors, the most important of which is the scale at which the site will be investigated and modeled. If the region of interest is very large, as compared to the contaminant source area, even sizable lagoons or landfills could be considered point sources.

The modeling objectives are also important in determining the way in which the source term should be modeled. For example, if simple scoping calculations are being performed, treating the source as a point will yield generally conservative approximations of contaminant concentrations because of limited dispersion. However, if more realistic estimates of concentrations and plume geometry are required, it will be generally necessary to simulate the source term characteristics more accurately, especially if the receptor is close to a relatively large source.

In addition to the geometry of the source, code selection is determined by whether the source is to be modeled as a continuous or time-varying release. 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 need to model the source as a constant or time-varying release primarily depends on the half-life of the radionuclide relative to the time period of interest and whether average impacts or time-varying impacts

of a release are of interest. In general, the simplest calculations, which assume a continuous release, are sufficient when determining the average annual doses to ground-water users at sites with relatively long-lived radionuclides.

Aquifer and Soil/Rock Characteristics

The most common site characteristics with regard to aquifers that influence code selection include the following:

- Confined aquifers

- Water-table (unconfined) aquifers

- Convertible aquifers

- Multiple aquifers/aquitards

- Heterogeneous aquifers

- Anisotropic aquifers

- Fractures/Macropores

- Layered soils/rocks

Recognizing when and if these processes need to be explicitly modeled is critical to the code selection process. There are no simple answers to these questions. However, the following general guidance may be helpful in making these determinations.

Confined versus Unconfined Aquifers

In most circumstances, the concern at a contaminated site is contamination of unconfined aquifers since sources of ground water generally become contaminated by leachate migrating from contaminated surface soil through an unsaturated zone of varying thicknesses to an aquifer. However, confined aquifers could be of concern at sites where contaminants were disposed in injection wells and layered sites with "leaky aquitards."

Multiple Aquifers/Aquitards

Computer codes have been developed that have the ability to simulate either single or multiple

hydrogeologic layers. Generally, a single-layer code is used if the bulk of the contamination is confined to that layer or if the difference in the flow and transport parameters between the various layers is not significant enough to warrant the incorporation of various layers. It generally does not make much sense to model discrete layers if estimated parameter values, separating different layers, fall within probable error ranges for the parameters of interest. Furthermore, unless the discrete hydrogeologic units are continuous over the majority of the flow path, it is often possible and preferable to model the system as one layer using average flow and transport properties.

Layered Soil/Rocks in the Unsaturated Zone

Rarely would soils and rocks within the unsaturated zone not exhibit some form of natural layering. The first consideration as to how this natural layering should be treated in the modeling analysis is related to whether the various soil layers have significantly different flow and transport properties. If these properties do not vary significantly from layer to layer, there would be little need for the code to have multiple-layer capability. On the other hand, if the layers have distinctive properties that could affect flow and transport, a decision needs to be made about how best to achieve the modeling objectives; i.e., should each layer be discretely treated or should all of the layers be combined into a single layer.

Macropores/Fractures

Modeling flow through the unsaturated zone is 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 water at velocities and concentrations that greatly exceed those in the surrounding matrix. Accordingly, it is critical to determine whether ground-water flow and contaminant transport at a site is dominated by macropores and fractures because this factor could determine whether a contaminant can reach the saturated zone almost immediately versus a transit time on the order of hundreds to thousands of years. This issue is especially important for radionuclides where radioactive decay in transit in the unsaturated zone

could virtually eliminate the concern over ground-water contamination.

Anisotropic/Isotropic

In a porous medium made of spheres of the same diameter packed uniformly, the geometry of the voids is the same in all directions. Thus, the intrinsic permeability of the unit is the same in all directions, and the unit is said to be isotropic. On the other hand, if the geometry of the voids is not uniform, and the physical properties of the medium are dependent on direction, the medium is said to be anisotropic.

In most sedimentary environments, clays and silts are deposited as horizontal layers. This preferential orientation of the mineral particles allows the horizontal velocity of the contaminants to greatly exceed those in the vertical direction. If anisotropy is not taken into account for the modeling analysis, the contaminants will be predicted to be more dispersed in the vertical direction than would probably be occurring in the real world. The result could be an under-prediction of the concentration of the contaminant in the centerline and an over-prediction of the contaminant concentration off-center in the vertical direction.

Homogeneous/Heterogeneous

A homogeneous unit is one that has the same properties at all locations. For example, for a sandstone, this would mean that the grain-size distribution, porosity, degree of cementation, and thickness vary only within small limits. As a result, the velocity and the volume of ground water would be about the same at all locations. In heterogeneous formations, hydraulic properties change spatially.

For example, if it is expected that the aquifer thickness will vary significantly (e.g., greater than ten percent), a computer code capable of simulating variable thicknesses is needed. If a code does not properly simulate the aquifer thicknesses, the contaminant velocities will be too large in areas where the simulated aquifer is thinner than the true aquifer thickness and too small in those regions that have too great a simulated thickness.

The ability to simulate aquifer heterogeneities may also be important during the remedial design phase of the investigation. If engineered barriers of low

permeability are evaluated as potential remedial options, it would be necessary to determine their overall effectiveness. In this scenario, it would not only be important to select a computer code that has the capability to simulate highly variable ground-water velocities but also to ensure that the sharp changes in ground-water velocities do not cause instabilities in the mathematical solutions.

Fate and Transport Processes

The transport of radionuclides will be affected by various geochemical and mechanical processes. Among the geochemical processes are adsorption on mineral surfaces and processes leading to precipi-tation. These processes are important primarily because they reduce the velocity of the radionuclides relative to the ground water (i.e., retardation), which increases the transit time to receptor locations and results in additional radioactive decay in transit.

The following summarizes the primary processes that affect the mobility and concentrations of radionuclides being transported by ground water, including:

- ! Advection
- ! Dispersion
- ! Matrix Diffusion
- ! Retardation
- ! Radioactive Decay

Advection

The process by which solutes are transported by the bulk movement of water is known as advection. The amount of solute that is being transported is a function of its concentration in the ground water and the flow rate of the ground water.

Computer codes that consider only advection are ideal for designing remedial systems (e.g., pump and treat) because the model output is in the form of solute pathlines (i.e., particle tracks) which delineate the actual paths that a contaminant would follow. Therefore, capture zones created by pumping wells are based solely on hydraulic gradients and are not subject to typical problems that occur when solving contaminant transport equations that include dispersion and diffusion.

Advective codes are also excellent in the remedial design stage for determining the number and placement of extraction or injection wells and in evaluating the effect that low permeability barriers may have on the flow system. They also tend to yield more accurate travel-time determinations of unretarded contaminants because the solution techniques are inherently more stable, and numerical oscillations, which artificially advance the contaminant front, are minimized. Another important advantage of advective codes is that the output (i.e., particle tracks) are a very effective means of ensuring that ground-water gradients, both vertical and horizontal, are consistent with the conceptual model.

Notwithstanding these advantages, advective codes have some drawbacks. The most significant of these are their inability to address adsorption and matrix diffusion. As discussed below, these processes can determine the length of time that a pump and treat system must operate before clean-up goals will be met. Without the ability to evaluate the effects that adsorption and diffusion may have on solute transport, it would be very difficult to estimate remediation times.

A second potential problem with advection-based codes is that dispersion will tend to spread contaminants over a much wider area than would be predicted if only advective processes are considered, thereby underestimating the extent of contamination. However, because dilution due to dispersion is under-accounted for, unrealistically high peak concentrations are generally obtained, which may be appropriate if conservative estimates are desired. An additional disadvantage is that pure advection-based problems result in hyperbolic instead of parabolic equations which cannot be solved numerically due to severe grid and time-step constraints.

Hydrodynamic Dispersion

In addition to advective transport, the transport of contaminants in porous media is also influenced by dispersion and diffusion, which tend to spread the solute 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, called hydrodynamic dispersion, 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 particles and also contributes to the dispersion process. Diffusion in solutions is the process whereby ionic or molecular constituents move in the direction of their concentration gradient. 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 concentrations of the contaminant.

Matrix Diffusion

The diffusion of radionuclides from water moving within fractures, or coarse-grained material, into the rock matrix or finer grained clays can be an important means of slowing the transport of the dissolved radionuclides, particularly for non-sorbing or low-sorbing soluble species.

Matrix diffusion is frequently insignificant and is often neglected in many of the contaminant-transport codes. However, a number of potential problems arise when matrix diffusion is ignored and contaminant velocities are based solely on advective-dispersive principles. For example, ground-water pump and treat remediation systems work on the premise that a capture zone is created by the pumping well and all of the contaminants within the capture zone will eventually flow to the well. The rate at which the contaminants flow to the well may, however, be very dependent on the degree to which the contaminants have diffused into the fine grained matrix (e.g., clays). This is because the rate at which they will diffuse back out of the fine grained materials may be strongly controlled by concentration gradients, rather than the hydraulic gradient created by the pumping well. Therefore, matrix diffusion can significantly retard the movement of contaminants, and, if the computer code does not explicitly account for this process, the overall effectiveness of the remediation system (i.e., clean-up times) could be grossly underestimated. Matrix diffusion processes can also lead to erroneous model predictions in the determination of radionuclide travel times, peak concentrations, and flushing volumes.

In general, matrix diffusion can be a potentially important process in silty/sandy soil which contains layers of clay or fractured rock. Through the process of matrix diffusion, the clay and rock can serve as reservoirs of contaminants that slowly leak back into the ground water over a long period of time.

Retardation

In addition to the physical processes, the transport of radionuclides is affected by chemical processes. The most important include:

- ! Sorption -- the sorption of chemical species on mineral surfaces, such as ion exchange, chemisorption, van der Waals attraction, etc., or ion exchange within the crystal structure.

- ! Ion exchange phenomena -- that type of sorption restricted to interactions between ionic contaminants and geologic materials with charged surfaces which can retard the migration of radionuclides.

A wide range of complex geochemical reactions can affect the transport of radionuclides, many of which are poorly understood and are primarily research topics. 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) 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 to the soil. Because the distribution coefficient is strongly affected by site-specific conditions, it is frequently obtained from batch or column studies in which aliquots of the solute, in varying concentrations, are well mixed with representative solids from the site, and the amount of solute removed from the water to the solid is determined.

From the perspective of model selection, virtually all computer codes explicitly address retardation through the use of retardation factors, which are derived from the distribution coefficient. The primary concern is that the retardation factors are appropriate for the site and conditions under consideration. Spacial and temporal changes in pH and the presence of chelating agents could invalidate the retardation factors selected for use at a site.

Radioactive Decay

Radionuclides decay to either radioactively stable or unstable decay products. For some radionuclides,

several decay products may be produced before the parent species decays to a stable element. These radioactive decay products may present a potentially greater adverse health risk than the parent. Accounting for the chain-decay process is particularly important for predicting the potential impacts of naturally occurring radionuclides, such as uranium and thorium, and transuranics. In considering this process over the transport path of radionuclides, one transport equation must be written for each original species and each decay product to yield the concentration of each radionuclide (original species and decay products) at points of interest along the flow path in order to estimate total radiological exposures. However, not all computer codes that simulate radioactive decay allow for ingrowth of the decay products, which may not cause a problem if the half-lives of the parent and daughters are very long (i.e., it takes a long time for the daughter products to grow in) or if the decay products are of little interest.

Multiphase Fluid Conditions

The movement of contaminants that are immiscible in water (i.e., non-aqueous phase liquids - NAPL) through the unsaturated zone and below the water table results in systems that have multiple phases (i.e., air, water, NAPL). This coexistence of multiple phases can be an important facet in many contaminant-transport analyses. However, only the water and the vapor phase are generally of concern when evaluating the transport of radionuclides. A limited number of radionuclides can form volatile species that are capable of being transported in a moving vapor or gas. Among these are tritium, carbon-14, radon-220/222, and iodine-129. Accordingly, if these radionuclides are present, vapor phase transport may need to be explicitly considered.

S.5 THE CODE SELECTION PROCESS

Given that an investigator understands the various waste/contaminant and site characteristics that need to be modeled in order to meet specific modeling objectives, there will often be several suitable computer codes that could potentially be chosen from a large number of published codes presented in the scientific literature. Ideally, each candidate code should be evaluated in detail to identify the one most appropriate for the particular site and modeling objectives. However, the resources to complete a detailed study are seldom available, and usually only one to two codes are selected based upon a cursory review of code capabilities and the experience of the modeler.

Regardless of whether a detailed or more cursory review is performed, it is important for the reviewer/investigator to be cognizant of the following factors and how they will affect code selection:

1. Code Capabilities consistent with:
   User needs
   Modeling objectives
   Site characteristics
   Contaminant characteristics
   Quality and quantity of data

2. Code Testing
   Documentation
   Verification
   Validation

3. History of Use Acceptance

The first aspect of the review concentrates on the appropriateness of the particular code to meet the modeling needs of the project. The reviewer must also determine whether the data requirements of the code are consistent with the quantity and quality of data available from the site. Next, the review must determine whether the code has been properly tested for its intended use. Finally, the code should have some history of use on similar projects, be generally accepted within the modeling community, and readily available to the public.

Evaluating a code in each of the three categories can be a significant undertaking, especially with respect to code testing. Theoretically, the reviewer should obtain a copy of the computer code, learn to use the code, select a set of verification problems with known answers, and compare the results of the model to the benchmark problems. This task is complicated, largely because no standard set of benchmark problems exists and the mathematical formulation for each process described within the code has to be verified through the benchmarking process. It is recommended, primarily for this reason, that the codes selected already be widely tested and accepted. Model validation, which involves checking the model predictions against independent field investigations designed specifically to test the accuracy of the model, would almost never be practical during the code evaluation and selection process.

The model evaluation process involves the following steps:

1. Contact the author of the code and obtain the following:

   - Documentation and other model-related publications
   - List of users
   - Information related to code testing

2. Read all publications related to the model, including documentation, technical papers, and testing reports.

3. Contact code users to find out their opinions.

4. Complete the written evaluation using the criteria shown in Table S-3.

Much of the information needed for a thorough evaluation can be obtained from the author or distributor of the code. In fact, inability to obtain the necessary publications can be an indication that the code is either not well documented or that the code is proprietary. In either case, inaccessibility of the documentation and related publications should be grounds for evaluating the code as unacceptable.

Most of the items in Table S-3 should be described in the code documentation, although excessive use of modeling jargon may make some items difficult to find. For this reason, some assistance from an experienced modeler may be required to complete the evaluation. Conversations with users can also help decipher cryptic aspects of the documentation.

The evaluation process must rely on user opinions and published information to take the place of hands-on experience and testing. User opinions are especially valuable in determining whether the code functions as documented or has significant errors (bugs). In some instances, users have performed extensive testing and benchmarking or are familiar with published papers documenting the use of the code. In essence, the evaluation process substitutes second-hand experience for first-hand knowledge (user opinions) to shorten the time it takes to perform the review.

Table S-3. Model Selection Criteria

CRITERIA
Section 5.2.1   **Administrative Data**
Author(s)
Development Objective (research, general use, education)
Organization(s) Distributing the Code
Organization(s) Supporting the Code
Date of First Release
Current Version Number
References (e.g., documentation)
Hardware Requirements
Accessibility of Source Code
Cost
Installed User Base
Computer language (e.g., FORTRAN)
Section 5.2.2   **Remedial Process**
Scoping
Characterization
Remediation
Section 5.2.3   **Site-Related Criteria**
Boundary/Source Characteristics
Source Characteristics
Multiple sources
Geometry
line
point
area
Release type
constant
variable
Aquifer System Characteristics
confined aquifers
unconfined aquifers (water-table)
aquitards
multiple aquifers
convertible
Soil/Rock Characteristics
heterogeneity in properties
anisotropy in properties
fractured
macropores
layered soils
Transport and Fate Processes
dispersion
advection
diffusion
density dependent
partitioning between phases
solid-gas
solid-liquid

CRITERIA
equilibrium isotherm:
linear (simple retardation)
Langmuir
Freundlich
nonequilibrium isotherm
radioactive decay and chain decay
speciation
Multiphase Fluid Conditions
two-phase water/NAPL
two-phase water/air
three-phase water/NAPL/air
Flow Conditions
fully saturated
variably saturated
Temporal Discretization (steady-state or transient)
Section 5.2.4   **Code-Related Criteria**
Source Code Availability
History of Use
Code Usability
Quality Assurance
code documentation
code testing
Hardware Requirements
Solution Methodology
Code Output
Code Dimensionality

SECTION 1

INTRODUCTION

1.1 BACKGROUND - PURPOSE AND SCOPE OF THE JOINT EPA/DOE/NRC PROGRAM

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

Though the joint program is concerned with all pathways, it has been determined that, due to the magnitude of the undertaking, it would be appropriate to divide the program into smaller, more manageable phases, corresponding to each of the principal pathways of exposure. It was also determined that in the first phase of the project greatest attention would be given to the ground-water pathways.

Ground-water pathways were selected for consideration first for several reasons. At a large number of sites currently regulated by the EPA and the NRC or owned by the DOE, the principal concern is the existence of, or potential for, contamination of the aquifers underlying the various sites. In addition, relative to the air, surface water, and terrestrial pathways, ground-water contamination is more difficult to sample and monitor, thereby necessitating greater dependence on models to predict the locations and levels of contamination in the environment.

The types of models used to simulate the behavior of radionuclides in ground water must be more complex than surface water and atmospheric pathway transport models in order to address the more complex settings and the highly diverse types of settings associated with different sites. As a result, the methods used to
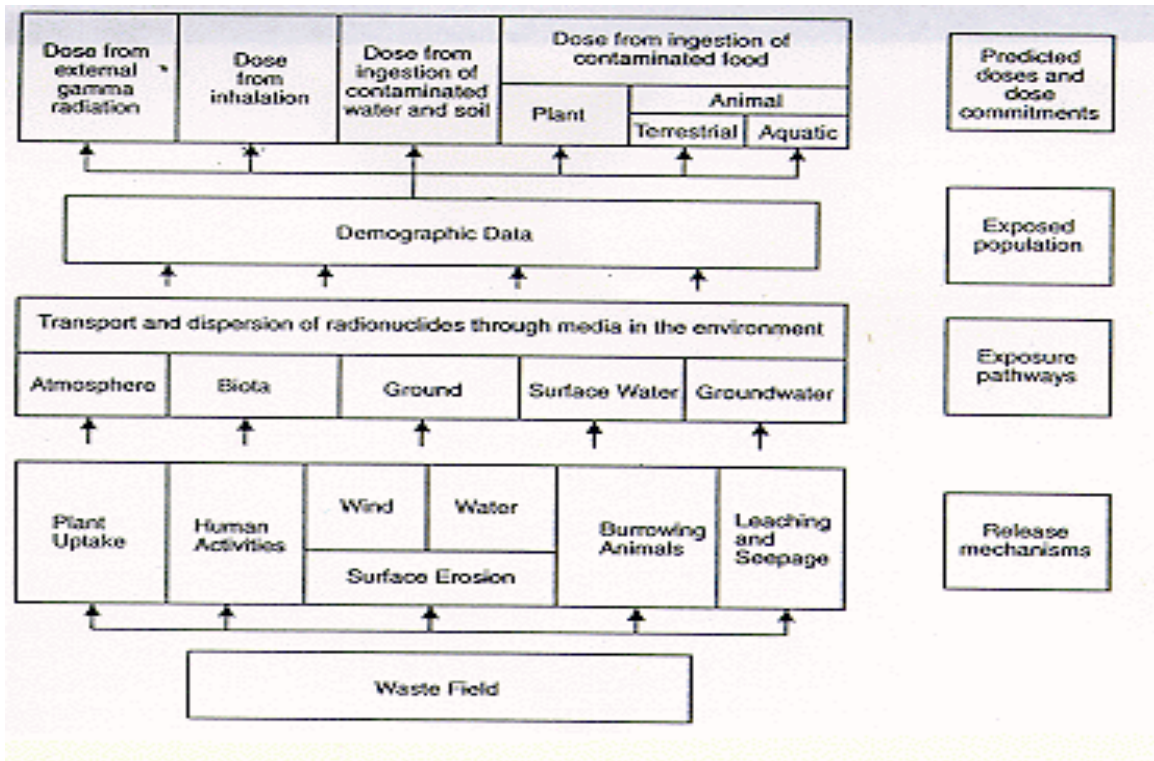

Figure 1-1. Exposure Pathways

model ground water have not been standardized to the same extent as has surface water and air dispersion modeling, and, therefore, there is considerably less regulatory guidance regarding appropriate methods for performing ground-water modeling.

In addition to pathways of exposure, the scope of Phase 1 of the joint program also considered the range of categories of sites that should be considered. The full range of sites in the United States that contain radioactive materials can be divided into the following categories:

! Federal facilities under the authority of 18 federal agencies, predominantly consisting of DOE and Department of Defense (DOD) sites and facilities, and sites listed on the National Priorities List (NPL),

! NRC and NRC Agreement State licensed facilities,

! State licensed facilities,

! Facilities and sites under the authority of the states but not governed by specific regulations. These include sites containing elevated levels of naturally occurring radionuclides (NORM).

All of these sites are of interest to the program. However, a number of categories of facilities and sites were excluded from consideration in the joint program because they are being licensed specifically to receive radioactive material for storage and disposal; i.e., licensed low-level and high-level waste storage and disposal sites. These sites are being managed within a highly structured regulatory context to receive radioactive materials, and, though models are used to support the siting and design of such facilities, they are not remedial sites.

It was also necessary to limit the range of the categories of sites of interest to the program in order to keep the number of categories of sites to a manageable size. It was determined that this phase of the project will be limited to (1) sites currently listed on the NPL that contain radioactive materials and (2) sites currently or formerly licensed by the NRC that are part of the Site Decommissioning Management Program (SDMP). The SDMP has been established by the NRC to decommission 46 facilities

that require special attention by the NRC staff.

Ground-water modeling needed to support remedial decision making at NPL sites containing radioactive materials is in many ways similar to the ground-water modeling needs of the SDMP.

These categories of sites were selected for consideration because decisions are currently being made regarding their decontamination and remediation, which, in many cases, require the use of models to support decision making and demonstrate compliance with remediation goals. Though the project is designed to address the modeling needs of these categories of sites, the information gathered on this project should have applicability to the full range of categories of sites concerned with the disposition of radioactive contamination.

In conclusion, in order to meet its mission of promoting the appropriate and consistent use of mathematical models in the remediation and restoration process at sites containing, or contaminated with, radioactive materials, this first phase of the joint program is designed to achieve the following four objectives:

1) Describe the roles of modeling and the modeling needs at each phase in the remedial process (MAU93);

2) Identify models in actual use at NPL sites and facilities licensed under RCRA, at DOE sites, and at NRC sites undergoing decontamination and decommissioning (D&D) (PAR92);

3) Produce detailed critical reviews of selected models in widespread use; and

4) Produce draft guidance for hydrogeologists and geoscientists tasked with the responsibility of selecting and reviewing ground-water flow and transport models used in the remediation, decommissioning, and restoration process.

This report fulfills the fourth objective of Phase 1 of the joint program. Specifically, this report describes a process for reviewing and selecting ground-water flow and transport models that will aid remedial decision making during each phase of the remedial process, from the initial scoping phase, to the detailed characterization of the site, to the selection and implementation of remedial alternatives.

1.2 PURPOSE AND SCOPE OF THIS REPORT

Remedial contractors, with the concurrence of the site managers, generally select and apply ground-water flow and transport models. However, unless specifically trained in ground-water flow and transport modeling, it is difficult for the site manager to participate actively in these decisions. Ground-water flow and transport modeling requires highly specialized training and experience, and, as a result, the site manager must usually depend heavily on the expertise and judgement of staff hydrogeologists as well as outside contractors and consultants. This report provides background information that should help hydrogeologists and geoscientists assist the site manager in making more informed decisions regarding the selection and use of ground-water flow and transport models and computer codes throughout the remedial process.

Previous reports in this series (MOS92, PAR92) have determined that the types of models and the processes that require modeling during the remedial process depend on a combination of the following five factors:

1. reasons for modeling,
2. contaminant waste characteristics,
3. site environmental characteristics,
4. site land use and demography, and
5. phase of the remedial process.

The principal reasons for modeling that, in part, influence model selection include: (1) development and refinement of the site conceptual model from which hypotheses may be tested, (2) the performance of risk assessments and the evaluation of compliance with applicable health and safety regulations, (3) the design of environmental measurements programs, primarily to determine the optimal location for boreholes, and (4) the identification, selection, and design of remedial alternatives. Each of these reasons for modeling influences modeling needs and model selection differently.

A review of the physical, chemical, and radiological properties of the waste at a number of remedial sites reveals that the waste characteristics can be diverse. At sites currently undergoing or scheduled for remediation, over 30 different types of radionuclides have been identified, each with its own radiological and chemical properties. The waste is found in a variety of chemical forms and physical settings, including contaminated soil, in ponds, in storage piles and landfills, buried in trenches, and in tanks and drums. Each of these physical and chemical settings influences the areal distribution of the contaminants and rate at which they may leach into the underlying aquifer, which, in turn, influences model selection.

In a similar manner, the environmental characteristics of remedial sites are highly diverse (PAR92). The sites containing radioactive materials that are currently undergoing remediation include both humid and dry sites, sites with and without an extensive unsaturated zone, and sites with simple and complex hydrogeological characteristics. These different environmental settings determine the processes that need to be modeled, which, in turn, influence the selection of models and computer codes.

The land use and demographic patterns at a site, especially the location and extent of ground-water use, affect the types and complexity of the models required to assess the potential impacts of the site on public health. At many of the sites contaminated with radioactive materials, the principal concern is the use of the ground water by current or future residents located close to, and downgradient from, the source of contamination. At other sites, the concern is the use of private and municipal wells located at some distance and in a variety of directions from the source. Each of these usage patterns influences the selection of ground-water flow and transport models and computer codes.

Superimposed on these waste and site-related issues are the different modeling needs associated with the various phases of the remedial process. The phase of the remedial process from scoping and planning, to site characterization, to remediation, creates widely different opportunities for modeling, which, together with the other factors, influences model and code selection.

This report describes the methods for selecting ground-water flow and transport models and computer codes that meet the modeling needs at sites contaminated with radioactive materials. The selection process is described in terms of the various site characteristics and processes requiring modeling and the availability, reliability, and costs of the computer codes that meet the modeling needs.

Though this report is limited to a discussion of the model selection process, it is recognized that the proper application of the selected models is as important, if not more important, than model selection. A model, no matter how well suited to a particular application, could give erroneous and highly

misleading results if used improperly or with incomplete or erroneous 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 used intelligently and with a full appreciation of the limitations of the model and the input data. It is not possible within the scope of this project to address model applications, quality control, and the presentation and interpretation of modeling results. Future reports prepared under this program will address these important topics.

1.3 PRINCIPAL SOURCES OF INFORMATION

In accomplishing its objectives, this report makes use of the information contained in the previous reports prepared on this program, including:

- ! "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.

- ! "Environmental Characteristics of EPA, NRC, and DOE Sites Contaminated with Radioactive Substances," EPA 402-R-93-001, March 1993.

- ! "Computer Models Used to Support Cleanup Decision Making at Hazardous and Radioactive Waste Sites," EPA 402-R-93-005, March 1993.

In addition, extensive use was made of:

- ! "Superfund Exposure Assessment Manual," EPA/540/1-88/001, April 1988.

- ! "Leachate Plume Management," EPA/540/2-85/004, November 1985.

- ! IMES, "Integrated Model Evaluation System," Prototype, Version 1, September 1991. Developed by Versar, Inc. for the Exposure Assessment Group, Office of Health and Environmental Assessment, Office of Research and Development, Environmental Protection Agency.

Finally, this report relies heavily on the experience gained by the project team during the review of three existing codes: RESRAD, VAM2D, and MT3D. As part of this project, these three computer codes were reviewed as if they were being considered for use on a remedial project. The review of these codes, including the process used to review these codes, has been documented in a separate report (EPA 402-R-93-005) in this series. The procedures used to perform these reviews contributed to the generic guidance presented in this report.

1.4 KEY TERMS

A glossary of terms used in this report is presented in Appendix A. In addition, an index directs the reader to the pages in the report where key terms are defined and discussed. Described below are three key terms/concepts that are fundamental to understanding the report.

Conceptual Model. The conceptual model of a site is a flow diagram, sketch, and/or 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 depicts the types of contaminants/wastes at a site, where they are located, and how they are being transported offsite by runoff, percolation into the ground and transport offsite in ground water, or suspension or volatization into the air and transport by the prevailing meteorological conditions. The conceptual model also attempts to help 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 regarding a site accumulates, the conceptual model is continually revised and refined.

Mathematical Model. A mathematical model translates the conceptual model into a series of equations which, at a minimum, describe the geometry and dimensionality of the system, initial and boundary conditions, time dependence, and the nature of the relevant physical and chemical processes. The mathematical model essentially transforms the conceptual model to the level of mathematical accuracy needed to support remedial decision making.

Computer Code. A computer code is simply a tool that is used to solve the equations which constitute the mathematical model of the site and display the results in a manner convenient to support remedial decision making.

1.5 ORGANIZATION OF THE REPORT

This report is divided into five sections. Following this introduction, Section 2 presents an overview of the types of ground-water modeling decisions facing the site remediation manager. The section is designed to help the site manager determine the role of, and need for, modeling in support of remedial decision making.

Section 3 addresses the construction of a conceptual model of a site and how it is used in the initial planning and scoping phases of a site remediation, especially as it pertains to the selection and use of ground-water flow and contaminant transport models.

Section 4 describes the various site characteristics and ground-water flow and contaminant transport processes that may need to be explicitly modeled. The purpose of this section is to help the site manager recognize the conditions under which specific model features and capabilities are needed to support remedial decision making during each phase in the site remediation process.

Section 5 summarizes the computer code attributes that should be considered for screening and selecting the potential computer codes that are best suited to meet site-specific modeling needs.

SECTION 2

MODELING DECISIONS FACING THE SITE
REMEDIATION MANAGER

A review of current regulations and guidelines pertaining to the remediation of sites on the National Priorities List and in the Nuclear Regulatory Commission's Sites Decommissioning Management Program (SDMP) reveals that fate and effects modeling is not explicitly required. However, in order to make informed and defensible remedial decisions, ground-water flow and transport modeling can be useful. This section presents a methodology for determining when ground water may be a significant pathway of exposure and discusses the roles ground-water modeling may play in support of remedial decision making. The section concludes with a discussion of the various resources available to the remediation manager to help in identifying and fulfilling modeling needs.

2.1 IS GROUND WATER A POTENTIALLY IMPORTANT EXPOSURE PATHWAY?

The ground-water pathway may be considered a potentially significant exposure pathway if: (1) the radionuclide concentrations in the ground water exceed the levels acceptable to the cognizant regulatory authorities; or (2) the contamination at the site could eventually cause the radionuclide concentrations in ground water to exceed the applicable criteria. On this basis, if the measured concentrations of radionuclides in ground water downgradient from the site, or in leachate at the site, exceed the applicable criteria, and the ground water in the vicinity of the site is being used, or has the potential to be used as a source of drinking water, it is likely that ground-water modeling will be useful, if not necessary, in support of remedial decision making at the site.

Until additional regulatory guidance is available, the drinking water standards set forth in 40 CFR 141 should guide remedial decision making. Section 1412 of the Safe Drinking Water Act (SDWA), as amended in 1986, requires EPA to publish Maximum Contaminant Level Goals (MCLGs) and promulgate National Primary Drinking Water Regulations for contaminants in drinking water which may cause any adverse effects on the health of persons and which are known or anticipated to occur in public water systems. On July 9, 1976, the EPA published "Interim Primary Drinking Water Regulations, Promulgation of Regulations on Radionuclides" (41 FR 28402).

The interim rule establishes maximum contaminant levels (MCL) for radionuclides in community water. The MCLs limit the concentration of radionuclides at the tap to:

!   5 pCi/L for Ra-226 plus Ra-228.

!   15 pCi/L for gross alpha, including Ra-226 but excluding radon and uranium.

!   that concentration of manmade beta/gamma emitting radionuclides that could cause 4 mrem/yr to the whole body or any organ.

The regulation applies to community public water systems regularly serving at least 25 persons year-round or having at least 15 connections used year-round.

In response to a need to finalize the rule, expand the regulations to include uranium and radon, and revise and refine the rule, the EPA published an Advanced Notice of Proposed Rulemaking (ANPR) on September 30, 1986 (51 FR 34836), and on July 18, 1991 the EPA issued an NPR entitled "National Primary Drinking Water Regulations; Radionuclides" (56 FR 33050). 40 CFR 191 is being finalized.

As in the interim rule, the proposed rule applies to all community, and all non-transient, non-community public water systems regularly serving at least 25 persons year-round or having at least 15 connections used year-round. The proposed standards establish the following requirements:

The Maximum Contaminant Level Goal (MCLG) for all radionuclides is zero since radionuclides are known carcinogens. MCLGs are non-enforceable health goals that are set at levels at which no known or anticipated adverse effects on the health of persons occur and which allow an adequate margin of safety.

The MCLs are as follows:

Radionuclide	MCL
Ra-226	20 pCi/L
Ra-228	20 pCi/L
Rn-222	300 pCi/L
Uranium	20 μg/L (30 pCi/L)
Beta and photon emitters (excluding Ra-228)	4 mrem/yr EDE
Adjusted gross alpha emitters (excluding Ra-226, U, and Rn 222)	15 pCi/L

MCLs are enforceable standards set as close to the MCLGs as is feasible, including economic factors. The proposed rule also establishes specific requirements regarding the use of control and treatment technologies and monitoring and reporting requirements.

The drinking water standards are fundamental health-based standards that apply to public sources of drinking water. In addition, the drinking water standards have also had extensive use as applicable or relevant and appropriate regulations (ARARs) for NPL sites. As an ARAR, if the observed concentrations of radionuclides in drinking water supplies covered by the rule exceed the MCLs, the rule applies directly and remedial actions are required. If the potential exists for ground-water contamination to exceed the MCLs, the rule is considered relevant and appropriate.

For NPL sites, the Hazard Ranking System (HRS) scoring package provides information that will help in determining if ground-water modeling is needed at a site. Specifically, Section 7.1.1 of the HRS requires the sampling and analysis of ground water to determine if ground-water contamination is present. If radionuclide concentrations in ground water in excess of background are found and exceed the Level I benchmarks delineated in Sections 2.5.2 and 7.3.2 of the HRS (these benchmarks are keyed to the MCLs), ground-water contamination is a concern at the site, and ground-water modeling will likely be needed to support the baseline risk assessment and remedial decision making.

At some sites, information may not be available regarding the levels of radionuclide contamination in ground water or leachate. Alternatively, radionuclide measurements may have been made, but yield inconclusive results. Under these conditions, an estimate needs to be made of the radionuclide concentrations in the soil or the waste at the site,

which can then be used to determine if the potential exists for exceeding the applicable criteria.

For NPL sites, the information needed to make this determination is likely to be available in the HRS scoring package addressing Hazardous Waste Quantity and Likelihood of Release. The preferred method for scoring Hazardous Waste Quantity (Section 7.2.5.1 of the HRS) requires information on the concentration of individual radionuclides at the site and the volume and area of the contamination.

Given the radionuclide concentrations in soil or waste, the radionuclide concentration in leachate can be estimated using partition factors. A partition factor establishes the equilibrium relationship between the average radionuclide concentration in soil or waste and that in leachate. If the product of the radionuclide concentrations with the appropriate partition factors results in radionuclide concentrations in leachate significantly in excess of the applicable criteria, it may be concluded that the radionuclide concentrations in ground water in the vicinity of the site could exceed the criteria, thereby requiring ground-water modeling to assess the potential impacts on nearby user locations.

Once the leachate comes into contact with the underlying soil, a new equilibrium begins to be established between the leachate and the soil. The equilibrium ratio of the radionuclide concentration in the soil to that in the water in intimate contact with the soil is referred to as the distribution coefficient (Kd). Once site-specific Kds are determined or appropriate generic Kds are identified, the radionuclide concentration in the soil divided by the Kd for each radionuclide yields a crude estimate of the concentration of the radionuclide in the soil pore water percolating through the soil.

Though partition factors are highly site specific, generic values have been used in the past for screening calculations which are designed to provide reasonable upper bound radionuclide concentrations in leachate and ground water. Examples of generic partition factors are provided in NRC86. Tabulations of Kd values that have had widespread application are provided in BAE83 and SHE90.

If either the measured or derived values for the radionuclide concentrations in ground water exceed the applicable criteria, resources need to be put into place to perform ground-water modeling.

2.2 REASONS FOR MODELING

Once it is determined that the ground-water exposure pathway is potentially important, ground-water flow and transport modeling can have a wide range of uses in support of remedial decision making. Table 2-1 presents the principal reasons for modeling on a remedial project. These uses can surface during any phase of the remedial process. However, some of these reasons are more likely to occur during specific phases of a remedial project.

In Table 2-1, scoping and planning occur early in the project, wherein regional, sub-regional, and site-specific data are reviewed and analyzed in order to define the additional data and analyses needed to support remedial decision making. In the site characterization phase, the plans developed during the scoping phase are implemented. These data are used to characterize more fully the nature and extent of the contamination at the site, to define the environmental and demographic characteristics of the site, and to support assessments of the actual or potential impacts of the site. The results of the site characterization phase are analyzed to determine compliance with applicable regulations and to begin to define strategies for the remediation of the site. In the site remediation phase, alternative remedies are identified, evaluated, selected, and implemented.

During scoping and planning, modeling can be used to identify the potentially significant radionuclides and pathways of exposure, which, in turn, can be used to support the design of comprehensive and cost-effective waste characterization, environmental measurements, and site characterization programs. During site characterization, modeling is used primarily in support of dose and risk assessment of the site and to evaluate the adequacy of the site characterization program. During the remediation phase, modeling is used primarily to support the selection and implementation of alternative remedies and, along with environmental measurements programs, is used to determine the degree to which the remedy has achieved the remedial goals.

Table 2-1 attempts to identify those opportunities for modeling that are more likely to surface during the different phases of the remedial process. In general, the remedial phase often dictates the types of remedial decisions that need to be made and the amount of site-specific information and time available to make these decisions. These, in turn, determine the role of modeling. For example, during scoping, it may not be feasible to gain access to sampling locations, and the only way to predict the potential impacts of a source of contaminants is by modeling. During site characterization, sampling locations are generally accessible; however, the contaminant may have not yet reached a receptor location. Accordingly, modeling is used to predict future impacts. During remedy selection, modeling is used to simulate the performance of a remedy in order to evaluate its cost-effectiveness and refine its design.

2.3 PLANNING FOR MODELING

2.3.1 Identifying Modeling Needs

Given the phase in the remedial process and the reasons for modeling, the types of models and the input data required to run the models are determined by the characteristics of the waste, the site hydrogeological setting and characteristics, and the current and projected ground-water use in the vicinity of the site. Accordingly, the role of and need for modeling, and the types of models and associated input data, are determined by a combination of five factors:

- ! phase of the remedial process,
- ! reasons for modeling,
- ! waste characteristics,
- ! hydrogeological characteristics, and
- ! local land use and demography.

In order to make informed decisions regarding the selection and application of ground-water flow and transport models and the interpretation of the results, the remediation manager will require site-specific information on each of these five factors. The first two factors are related and are largely determined by the regulatory structure within which remedial decisions are being made. The last three factors are of a more technical nature and usually require highly specialized expertise to relate the waste, hydrogeologic, and demographic characteristics of a site to the models suited to these characteristics and the reasons for modeling.

Table 2-1. Matrix of Reasons for Modeling

Opportunities for Modeling	Scoping[1]	Site Characterization[1]	Remediation[1]
1. When it is not feasible to perform field measurements, i.e., ! Cannot get access to sampling locations ! Budget is limited ! Time is limited	M	F	F
2. When there is concern that downgradient locations may become contaminated at some time in the future.	M	M	M
3. When field data alone are not sufficient to characterize fully the nature and extent of the contamination; i.e., ! when field sampling is limited in space and time and needs to be supplemented with models ! when field sampling results are ambiguous or suspect	M	M	M
4. When there is concern that conditions at a site may change, thereby changing the fate and transport of the contaminants; i.e., ! seasonal changes in environmental conditions ! severe weather (floods, tornadoes) ! accidents (fire)	F	M	M
5. When there is concern that institutional control at the site may be lost at some time in the future resulting in unusual exposure scenarios or a change in the fate and transport of the contaminants; i.e., ! trespassers ! inadvertent intruder ! (construction/agriculture) ! drilling, mineral exploration, mining ! human intervention (drilling, excavations, mining)	F	M	M
6. When remedial actions are planned and there is a need to predict the effectiveness of alternative remedies.	F	F	M
7. When there is a need to predict the time when the concentration of specific contaminants at specific locations will decline to acceptable levels (e.g., natural flushing).	F	M	M
8. When there is concern that at some time in the past individuals were exposed to elevated levels of contamination and it is desirable to reconstruct the doses.	F	M	F

1. **M** Denotes an important role.
    F Denotes a less important role.   2-4

Table 2-1. (Continued)

	Opportunities for Modeling	Scoping[1]	Site Characterization[1]	Remediation[1]
9.	When there is concern that contaminants may be present but below the lower limits of detection.	F	M	F
10.	When field measurements reveal the presence of some contaminants and it is desirable to determine if and when other contaminants associated with the source may arrive, and at what levels.	F	M	F
11.	When field measurements reveal the presence of contaminants and it is desirable to identify the source or sources of the contamination.	M	M	F
12.	When there is a need to determine the timing of the remedy; i.e., if the remedy is delayed, is there a potential for environmental or public health impacts in the future?	F	F	M
13.	When there is a need to determine remedial action priorities.	F	F	M
14.	When demonstrating compliance with regulatory requirements.	M	M	M
15.	When estimating the benefit in a cost-benefit analysis of alternative remedies.	F	F	M
16.	When performing a quantitative dose or risk assessment.	F	M	M
17.	When designing the site characterization program and identifying exposure pathways of potential significance.	M	F	M
18.	When there is a need to compute or predict the concentration distribution in space and time of daughter products from the original source of radionuclides.	M	F	F
19.	When there is a need to quantify the degree of uncertainty in the anticipated behavior of the radionuclides in the environment and the associated doses and risks.	M	F	F
20.	When communicating with the public about the potential impacts of the site and the benefits of the selected remedy.	M	F	M

Source: EPA93

1. **M** Denotes an important role.
    F Denotes a less important role.   2-5

Recognizing the need for modeling, and identifying and applying the models that meet these needs, unfolds as the project matures. Modeling decisions are based on site-specific information pertaining to each of the above five factors and the combined judgement of regulatory and technical specialists. Modeling decisions cannot be made in a "cookbook" fashion. Accordingly, during the initial phases of a remedial project and throughout the remedial process, the remediation manager must continually assess the need to employ models. Table 2-1 can be useful in determining when these needs exist or may arise.

Once the modeling needs are recognized, it is appropriate to determine or define the form of the results or output of the modeling exercise. The following presents the various types of output resulting from a given modeling exercise for sites containing radioactive material.

! The time-averaged and time-varying radionuclide concentrations in air, surface water, ground water, soil, and food items. These are usually expressed in units of pCi/L of water or pCi/kg of soil or food item. The time-averaged values are used to determine the annual radiation doses and risks and/or compliance with ARARs that are expressed as average, as opposed to peak values. The time-varying values are useful in determining arrival times of contaminants at receptor locations, which can help in prioritizing sites, or the impacts of accidental releases, which are often one-time, short-term occurrences.

! The radiation field in the vicinity of radioactive material, expressed in units of $\mu R/hr$. Estimates of exposure rate, whether measured or predicted, are useful in protecting members of the public or workers who may be present in, or need to enter, the radiation field.

! The transit time or time of arrival of a radionuclide at a receptor location. This measure is useful in determining at what point in the future a source of contamination has the potential to adversely affect receptors.

! The volume of water contained within or moving through a hydrogeological setting.

! Potentiometric surfaces (i.e., heads) are commonly output from ground-water flow models from which ground water/contaminant flow paths and/or capture zones can be determined.

! Radiation doses to individual members of the public under quasi-steady state and changing conditions and following accidents. The doses are evaluated for the site in its current condition (i.e., the no action alternative) and during and following a broad range of feasible alternative remedies. These are usually expressed in units of mrem/yr effective dose equivalent (EDE) for continuous exposures and mrem per event (EDE) for transients and postulated accidents. Most radiation protection standards are expressed in units of the dose to individuals.

! Radiation risks to individual members of the public under expected and transient conditions and following accidents. The risks are evaluated for the no action alternative and during and following a broad range of feasible remedies. These are usually expressed in units of individual lifetime risk of total and fatal cancers. In addition to individual dose, individual risk is used to characterize the impacts on public health and is required by the National Contingency Plan (NCP).

! Cumulative radiation doses to the population in the vicinity of the site under expected and transient conditions and following accidents. The cumulative doses are evaluated for the no action alternative and during and following a broad range of feasible remedies. These are usually expressed in units of person rem/yr (EDE) for continuous exposures and person rem per event (EDE) for transients and accidents.

! Cumulative radiation risks to the population in the vicinity of the site under expected and transient conditions and following accidents. The cumulative population risks are evaluated for the no action alternative and during and following a broad range of feasible remedies. These are usually expressed in units of total and fatal cancers per year for continuous exposures or per event for transients and accidents in the exposed population.

! Radiation doses and risks to remedial workers for a broad range of alternative remedies. The units of dose and risk for individual and cumulative exposures are the same as those for members of the public.

! Uncertainties in the above impacts, expressed as a range of values or a cumulative probability

distribution of dose and risk.

The specific regulatory requirements that apply to the remedial program determine which of these "end products" is needed. In general, these modeling results are used to assess impacts or compliance with applicable regulations; however, information regarding flux, transport times, and plume arrival times is also used to support a broad range of remedial decisions.

These modeling endpoints must be clearly defined, since the type of endpoint will help to determine the type of ground-water flow and transport model that will support the endpoint of interest. For example, a baseline risk assessment at a site contaminated with radioactive material is used in determining the annual radiation dose to an individual drinking water obtained from a potentially contaminated well. The endpoint in this case is the dose to an individual expressed in units of mrem/yr. In order to estimate this dose, it is necessary to estimate the average concentration of radionuclides in the well water over the course of a year. The models, input parameters, and assumptions needed to predict the annual average radionuclide concentration are different than those needed to predict the time-varying concentration at a given location. The latter usually requires much more input data and models capable of simulating dynamic processes.

2.3.2   Sources of Assistance

Once the remediation manager has identified the role modeling will play on the remedial project (see Table 2-1) and the forms of the results of the modeling exercise, resources must be put into place to meet these needs. These resources include access to technical expertise and a broad range of ground-water flow and transport models.

In response to the need for ground-water flow and transport modeling in support of remedial decision making, guidance and assistance are becoming increasingly available. Appendix B briefly summarizes some of the resources available to a remediation manager, organized according to the following categories:

- ! Branches and Divisions within Agencies
- ! Expert Systems
- ! Electronic Bulletin Boards
- ! Electronic Networks

2.3.2.1   Branches and Divisions Within Agencies

Environmental Protection Agency

Technical assistance available to EPA remediation managers is described in "Technical Assistance Directory," CERI-91-29, July 1991.

Nuclear Regulatory Commission

Technical assistance to NRC personnel with regulatory oversight responsibility for the decontamination and decommissioning of licensed facilities is available from the Office of Nuclear Material Safety and Safeguards (NMSS).

Department of Energy

Technical guidance for DOE and DOE contractor personnel with responsibility for environmental restoration and waste management at DOE facilities is provided through the Office of Environmental, Safety, and Health. In addition, since many of the DOE sites are on the NPL, EPA technical assistance can also be accessed.

2.3.2.2   Electronic Media

Electronic communication media are becoming a common means by which individuals participate in forums where expertise is freely shared. Institutions whose mandate includes the dissemination of expert advice and information also use these media. These forms of communication result from the direct transmittal of computer media (e.g., tape, diskette, CD-ROM, etc.) or utilize remotely accessed computer systems consisting of dedicated hardware and associated software. In remote systems, the user can access the system via modem or some other hard-wired connection and retrieve from or transmit to the system information as required.

Electronic media offer great potential to assist ground-water model users and reviewers. It is possible to classify these media into three types, namely bulletin boards (restricted access), networks (general access), and expert systems. Although the first two systems operate similarly and share some approaches to providing their services, they differ in the way that they are used. A brief overview of these instruments follows. Specific examples of these resources are presented in Appendix B.

Bulletin Boards

Bulletin boards exist at a specific location maintained by an identifiable individual or institution. Bulletin boards usually contain facilities for posting electronic mail and allow the user to participate in one or more conferences - more-or-less structured discussions on specific topics. In addition, most bulletin boards contain archives of files consisting of various data bases, executable programs, and notices.

Networks

A computer network consists of a number (in some cases many thousands) of individual computers (nodes) tied together by hardware and some network software that regulates access to the system and the transfer of information between nodes. Most network discussion groups are moderated by an individual or group of individuals. Networks can be and are used to post electronic mail in much the same way as one would post mail on a bulletin board. However, they have the additional capability of "broadcasting" information to a much more general audience. Networks are a good way to get answers to problems when the user is unsure of who might possibly provide those answers. An even more powerful aspect of some networks is the ability to run software on one of the network nodes in real-time from a

remote location with immediate feedback. Most bulletin boards don't allow that level of access.

Expert Systems

Expert systems are software packages which guide a user through the solution of a problem by asking a series of questions and/or by providing a series of pre-programmed answers to those questions. An example of such a system that can be used in the selection of an appropriate code for air, surface, or ground-water modeling is the Integrated Model Evaluation System available from the Environmental Protection Agency.

Both bulletin boards and networks are effective in obtaining non-urgent help on focused issues and for keeping up with fast-changing subjects - they are not particularly useful if the user needs information quickly or cannot phrase a question succinctly and clearly. Many bulletin boards and networks are free to the user while others are based on some fee system. Nearly all remotely accessed electronic media require some form of registration before use, either by written request and registration or by on-line registration during the user's first session. Expert systems will usually offer the fastest and most in-depth answers to specific problems. But expert systems can be quickly outdated if the data (knowledge) base on which they depend changes. The "learning curve" for all three types of electronic information exchange is fairly quick - a user can request and/or obtain useful information in a matter of minutes to hours.

SECTION 3

CONSTRUCTING AND REFINING THE CONCEPTUAL MODEL
OF THE SITE

For sites on the NPL, the development of a conceptual model of the site is identified as a specific step in the scoping stage of the RI/RS process (see EPA88). However, the need for conceptual modeling applies to any site undergoing remediation. Figure 3-1, taken from EPA88, is an example of a conceptual model. It identifies the various pathways that may contribute to the potential current and future impacts of the site on public health and the environment. Accordingly, the construction of a conceptual model of a site is the first step in determining modeling needs and identifying models that meet these needs. This section presents a brief discussion of basic concepts pertinent to the construction of a conceptual model of the site with respect to the ground-water pathway for sites contaminated with radionuclides.
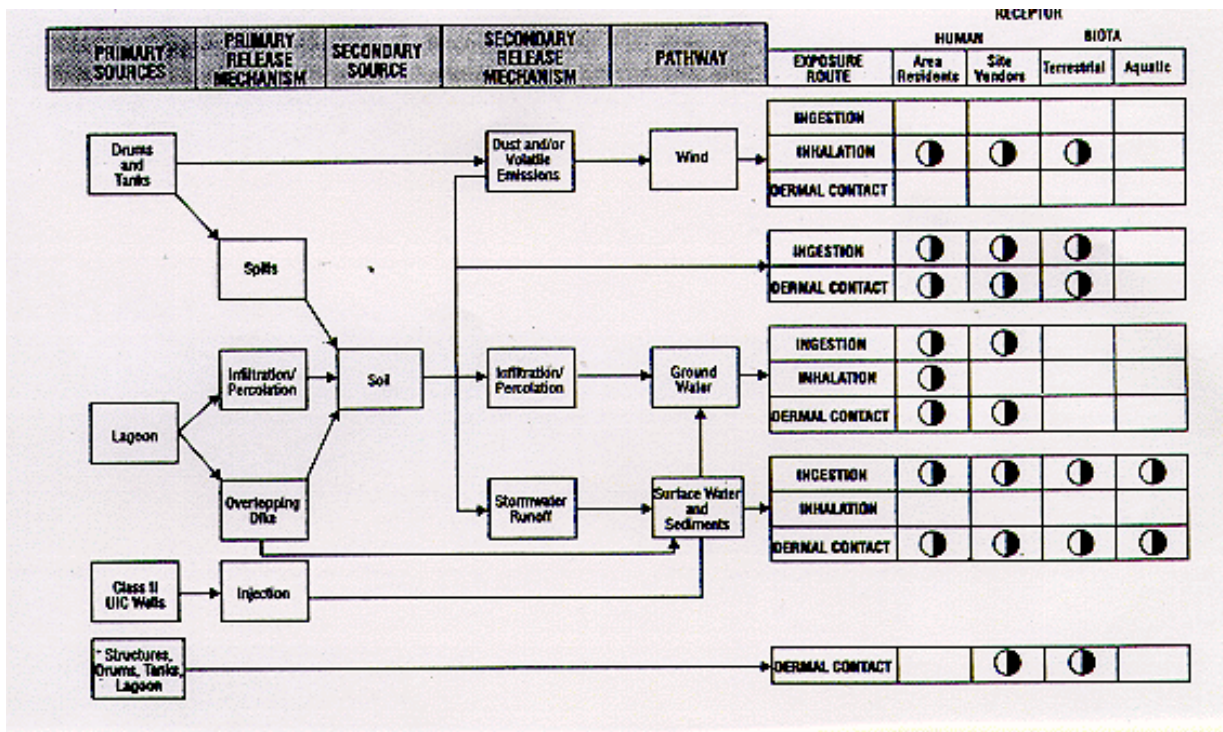

Figure 3-1. Example Conceptual Model

3.1 BASIC QUESTIONS THAT WILL NEED TO BE ANSWERED

For sites where ground-water contamination is identified as a potentially important exposure pathway, the planning effort should attempt to answer the following typical questions:

! Do the radionuclides have relatively long or short half-lives and do they have radioactive daughters?

! Do the contaminants enter the ground-water flow system at a point, or are they distributed along a line or over an area (or volume)?

! Does the source consist of an initial pulse of contaminant or is it constant over time?

! Is there a thick unsaturated zone?

! Is the lithography relatively homogeneous or does it contain multiple layers?

! How will the hydrogeology affect flow and transport?

! At what rate will the radionuclides be transported relative to ground-water flow?

! Are there nearby wells or other hydraulic boundaries that could influence ground-water flow?

! What is the nature of the system boundaries?

! Where are the current or future receptors located? Can they influence ground-water flow?

The answers to these questions will help to identify the types of processes that may need to be modeled at the site, which, in turn, will help in screening the types of models and computer codes appropriate for the site. A discussion of the various flow and transport processes and the site characteristics that influence these processes is provided in EPA88.

During the scoping phase, it will not be possible, nor necessary, to answer these questions with certainty. However, as site characterization proceeds, information will become available that will help to develop more complete answers to these questions. In fact, a well-designed site characterization program will obtain data that will help answer these questions.

3.2 COMPONENTS OF THE CONCEPTUAL MODEL FOR THE GROUND-WATER PATHWAYS

The components that make up the initial conceptual model of the site include:

1. the contaminant/waste characteristics,

2. the site characteristics, and

3. land use and demography.

As the remedial process progresses from initial scoping and planning to detailed characterization to remediation, the site characterization becomes more precise and complete. The following sections discuss each of these components of a conceptual model and how they can influence model selection.

3.2.1 Contaminant/Waste Characteristics

To the extent feasible, the site conceptual model should address the following characteristics of the waste:

! Types of radionuclides

! Waste form and containment

! Source geometry (e.g., volume, area, depth, homogeneity)

! Physical and chemical properties of the radionuclides

! Geochemical setting

Within the context of ground-water modeling, these characteristics are pertinent to modeling the source term, i.e., the rate at which radionuclides are mobilized from the waste and enter the unsaturated and saturated zones.

Types of Radionuclides

One of the most important characteristics in developing a conceptual model of the site is identifying the type and approximate quantities of the radionuclides present. This will not only determine the potential offsite impacts of the site, it will also help

to identify the potential magnitude of the risks to workers, the mobility of the radionuclides, and the time period over which the radionuclides may be hazardous. The types of radionuclides will also determine whether radioactive decay and the ingrowth of daughters are important parameters that will need to be modeled.

Waste Form and Containment

Radioactive contaminants are present in a wide variety of waste forms that influence their mobility. However, in most cases, the radionuclides of concern are long-lived, and the integrity of the waste form or container cannot be relied upon for long periods of time. Therefore, the source term is often conservatively modeled as a uniform point, areal, or volume source, and no credit is taken for waste form or containerization (EPA92).

If it is desired to model explicitly the performance of the waste form (e.g., rate of degradation of solidified waste or containerized waste) or transport in a complex geochemical environment (changing acidity, presence of chelating agents or organics), complex geochemical models may be needed. Depending on the waste form and container, such models would need to simulate the degradation rate of concrete, the corrosion rate of steel, and the leaching rate of radionuclides associated with various waste forms (i.e., soil, plastic, paper, wood, spent resin, concrete, glass, etc.). These processes depend, in part, on the local geochemical setting. However, it is generally acknowledged that it is not within the current state-of-the-art to explicitly model the geochemical processes responsible for the degradation of the waste containers or the waste itself (NRC 90).

Physical and Chemical Properties of the Radionuclides

If feasible, the conceptual model of the site should describe the radionuclides and their physical and chemical characteristics. These parameters may be pertinent to model selection because certain radionuclides have properties that are difficult to model. For instance, most of the NPL and SDMP sites are contaminated with thorium and uranium, both of which decay into multiple daughters which may differ from their parents both physically and chemically. Some of the radionuclides (e.g., uranium) exhibit complex geochemistry and their mobility is dependent

upon the redox conditions at the site. Though the chemical form of the radionuclides and the geochemical setting can have a profound effect on the transport of the radionuclides, it is generally acknowledged reliable modeling of the various geochemical processes is not often feasible. Accordingly, during the construction of a site conceptual model, detailed information regarding the chemical composition of the radionuclides may not be necessary. The degree to which this type of information will be needed to support remedial decision making will surface as site characterization proceeds.

Geochemical Setting

In addition to the standard chemical properties of radionuclides, it is important to understand the geochemical properties and processes that may affect transport of the radionuclides that are specific to the site. These properties and processes include the following:

! Complexation of radionuclides with other constituents

! Phase transformations of the radionuclides

! Adsorption and desorption

! Radionuclide solubilities at ambient geochemical conditions

If it is desired to model these processes explicitly, as opposed to using simplifying assumptions, such as default or aggregate retardation coefficients, more complex geochemical models may be needed. However, as discussed above, it is currently not often feasible to explicitly model complex geochemical processes.

3.2.2 Environmental Characteristics

The conceptual model of the site should begin to address the complexity of the environmental and hydrogeological setting. A complex setting, such as a complex lithology, a thick unsaturated zone, and/or streams or other bodies of water on site (i.e., a complex site), generally indicates that the direction and velocity of ground-water flow and radionuclide transport at the site cannot be reliably simulated using simple one-dimensional, analytical models (see Appendix C).

At more complex sites, such as many of the defense facilities on the NPL, the remedial process is generally structured so that, as the investigation proceeds, additional data become available to support ground-water modeling. An understanding of the physical system, at least at a sub-regional scale, may allow an early determination of the types of models appropriate for use at the site. Specifically, during the early phases of the remedial process, when site-specific data are limited, the following site characteristics may be extrapolated from regional-scale information and will, in part, determine the types and complexity of models required:

!   Approximate depth to ground water

!   Ground-water flow patterns

!   Lithology of the underlying rocks (e.g., limestone, basalt, shale)

!   Presence of surface water bodies

!   Land surface topography

!   Sub-regional recharge and discharge areas

!   Processes or conditions that vary significantly in time

Even at complex sites, complex computer models may not be needed. For example, if a conservative approach is taken, where transport through the unsaturated zone is assumed to be instantaneous, then the complex processes associated with flow and transport through the unsaturated zone would not need to be modeled. Such an approach would be appropriate at sites that are relatively small and where the extent of the contamination is well defined. Under these conditions, the remedy is likely to be removal of the contaminated surface and near-surface material. Examples of these conditions are many of the SDMP sites and several of the non-defense NPL sites. In these cases, the use of conservative screening models, along with site data, may be sufficient to support remedial decision making throughout the remedial process.

Depth to Ground Water

Sites located in the arid west and southwest (e.g., Pantex, Hanford, and INEL) generally have greater

depths to ground water. The simulation of flow and transport through the unsaturated zone will generally require more complex computer codes due to the non-linearity of the governing equations. Modeling of the unsaturated zone is further hampered because the necessary data are often difficult to obtain.

Ground-Water Flow Patterns

The intricacy of the ground-water flow patterns will have a significant impact on the complexity of the required modeling. The dominating factors that control the flow patterns are both the geology and hydraulic boundaries. Flow in the saturated zone will tend to be uniform and steady in hydrogeologic systems that have uncomplicated geology and boundary conditions that are relatively stable with time. Uniform flow refers to flow that is in one direction and does not vary across the width of the flow field. Steady flow does not change over time. Boundary conditions, such as constant pumping/injection and recharge from perennial lakes and streams, are generally constant over time.

Hydrogeological features that indicate that flow may be unsteady and nonuniform are areas where discrete geologic features are known to exist (e.g., faults, fractures, solution channels), as well as hydraulic boundaries which may consist of ephemeral streams, highly variable rainfall, and areas occasionally indurated by flooding.

Sub-Regional Lithology

The lithology of the underlying rocks also provides insight into the expected level of difficulty of modeling. A number of the NPL sites overlie areas where fractures are probably dominant mechanisms for flow and transport. These sites include Hanford, Idaho National Engineering Laboratory (INEL), Maxey Flats, Jacksonville, Oak Ridge, West Valley, and Pensacola Air Stations. In some cases, such as at Hanford, the fractured zone is deep below the site, and concerns regarding ground-water contamination are limited primarily to the near-surface sedimentary rock.

It is unlikely that analytical models could be used to adequately describe flow and transport in the fractured systems because radionuclide transport and ground-water flow in fractured media are much more complex than in unfractured granular porous media. For that

matter, it generally requires very specialized numerical codes to simulate flow and transport in fractured media. This is because of the extreme heterogeneity and anisotropy associated with the fractures.

Surface Water Bodies

Virtually all of the NPL sites and many of the SDMP sites have surface water bodies at or in the immediate vicinity of the site. Bodies of water often have a significant impact on the ground-water flow and can seldom be neglected in the modeling analysis. In general, analytical models are limited in their ability to simulate properly the effect that surface water bodies have on contaminant flow and transport, particularly if the surface water body behaves episo-dically, such as tidal or wetland areas. Several of the NPL sites are inundated with wetlands, including Oak Ridge, Himco, and Shpack Landfill. At least two sites, Pensacola and Jacksonville, are close to estuaries, which suggests that tidal as well as density-dependent flow and transport may be significant.

Sub-Regional Topography

The land surface topography is often overlooked in developing a site conceptual model but may be an important factor in evaluating the need for, and complexity of, ground-water modeling. Topography may significantly influence ground-water flow patterns. For instance, Maxey Flats is situated atop a relatively steep-sided plateau with a stream located at the bottom of the slope. The steep topo-graphy strongly controls the direction of ground-water flow, making it much more predictable. Furthermore, estimating the flux of ground water moving into the system from upgradient sources becomes much simpler if the area of interest is a local recharge area, such as a hill or mountain.

Steep topography can also complicate the modeling by making it more difficult to simulate hydraulic heads that are representative of the hydrologic units of interest.

Regional Recharge/Discharge

The ground-water flow paths will largely be controlled by regional and sub-regional ground-water recharge and discharge areas. It is generally necessary to ensure that the conceptual model of flow and transport on a local scale is consistent with the sub-regional and

regional scale. If the site is located in an aquifer recharge area, the potential for widespread aquifer contamination is significantly increased, and reliable modeling is essential.

3.2.3 Land Use and Demography

The site conceptual model will need to identify the locations where ground water is currently being used, or may be used in the future, as a private or municipal water supply. At sites with multiple user locations, an understanding of ground-water flow in two or three dimensions is needed in order to predict realistically the likelihood that the contaminated plume will be captured by the wells located at different directions, distances, and depths relative to the sources of contamination.

Simple analytical ground-water flow and transport models typically are limited to estimating the radionuclide concentration in the plume centerline downgradient from the source. Accordingly, if it is assumed that the receptors are located at the plume centerline, a simple model may be appropriate. Such an assumption is often appropriate even if a receptor is not currently present at the centerline location because the results are generally conservative. In addition, risk assessments often postulate that a receptor could be located directly downgradient of the source at some time in the future.

The need for complex models increases if there are a number of public or municipal water supplies in the vicinity of the source. Under these circumstances, it may be necessary to calculate the cumulative population doses and risks, which requires modeling the radionuclide concentrations at a number of specific receptor locations. Accordingly, off-centerline dispersion modeling may be needed.

SECTION 4

CODE SELECTION - RECOGNIZING IMPORTANT MODEL CAPABILITIES

The greatest difficulty facing the investigator during the code selection process is not determining which codes have specific capabilities, but rather which capabilities are actually required to support remedial decision making during each remedial phase at a specific site. This section is designed to help the remediation manager and support personnel recognize the conditions under which specific model features and capabilities are needed to support remedial decision making.

4.1 INTRODUCTION

The influence that site and code related characteristics have on code selection can be both global in nature as well as very specific and exacting. For this reason, this section is divided into two distinct parts. The first part addresses general considerations of the code selection process. The discussion provides an overview of how the code selection process is influenced by the interdependency between the modeling objectives and the site and code characteristics. The second part of the section focuses primarily on specific considerations related to the code selection process. The discussion provides the information necessary to determine which specific site characteristics need to be explicitly modeled and when attempting to model such characteristics is impossible, unjustified, or possibly even detrimental to the modeling exercise.

4.2 GENERAL CONSIDERATIONS - CODE SELECTION DURING EACH PHASE IN THE REMEDIAL PROCESS

Successful ground-water modeling must begin with the selection of a computer code that is not only consistent 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. There are no fail-safe methods for selecting the most appropriate computer code(s) to address a particular problem. However, the entire process of code selection can be relatively straightforward if it is given adequate attention early in the project development.

One of the primary goals of mathematical modeling is to synthesize the conceptual model, as discussed in section 3, into mathematical expressions, which, in turn, are solved by selecting an appropriate computer code. This section discusses how the different components of the conceptual model, in conjunction with the modeling objectives, influence the modeling approach and ultimately the selection of the most appropriate computer code.

The underlying premise of this section 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 sophisticated models.

Table 4-1 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 selection mistakes are selecting 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 typical 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 need to be considered which involve the underlying assumptions in the selection of a modeling approach and the physical processes which are to be addressed. If the modeler is not practical, sophisticated codes are 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.

Table 4-1. General Modeling Approach as a Function of Project Phase

Attributes	Scoping	Characterization	Remediation
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	One-Dimensional	1,2-Dimensional/Quasi-3-Dimensional	Fully 3-Dimensional/Quasi-3-Dimensional
Boundary and Initial Conditions	Uncomplicated Boundary and Uniform Initial Conditions	Non-Transient 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

One should begin with the simplest code that would satisfy the objectives and progress toward the more sophisticated codes until the modeling objectives are achieved.

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 that are available in the early stage of the remedial process may limit the modeling to one or two dimensions. In certain cases, this may be sufficient to support remedial decision making. If the modeling objectives cannot be met in this manner, additional data will be needed to support the use of more complex models. The selection of more complex models in the later phases often depends on the modeling results obtained with simpler models during the early phases.

Generally in the later phases of the investigation, sufficient data have been obtained 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 the respective phase of the project. All too often modeling is performed without developing a clear rationale to meet the objectives, and only after the modeling is completed are the weaknesses in the approach discovered.

The modeling objectives must consider the decisions that the model results are intended to support. The selected modeling approach should not be driven by the data availability, but by the modeling objectives which should be defined in terms of what can be accomplished with the available data. It is important to keep in mind that the modeling objectives should be reviewed and possibly revised during the modeling process. Furthermore, ground-water modeling should not be thought of as a static or linear process, but rather one that must be capable of continuously adapting to reflect changes in modeling objectives, data needs, and available data.

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

The following discusses computer code selection during each phase of the remedial process. The emphasis is placed on the processes and assumptions inherent in the mathematical models used in computer codes. The discussion is organized according to the factors delineated in Table 4-1.

4.2.1   Scoping

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 using 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. How-ever, at relatively simple sites, early remediation decisions can be made, thereby avoiding the unneces-sary delays and costs associated with a possibly pro-longed site characterization and modeling exercise.

A large part of code selection in the early phase of the investigation is understanding the project decisions that need to be made, and, of these, which can be assisted through the use of specific codes under the constraints of both limited data and an incomplete understanding of the controlling hydrogeologic processes at the site. It is not always necessary to select a computer code or analytical method that is consistent with all aspects of the conceptual model. It is often useful to model only certain components of the conceptual model. 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.

Because general trends, rather than accuracy, are most important during the scoping phase, a computer code or analytical method would need to be capable only of accommodating the following:

! Conservative Approximations

! Steady-State Assumptions

! Restricted Dimensionality

! Uncomplicated Boundary and Initial Conditions

! Simplified Flow and Transport Processes

! System Homogeneity

These model attributes generally translate to modeling approaches that are consistent with the available data during the scoping phase. They are discussed in greater detail in the following sections.

4.2.1.1   Conservative Approximations

In the scoping phase of the investigation, the objectives are generally focused 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 a number of parameters and flow and transport processes which typically would not have been fully characterized in the early phase of the investigation. The parameters include recharge, hydraulic conductivity, effective porosity, hydraulic gradient, distribution coefficients, aquifer and confining unit thicknesses, and source concentrations. Questions during the early phases regarding flow and transport processes are typically limited to more 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).

One of the most useful analyses at this point in the remedial program is to evaluate the potential effects of the controlling parameters on flow and transport. One objective of the early analyses is to assess the relationship 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 would assist in properly focusing the site characterization activities and ensuring that they are adequately scoped. Obviously, it would also be desirable to evaluate the effects that various processes

would have on controlling flow and transport; however, this would generally have to be deferred until additional information is obtained during site characterization. Furthermore, some caution is needed in that 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 parameter variations.

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 of interest. At this phase in the remedial process, it is important to select a modeling method where individual parameter values can be systematically selected from the parameter range and easily substituted into the governing mathematical equations which 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 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. It is important to ensure that the range of individual parameter values and parameter combinations selected allow for a conservative analysis of the flow and transport processes.

In many cases, the possible range of values of important parameters is unknown or very large. As a result, 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 can also be used incorrectly. For example, individuals not familiar with the scoping process could come to grossly inappropriate conclusions regarding the potential public health impacts of the site based on the results of scoping analyses. 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 the detailed sensitivity analysis is a conservative bounding approach. In this less demanding analysis, values are selected from the parameter range 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 distribution coefficients would tend to maximize the predicted contaminant migration rates although the concentrations at receptors may be underestimated.

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

Other processes that could render an otherwise conservative analysis with erroneously optimistic results 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 be predicted by their respective distribution coefficients. Furthermore, discrete features are rarely considered in early analyses, even though it is well known that discrete features, such as soil macropores, can allow contaminant movement on the order of meters per year in the vadose zone. The result could be 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 scoping phase. Therefore, the potential exists that what would normally be considered conservative modeling results are actually underestimating the contaminant velocities and concentrations. This possibility highlights the need for confirmation of modeling results with site-specific field data even if a conservative approach has been undertaken.

As far as code selection is concerned, three basic choices are available: analytical, semi-analytical, or numerical codes (Appendix C). 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 (Section 4.3.2.1). Several analytical models are set up specifically for performing sensitivity analyses.

In contrast, numerical methods do not lend themselves to the same kind of "simplified" applications. The primary reasons are that numerical models are difficult to set up, require a large amount of data input to calibrate the model, and multiple parameter substitutions are generally very cumbersome. However, the bottom line is that simply not enough data exist in the early phases of a remedial project to construct and perform defensible numerical modeling.

4.2.1.2 Steady-State Solutions

In the scoping phase, the data that are generally available have been collected over relatively short time intervals. Therefore, modeling objectives would be limited to those which could be met without a detailed understanding of the temporal nature of processes affecting flow and transport. For example, a typical analysis that would not require 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 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 be associated with a high degree of uncertainty.

Analytical transport solutions are generally able to simulate only systems that assume steady-state flow conditions, but, 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.

4.2.1.3 Restricted Dimensionality

Ground-water flow and contaminant transport are seldom constrained to one or two dimensions. However, during scoping, modeling objectives must take into account that there is rarely sufficient information 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, two-dimensional areal analyses may be appropriate.

Figures 4-1 through 4-4 may be useful in visualizing the differences between one-, two-, and three-dimensional modeling. In one-dimensional modeling, the radionuclide concentration is predicted in the plume centerline in the x direction, and no information is provided on the radionuclide concentration in the y or z direction (Figure 4-1).
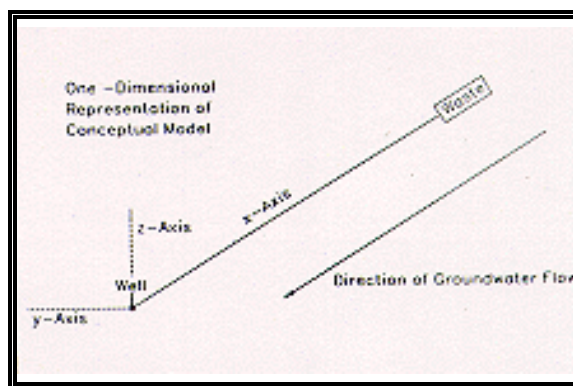
Figure 4-1.   One-Dimensional Representation of Conceptual Model

In two-dimensional cross-sectional models for the unsaturated zone, the radionuclide concentration is calculated for the x and z direction and it is assumed to be the same at any slice through the plume in the y direction (Figure 4-2).
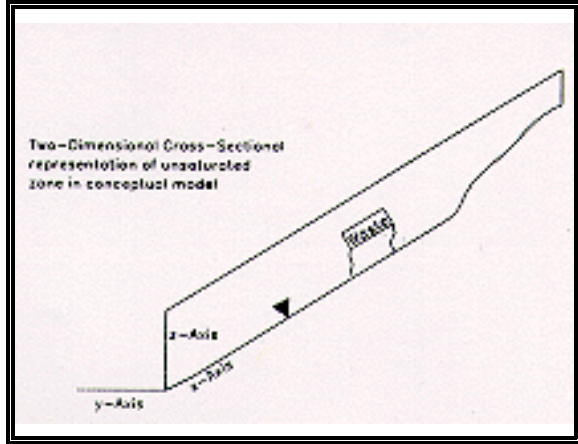
Figure 4-2.   Two-Dimensional Cross-Sectional Representation of Unsaturated Zone in Conceptual Model

In saturated zone areal models, the radionuclide concentrations are predicted for the x and y directions, but it is assumed the radionuclide concentration is the same in any slice in the z direction (i.e., the concentration at any location is the same at all depths) (Figure 4-3).
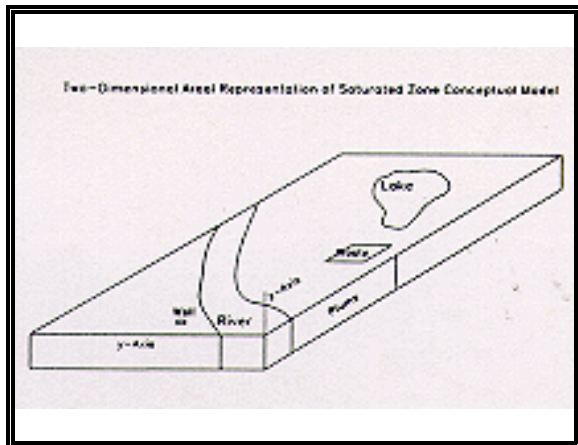
Figure 4-3.   Two-Dimensional Areal Representation of Saturated Zone Conceptual Model

Cross-sectional modeling of the saturated zone in which flow is assumed to be in the lateral and vertical

directions (e.g., transverse flow is ignored) may also be performed. A quasi-three-dimensional modeling approach is also commonly used when vertical components of flow within aquifers are deemed unimportant. This approach assumes that ground-water flow through any confining units that separate aquifers is in only one dimension (i.e., vertical). Furthermore, flow within the aquifers is two dimensional (i.e., vertical flow component is ignored). In this manner, the effects of the hydraulic interconnection among interbedded aquifers and confining units can be simulated without having to rely on fully three-dimensional models.

Three-dimensional models will calculate the radionuclide concentrations at any x, y, z coordinate, taking into consideration the variations in the lithography and hydrogeology in three dimensions (Figure 4-4).
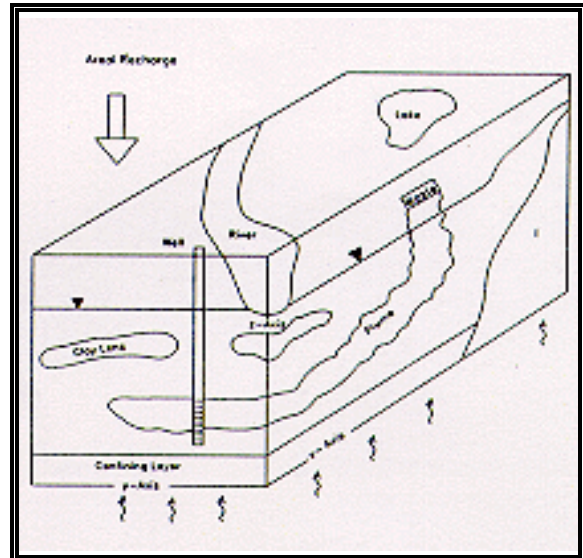
Figure 4-4.   Three-Dimensional Representation of Conceptual Model

A typical three-dimensional problem would be one which would be designed to evaluate the geometry of hypothetical capture zones if one or more extraction wells were planned for the remediation of the ground water. The vertical ground-water gradient that would be artificially created by the pumping wells, as well as the induced vertical leakage from overlying and underlying hydrogeologic units, would be very important to consider in this analysis. If this leakage were not accounted for, the effectiveness of the remedial system would be substantially overestimated

because the radii of the capture zones would be too large.

As a general rule, analytical methods, which can be performed on a hand-held calculator, are developed for predicting concentrations along the centerline of the plume and are limited to one dimension. Two- and three-dimensional analyses are customarily performed with the assistance of a digital computer. Although analytical solutions are available for two- and three-dimensional analysis, the limitations that are placed upon the solution techniques are so severe that they can be used only to simulate gross system behavior. Therefore, the three-dimensional example provided above could not be satisfactorily addressed by an analytical model because of computational limitations, such as simple boundary conditions and uniform geology. However, attempts to circumvent the limitations of analytical methods at this phase by adopting numerical methods would only complicate the problem for reasons previously discussed, as well as now having to provide parameter estimates in the second or third dimension.

At this phase, the question is not really whether to use analytical or numerical methods but rather how many dimensions should be included in the analytical

modeling. The advantages of adding a second or third dimension must be carefully weighed against the further complications of performing the sensitivity analysis which provides the real strength behind the application of analytical methods.

4.2.1.4 Uncomplicated Boundary and Uniform Initial Conditions

Boundary conditions are the conditions the modeler specifies as known values in order to solve for the unknowns in the problem domain (Figure 4-5). 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, rainfall, 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 which are initially assumed to be present in the area of interest.

Governing equations that describe ground-water flow and contaminant transport and associated boundary and initial conditions may be solved either analytically or numerically. Analytical solutions are preferable because they are easily adapted to sensitivity analyses; however, in most cases, analytical methods are not possible because of irregularly shaped boundaries and heterogeneity of
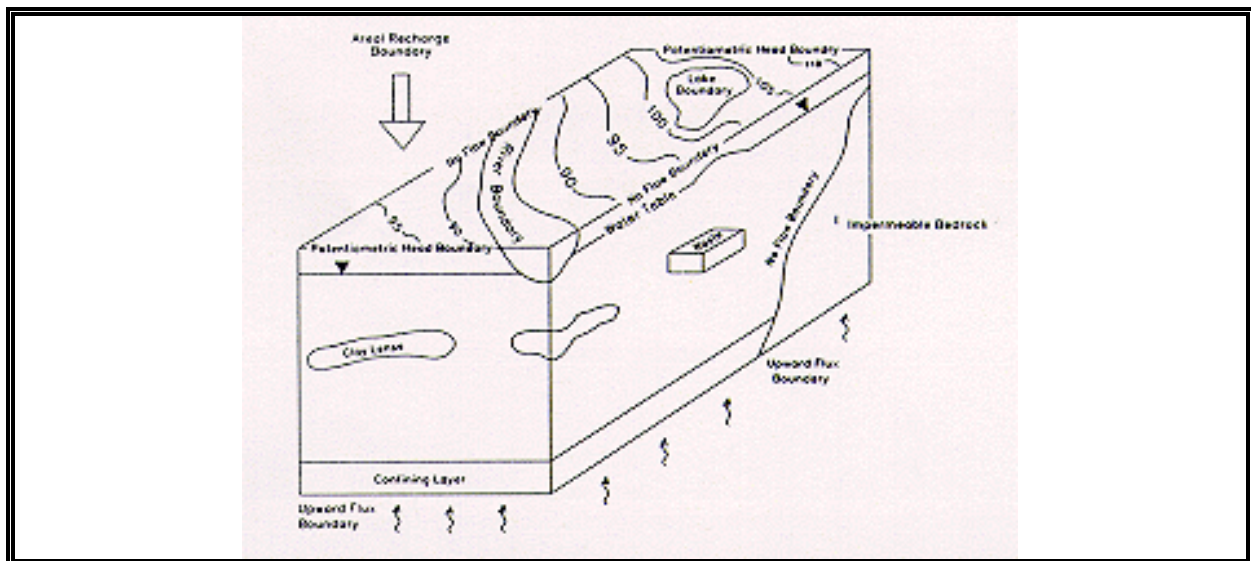

Figure 4-5.   Typical System Boundary Conditions

both the geology and flow field. If very few data are available for the site, it would be very unlikely that reliable ground-water elevations and flow volumes could be assigned to calculate the unknowns in the domain of a numerical model. Furthermore, the boundary conditions in the numerical model are not supposed to be subject to radical adjustments and are generally excluded from detailed sensitivity analyses. In contrast to numerical methods, analytical methods are conducive to testing and evaluating both the boundary and initial conditions. In fact, analytical methods do not require that boundary values be known and assigned for the planes and surfaces that surround the modeled region. However, this is also a limitation of analytical methods in that, if boundary conditions vary within the problem domain, they cannot be adequately simulated.

The lack of site-specific data available in the scoping phase will generally not allow a good definition of the system boundary and initial conditions; therefore, the objectives will be confined to very limited calculations of approximate travel distances and contaminant concentrations.

Most analytical models will not accommodate non-uniform boundary or initial conditions. Therefore, if the domain includes areas where recharge is variable or a lake or stream exhibits strong effects on the flow field, analytical modeling will not provide good agreement with the overall system behavior. It follows that, if the flow field is uniform, which can generally be described with simple uniform boundary conditions, analytical models provide a better method for testing the boundary conditions than do numerical methods. However, the true nature of the flow field cannot be determined until the site is characterized.

4.2.1.5 Simplified Flow and Transport Processes

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

However, the effects of dilution due to the lateral spreading of the plume over a uniform flow field can be considered as well as the radionuclide half-lives.

Discrete features, such as macropores, fractures, and faults, would generally have to be neglected for the flow and transport analysis, and distribution coefficients would be selected from literature values judged to be conservative. Movement through the unsaturated zone would be simulated with simplified versions of more complex equations describing the unsaturated flow and transport.

Unless there were sufficient data to prove to the contrary, it would be assumed that the flow field was uniform, and, at this time, there would be few advantages to selecting a numerical model over an analytical one. Analytical methods do exist that describe the flow and transport of radionuclides through fractures. However, the fracture-flow modeling would have to be performed as a sensitivity analysis, as the information to adequately describe the geometry of the fractures would seldom be available before site characterization.

4.2.1.6 Uniform Properties

Homogeneity describes a system where all of the characteristics 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, if, for example, an otherwise homogeneous sandstone aquifer has a greater hydraulic conductivity in the horizontal direction than in the vertical. Therefore, hydrogeologic units may have anisotropic qualities but still be considered uniform throughout, provided the anisotropy does not vary within the unit.

Prior to site characterization, only the most general assumptions may be made regarding the relative flow properties of the aquifers. For example, as a rule of thumb, 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.

Except for some radial flow problems, almost all available analytical solutions belong to systems having a uniform steady flow. This means that the magnitude and direction of velocity throughout the system are invariable with respect to time and space, which

requires the system to be homogeneous and isotropic with respect to thickness and hydraulic conductivity. Therefore, analytical methods will not allow the simulation of flow and transport through layers of aquifers and aquitards. Furthermore, if there is a divergence from these uniform properties within the aquifer, such as direction flow properties of buried stream channels, analytical models would be unable to simulate the effect that these features would have on flow and transport. However, it is unlikely that this detailed information would be available prior to the site characterization program.

4.2.2   Site Characterization

The primary reasons for ground-water modeling in the site characterization phase of the remedial process are to: (1) refine the existing site-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 many instances, the unsaturated zone.

A properly designed site characterization program will expand the data base to enable very specific and often demanding objectives to be addressed. To meet the more rigorous requirements, the simplified modeling approaches undertaken in the scoping phase give way to more sophisticated means of data evaluation. However, this added sophistication and heightened expectations also convey far more complications in selecting the proper modeling approach. As discussed previously, the two general types of modeling options that could be selected during the site characterization program include analytical and numerical modeling methods.

In many instances, several different modeling approaches will be taken to accomplish the objectives at a particular phase in the investigation. 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. It must always be kept in mind that, regardless of the phase of the remedial process, the simplest modeling approach that meets the modeling objectives should be taken.

The site characterization program is the first time in the investigation where flow and transport processes are identified and investigated. Prior to site characterization activities, the investigator could only evaluate the effects of various parameter values on flow and transport. In the scoping phase, the modeling focuses on parameter estimations rather than on the effects that geochemical and physical flow mechanisms could have on the fate and transport of contaminants. Examples of these mechanisms include processes related to fractures, density dependence, phase transformations, and changes in the geochemical environment.

It is important during the site characterization to gain an appreciation for the governing geochemical processes, as these reactions may have a significant impact on the transport of contaminants and can be simulated indirectly in the analysis by assuming a specified amount of contaminant retardation. 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 a better understanding of the hydrogeology is achieved, the modeling approach and code selection become more involved. Without the data limitations that constrained the choice of methods to those of an analytical nature in the scoping phase, the number of possible alternatives in the modeling approach and code selection process increases significantly.

Rather than examine many of the available computer codes and their inherent limitations and capabilities, the following discussion addresses the rationale for adopting a modeling approach that will be consistent with the objectives. This is important because it is relatively easy to determine the various attributes of the existing computer codes; however, it is far more difficult to understand the relevance of these attributes as they apply to a specific site and the modeling objectives.

The following subcategories, keyed to Table 4-1, are analogous to those presented in the scoping phase. Because the modeling objectives of the site characterization phase differ from those of the scoping phase, the approach to modeling is also different.

Basically, analytical methods will be replaced by numerical methods in order to use less restrictive and more realistic assumptions. The following discussions provide an overview of the concepts, terminology, and thought processes necessary to facilitate the model and computer code selection process. The modeling approach in the site characterization program will generally be based upon the following:

- ! Site-Specific Approximations

- ! Steady-State Flow/Transient Transport

- ! Multi-Dimensional

- ! Constant Boundary and Non-uniform Initial Conditions

- ! Complex Flow and Transport Processes

- ! System Heterogeneity

Obviously, if the site characterization activities discover that the system is very simple and the objectives can be addressed with analytical modeling, an approach similar to that outlined in the scoping phase can be taken.

4.2.2.1 Site-Specific Approximations

In the scoping phase of the investigation, the 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.

Many of the objectives defined for the site characterization phase of the investigation cannot be met solely with conservative analyses. If parameter values are not known, it may be necessary to make conservative estimates; however, the implications that a conservative approach may have on other aspects of the remedial program must also 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 and may underestimate the contaminant concentrations at downgradient receptors. Furthermore, 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 the formulation of a more specific site-conceptual model will have on the modeling approach is that now parameter ranges have been narrowed by additional data acquisition, and sensitivity analyses can become more focused. This parameter value refinement diminishes the need to perform a multitude of sensitivity analyses. In conjunction with the increased demand to more accurately simulate the controlling flow and transport processes, the primary advantages of analytical models are superseded by their inability to simulate more complex conditions. Therefore, the model selection process is reduced to determining which numerical model will best suit the objectives.

4.2.2.2 Steady-State Flow/Transient Transport

The data obtained during the site characterization program are generally collected over relatively short time intervals and frequently do not reflect the temporal nature of the hydrogeologic system. Unfortunately, objectives that need to be addressed during the site characterization phase often involve the prediction of temporal trends in the data. For instance, the risk assessment would generally include an analysis of the peak arrival times of radionuclides at downgradient receptors. This incompatibility between the objectives and data availability 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 will generally assume a steady-state flow field and accommodate the transient nature of the system through the contaminant transport analysis. Steady or transient leaching rates would be used in conjunction with the existing plume concentrations for initial conditions. Therefore, the system is actually modeled as a steady flow system and 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 are when records are available pertaining to the volumes of radioactive liquids that were dumped over time into absorption trenches or when correlations between rainfall events and source leaching rates may be extrapolated.

Analytical methods are able only to simulate systems that assume steady-state flow conditions, although some analytical codes will allow for the simulation of a transient source term. Therefore, analytical methods can be used to simulate the temporal nature of the contaminant plumes to predict probable maximum concentrations and contaminant arrival times. However, other limitations within the analytical codes often preclude their use during the site characterization phase.

Almost all of the numerical transport codes written for radioactive constituents are able to simulate constant radionuclide source terms with radioactive decay. However, if the simulation of a pulse-like source term is desired, special care is needed to ensure that this capability has been written into the code. Otherwise, the source release would have to be manually simulated using a code that models a single pulse in an iterative fashion for each separate pulse.

4.2.2.3 Multi-Dimensional

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 rationale 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 a 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 to meet 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, much of the modeling performed for site characterization will be on a scale where the vertical components of flow are usually 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 at different depths provide excellent information on the vertical 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 support a base-line risk assessment. Again, this example illustrates that the decision on how many dimensions to include in the modeling must be tied back to the objectives and the need to be aware of the limitations imposed upon the results if one or more dimensions are eliminated.

The recent development of more sophisticated pre- and post-processors greatly facilitate 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, there are far more concerns associated with constraining the analysis to two dimensions than including the third dimension, even if many of the parameters in the third dimension have to be estimated.

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.

The objectives for most characterization programs will be met only by modeling approaches and models that are multi-dimensional. Analytical models do exist that are two- and three-dimensional, but they have very little versatility and would rarely suffice in meeting complicated objectives. Furthermore, the likelihood that analytical methods could be effectively used in the remedial design and evaluation are even more remote. Therefore, numerical methods should almost always be

chosen if detailed analysis is required to meet the site characterization objectives.

There are numerous two- and three-dimensional flow and transport codes to describe the saturated zone. However, only a handful of three-dimensional codes exist that describe flow and transport through the unsaturated zone. A number of codes exist that are generally three-dimensional; however, certain transport properties (e.g., dispersion) within these codes are simulated in only two dimensions. Special attention should be given to ensure that the controlling flow and transport processes are described in the number of dimensions desired to meet the objectives.

Code selection should not only take into account the required dimensionality of the site characterization analysis, but also the projected modeling needs of the remedial design and evaluation phase. It is much easier to use a code with three-dimensional capability for a two-dimensional analysis and later expand to the third dimension than it is to set up a three-dimensional code from output obtained from a separate two-dimensional model.

4.2.2.4 Constant Boundary 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; (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.

The most common contaminant-source type boundaries either specify the source concentration or prescribe the mass flux of contamination entering the system. The concentration is generally prescribed when the release rate is largely controlled by the solubility limits of the contaminant. 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 the source to radioactively decay. The ability of the code to treat source decay may not be important if the parents and daughters have a relatively long half-life when 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, the 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 are solely dependent 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 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 fully describing and simulating the contaminant plume(s).

Analytical models are written for very specific boundary conditions and uniform initial conditions. In essence, this means that the boundary conditions cannot vary spatially and, in most instances, only one type of boundary condition can be accommodated. Furthermore, analytical methods do not allow for the contaminant source concentrations to change through time and the measured plume values (i.e., non-uniform initial conditions) cannot be input directly to the model. Understandably, these restrictions would impose significant limitations on analyzing the data collected during the site characterization program.

Numerical models are broadly designed to adapt to many different types of boundary geometries and initial conditions. Non-uniform initial conditions for a single contaminant plume can almost always be varied spatially, depending upon the dimensionality of the code.

The ability of numerical models to handle complex boundaries and non-uniform initial conditions bestow a versatility to the analysis which should be compatible with the objectives. This approach is consistent with the principles behind coupling the sophistication of the modeling with that of the existing knowledge base.

4.2.2.5 Complex Flow and Transport Processes

Site-specific information describing the flow and transport processes which dominate the migration of radionuclides would not have been available during the scoping phase of the investigation. As the site characterization activities progress, greater attention is focused upon the physical, chemical, and biological processes that are affecting ground-water flow and contaminant transport. Up until this time, the attention has been placed primarily upon estimating parameter ranges and variances within these ranges via the 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. The means by which this parameter-based approach is expanded is 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 present, each of these processes can invalidate the output of models that are based on the assumption that uniform flow and transport are occurring through a homogenous porous media.

It is still likely that all of the geochemical reactions that affect the radionuclide transport would be lumped together into the 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 utilize geochemical models in order to explicitly address specific geochemical reactions by relying upon thermodynamically based geochemical models.

Movement through the unsaturated zone could be simulated in a number of different ways depending upon the objectives. If the unsaturated zone is relatively thin and travel times are short, it may be that simplified versions of more complex equations describing the unsaturated flow and transport would 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 in this fashion can it be assured that data are sufficient to perform modeling at the necessary level of complexity. All too often, limitations within the data, rather than the modeling objectives, drive the sophistication of the modeling.

Analytical methods are not well suited to simulate complex flow and transport processes. Further, even numerical methods do not satisfactorily describe some flow and transport processes. These processes include facilitative transport and non-Darcian flow, which are discussed in section 4.3.

4.2.2.6 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 the accurate simulation of heterogeneous rocks is required to meet the modeling objectives, analytical methods would be inappropriate as they assume the rocks to all have the same properties. In contrast, most numerical codes allow for zones with different porous rock properties; however, relatively few codes can simulate discrete features, such as faults, fractures, solution features, or macropores. Numerical codes vary from one another in their ability to simulate sharp contrasts in rock properties. For example, many codes would have a problem arriving at a solution (i.e.,

convergence) if very impermeable rocks dissected highly permeable rocks. Therefore, if the site was situated in an alluvial flood plane bordered by low permeability bedrock, special care would be needed to select a code that will not have numerical convergence problems caused by permeability contrasts.

In selecting a computer code to be applied during the site characterization, consideration should also be given to what scenarios may be modeled during the remedial investigation. If a low-permeability slurry wall or sheet pile cut-off walls may be installed, it would be important that the computer code be able to simulate these features through permeability contrasts.

4.2.3 Remedial Phase

As the site investigation proceeds into the remedial phase, data are acquired that will assist in the identification of feasible remedial alternatives. These data, in combination with models, are used to simulate the flow and transport in support of the selection, design, and implementation of the remedial alternatives. The data and models are used to predict the behavior of ground-water flow and the transport of radionuclides and thereby aid in the selection and design of the remedy and demonstrate that the selected remedy will achieve the remedial goals.

The modeling objectives associated with remedial alternative design are generally more ambitious than those associated with the site characterization phase of the remedial process. Therefore, it is often necessary either to select a computer code with more advanced capabilities, or modify the existing model in order to simulate the more complex conditions inherent in the remedial design. The following are specific examples of processes that may not be important to the baseline risk assessment and 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);

- the capability to move from confined to unconfined conditions (pump and treat); and

- ability to simulate complex flow conditions (pumping wells, trenches, injection wells).

From a modeling standpoint, the remedial design is the most challenging phase of the remedial investigation. Frequently, it is the first time in the process that sufficient data are available to enable the model predictions to be verified. The very nature of many of the 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 and enable the model to become a very powerful management tool.

The following describes modeling during the remedial phase of the investigation. The modeling approaches taken at various sites would generally have the following characteristics in common:

- Remedial Action Specific

- Transient Flow and Transport

- Multi-Dimensional

- Prescribed Boundary and Non-uniform Initial Conditions

- Specialized Flow and Transport Processes

- System Heterogeneity

4.2.3.1 Remedial Action Specific

As the site characterization process comes to an end and the Remedial Design and Selection Phase is entered, data have been acquired which will define the remedial alternatives. 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 their 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

- Biotic
  - 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

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 geochemical environment

! Determination of the alteration of the physical rock properties that govern flow and transport

! 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. 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)

! Chemical
  - ion-exchange barriers

! Biotic
  - 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 be due to cracking, hydrofracturing, tunnelling 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 that would be consistent with simulating the effects that flow barriers would have on the fate and transport of radionuclides are closely tied to the ability of the code to accommodate a number of factors, including: 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

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 disbursed by the wind. The technologies that are most commonly applied to remove solid, liquid, and vapor (e.g., tritium) radionuclides include the following:

- Physical
  - soil excavation (solid)
  - pump and treat (vapor)
  - in-situ vaporization (liquid)

- Biotic
  - 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 relatively 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

- Biotic Properties and Processes
  - physical injection and withdrawal of the biomass
  - microbial population modeling

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. Specific examples of how these considerations are tied into the modeling approach are provided in the sections that follow.

4.2.3.2 Transient Solutions

The data that are available by the time the remedial design phase is entered usually span a relatively long time frame, which often allows the temporal nature of

the hydrogeologic system to be relatively well defined. If this is the case, the remedial design objectives could involve many criteria that could not have been met during the modeling activities in the site characterization phase. Many of these additional criteria of the design phase objectives may require that the code have the capability to perform transient flow and transport simulations. This capacity would be necessary to evaluate the effectiveness of a number of remedial alternatives. One such alterna-tive would be the placement of earthen covers and a broad range of natural and synthetic barriers, which are engineered to establish a cap over surface and subsurface soil. One of the objectives of the cover is to prevent rainwater from percolating through contaminated soil and carrying radionuclides to the ground water. In the site characterization program, the objectives were such that they could probably have been met by assuming constant areal recharge over the modeled area. However, this steady-state approach would not account for recharge rates which vary through time, which would be needed to simulate the deterioration of the cap and the subsequent effect on the radionuclide leaching rates.

Soil excavation of radioactively contaminated soil will result in some amount of residual radioactivity remaining in the soil contiguous to the removal operations. It could also result in the redistribution of 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.

4.2.3.3 Multi-Dimensional

The need to perform three-dimensional modeling during the remedial phase will largely depend upon what remedial alternatives are under consideration and how the effectiveness of the selected alternative 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. Under many circumstances, the vertical ground-water gradients, prior to these imposed stresses, would be several orders of magnitude less than the horizontal gradients and,

therefore, could be ignored in a one- or two-dimensional flow analysis. However, when the hydraulic gradients are significantly altered by imposed stresses, three-dimensional flow fields generally develop. Without the capability to simulate the actual flow field in three dimensions, it would be very difficult to effectively determine capture zones and influent contaminant concentrations. This is largely because vertical leakance from units above and below the screened interval of the extraction well would be ignored as well as vertical concentration gradients.

Another remedial alternative that generally creates three-dimensional flow fields are physical barriers to ground-water flow. Whether the barriers consist of grout injection techniques, sheet pile cutoff walls, or bentonite slurry walls, all of these procedures will have a common problem which is that the hydraulic head will build up behind the structures and induce vertical gradients allowing ground water to flow under the barriers. In these cases, the analysis of vertical flow is essential in determining probable leakage rates and the volume of water that would potentially flow through the structure.

4.2.3.4 Transient Boundary and Non-Uniform Initial Conditions

Most of the modeling analysis up until the remedial phase can be performed with constant boundary conditions. This means that physical features within the modeled area, such as the water elevations of surface water bodies and areal recharge, can be simulated with values that remain constant with time. Once the remedial phase is reached, however, the modeling objectives may require that the transient nature of these boundaries are incorporated into the analysis, and time-weighted averages may no longer be applicable. For instance, water bodies, such as radioactively contaminated waste lagoons, would probably have been treated as constant boundaries during the site characterization modeling, 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 through time. This would be done by prescribing the boundaries of the

lagoon(s) to change with time in order to simulate the expected extraction rates.

The ability to prescribe boundaries within the model would also 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 through time to reproduce the effects that various rates of flushing would have on the ground-water flow and contaminant transport.

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 from the source of contaminants. If properly designed and emplaced, barriers to flow can last for several decades, barring any geological disturbances, such as tremors, ground settling, significant changes in hydraulic gradients, etc. However, if a barrier should fail following installation, water may infiltrate the site, and contaminated leachates may move beyond the site. Therefore, the effects that the failure of a barrier would have on contaminant flow and transport should be evaluated through modeling. There are a number of ways that the failure of the barrier could be simulated. 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 and behind the barrier. Therefore, a code selected for this simulation should have the capability to incorporate transient boundaries.

4.2.3.5 Specialized Flow and Transport Processes

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

As mentioned previously, numerical models that satisfactorily couple ground-water flow and contaminant transport to complex geochemical reactions simply do not exist. The complex geochemical models are based upon the laws of thermodynamics, which means that they predict whether the potential exists for a particular reaction to

occur within a closed system. Despite many shortcomings inherent within the methods for analyzing complex geochemical reactions, it is important that the controlling geochemical reactions be examined, possibly in laboratory benchscale or field studies. This is particularly important when physical/chemical stabilization processes are under consideration whereby physical or chemical agents are added to, and mixed with, a waste (typically sludge in pits, ponds, and lagoons), with the objective of improving the handling or leaching characteristics of the waste destined for land disposal.

A detailed understanding of the geochemistry can also be very useful in estimating leach rates for uranium mill tailings which otherwise would be associated with possibly 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 rocks where diffusion governs contaminant transport rather than advection and dispersion. Pump and treat systems will 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 contaminant movement will be based solely upon ground-water velocities rather than the diffusion term. Ground-water velocity will generally move the contaminant much more rapidly than diffusion, and clean-up times may be dramatically underestimated.

In-situ vitrification (ISV) of soils is a thermal treatment and destruction process that achieves stabilization by converting contaminated soil and wastes into chemically inert, stable glass and crystalline products, resembling obsidian. Predicting the effectiveness of ISV and its implementability would require a number of specialized processes to be modeled. One such process would be vapor transport of radionuclides, such as tritium, which would be an important health consideration if the media were to be heated.

A mechanism that appears to affect the transport of radionuclides under some conditions is microbial fixation. Radionuclides may be immobilized and/or mobilized by organisms or plants. Immobilization may occur if radionuclides are incorporated in 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. Modeling of microbial processes requires a code that, at a bare minimum, allows a degradation rate to be assigned to the contaminant(s).

4.2.3.6 System Heterogeneity

The ability of a code to accommodate severe contrasts in soil and rock properties is particularly important during the design and evaluation of 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 would be important that the code allow the incorporation of multiple stratigraphic layers as well as sharp hydraulic conductivity contrasts. Only in this manner could the effect on contaminant flow and transport due to the effects of leakage through the barrier wall and basement strata be evaluated.

4.3 SPECIFIC CONSIDERATIONS

The purpose of this section is to guide the Remediation Manager and support personnel in determining what specific capabilities are needed from a computer code to address the modeling objectives. The discussion focuses on explanations as to how specific site and code characteristics will provide the information necessary to decide whether various code attributes could potentially assist in the analysis or be detrimental to the analysis, or whether they are simply unnecessary.

After the conceptual model is formulated and the modeling objectives are clearly defined in terms of the available data, the investigator should have a relatively good idea of the level of sophistication that the anticipated modeling will require. It now becomes necessary to select one or more computer code(s) that have the attributes necessary to describe mathematically the conceptual model at the desired level of detail. This step in the code selection process requires detailed analysis of the conceptual model to determine the degree to which specific waste and site characteristics need to be explicitly modeled.

Fundamental questions that need to be answered at this stage in the code selection process are presented in Table 4-2. In answering these questions, the investigator must decide whether a particular code has

the required capabilities and the importance of individual aspects of the conceptual model in the modeling analysis. It is generally relatively straightforward to ascertain whether a code has a specific capability, and many documents are already available which provide this kind of information. It is far more difficult to decide whether or not a certain attribute of a model is needed to accomplish the modeling objectives. Furthermore, other factors must be considered in the code selection process which are independent of the waste, site characteristics, and modeling objectives. These factors are inherent in the individual computer codes and include: solution methodology, availability of the code, hardware requirements, usability of the code, and the degree to which the code has been tested and accepted.

Accordingly, this section has two goals:

1. to describe the detailed waste and site characteristics and flow and transport processes that may need to be explicitly modeled in order to achieve the modeling objectives, and

Table 4-2. Questions Pertinent to Model Selection

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Site-Related Features of Flow and Transport Codes

Source Characteristics

    Does the contaminant enter the ground-water flow system at a point, or is it distributed along a line or over an area?

    Does the source consist of an initial pulse of contaminant, is it constant over time, or does it vary over time?

    Is the contaminant release solubility controlled?

Soil/Rock Characteristics

    Are anisotropy and heterogeneity important?

    Will fractures or macropores influence the flow and transport?

    Are discrete soil layers relevant to the analysis?

Aquifer System Characteristics

    What type of aquifers does the model need to simulate? Confined, unconfined, or both?

    Does the model need to simulate complete dewatering of a confined aquifer?

    Does the model need to simulate aquitards?

    Does the model need to simulate the dewatering and resaturation of an aquifer?

    Do multiple aquifers need to be accounted for?

Transport and Fate Processes

    Which transport and fate processes need to be considered in the analysis (e.g., retardation, chain decay reactions, matrix diffusion)?

Multiphase Fluid Conditions

    Are all of the wastes miscible in water?

    Is the gas phase important to the analysis?

    Are density effects important?

Flow Conditions

    Will flow be under fully saturated or partially saturated conditions?

</div>

Table 4-2. (Continued)

<div style="border:2px solid black; padding:1em;">

Code-Related Features of Flow and Transport Codes

Time Dependence

    Are the fluctuations in the hydrogeologic system significant, requiring transient analyses, or can they be ignored and simulated as steady state?

Solution Methodology

    How will the various mathematical methods used to solve the flow and transport equations affect the model results and therefore code selection?

    What will be the hardware requirements?

Code Geometry

    In how many dimensions is the code capable of modeling the representative flow and transport processes?

Source Code Availability

    Is the code publicly available?

    If not, how much does it cost and is the source code available?

Code Testing

    Has the code been verified?

    Has the code been field-validated?

    Has the code been independently peer reviewed?

Code Input and Output

    What input data parameters are required?

    Does the code have a pre- or post-processor?

    Will the code provide breakthrough curves?

    How will the output depict plume extent?

</div>

2. to describe the characteristics inherent in a computer code that could influence the practical usefulness of the code, including the usability of the code and the extent to which the code has been tested.

Once these two objectives are accomplished, the code selection process becomes simply identifying the codes that meet the modeling needs.

In light of these goals, this section is divided into two parts, one addressing the site-related characteristics and the other addressing code-related characteristics that must be considered when selecting a code. Table 4-3 presents a matrix relating various site characteristics and an example of codes that explicitly model those characteristics. Table 4-4 presents a matrix relating various code characteristics and an example of codes that have those characteristics. The following sections discuss the conditions and circumstances under which the various characteristics are important.

Referring to Tables 4-3 and 4-4, it is not the intention of this section to construct comprehensive reference tables listing all available codes, but rather to provide tables that clearly illustrate the criteria generally considered in the identification of candidate computer codes. Each of the criteria is discussed individually in context to its relevance in answering the questions identified in Table 4-2.

Once one or more computer code(s) are identified as potential candidates, the codes should undergo further review as a cross-check to ensure that the code has the capabilities that are specified in the literature. Furthermore, a more detailed review can provide valuable insight into the nuances of the code which are generally not available from cursory code reviews.

4.3.1 Site-Related Characteristics

The general components of the conceptual model that need to be considered when selecting an appropriate computer code are the following:

- ! Source Characteristics
- ! Aquifer and Soil/Rock Characteristics
- ! Transport and Fate Processes
- ! Fluid Conditions
- ! Flow Conditions

Each of these topics is presented as a major heading in Table 4-3. These broad subjects are further divided into their individual components both in the table and in the discussion that follows.

The objective of the subsequent presentation is not only to discuss the relevance that each of the site- related characteristics may have to the code selection process, but also to provide criteria to determine whether a particular attribute of a code will be important in the analysis.

4.3.1.1 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 is a general lack of data that characterize the nature and extent of the contamination as well as the release history. Computer codes can accommodate the spatial distribution of the contaminant source in several ways. The most common are the following:

- ! Point source
- ! Line source
- ! Areal source

Each of these source types can have an associated release mechanism in which either the mass flux or concentration is specified. The two general types of source-term boundary conditions include the following:

- ! Concentration is prescribed
- ! Contaminant mass flux is prescribed

Source Delineation

The determination of how the spatial distribution of the source term should be modeled (i.e., point, line, or area) depends on a number of factors, the most important of which is the scale at which the site will be investigated and modeled. If the region of interest is very large, when compared with the contaminant source area, even sizable lagoons or landfills could be considered point sources.

Typically, a point source is characterized by contaminants entering the ground water over a very small area relative to the volume of the aquifer (e.g., injection well). Line sources are generally used

Table 4-3. Site-Related Features of Ground-Water Flow and Transport Codes

Section 4.3.1.1	Source Characteristics
	Point Source
	Line Source
	Areally Distributed Source
	Multiple Sources
	Specified Concentration
	Specified Source Rate
	Time-Dependent Release
Section 4.3.1.2	Aquifer and Soil/Rock Characteristics
	Confined Aquifers
	Confining Unit(s)
	Water-Table Aquifers
	Convertible Aquifers
	Multiple Aquifers
	Homogeneous
	Heterogeneous
	Isotropic
	Anisotropic
	Fractures
	Macropores
	Layered Soils
Section 4.3.1.3	Fate and Transport Processes
	Dispersion
	Advection
	Matrix Diffusion
	Density-Dependent Flow and Transport
	Retardation
	Non-linear Sorption
	Chemical Reactions/Speciation
	Single Species First Order Decay
	Multi-Species Transport with Chained Decay Reactions
Section 4.3.1.4	Multiphase Fluid Conditions
	Two-Phase Water/NAPL
	Two-Phase Water/Air
	Three-Phase Water/NAPL/Air
Section 4.3.1.5	Flow Conditions
	Fully Saturated
	Convertible Aquifers
	Variably Saturated/Non-Hysteretic
	Variably Saturated/Hysteretic
Section 4.3.1.6	Time Dependence
	Steady-State
	Transient

Table 4-4. Code-Related Features of Ground-Water Flow and Transport Codes

Section 4.3.2.1	Geometry 　　　　1-D Vertical/Horizontal 　　　　2-D Cross Sectional 　　　　2-D Areal 　　　　Quasi 3-D (Layered) 　　　　Fully 3-D
Section 4.3.2.2	Source Code Availability 　　　　Proprietary
Section 4.3.2.3	Code Testing and Processing 　　　　Verified 　　　　Field-Validated 　　　　PC-Version 386-SR486 　　　　Pre and Post Processors
Section 4.3.2.3	Model Output 　　　　Contaminant Mass/Rate of Release to Ground Water 　　　　Contaminant Plume Extent 　　　　Contaminant Concentration as a Function of Distance 　　　　As a Function of Depth from Surface 　　　　Continuously Distributed in Space 　　　　Average at Selected Points or Cells 　　　　Profiles at Selected Points Over Time
Appendix C	Solution Methodology 　　Analytical 　　　　Approximate Analytical 　　　　Exact Analytical 　　　　Semi-Analytical 　　Numerical 　　　　Spatial Discretization 　　　　　　Finite Difference 　　　　　　Integrated Finite-Difference 　　　　　　Finite Element 　　　　　　Method of Characteristics 　　　　Temporal Discretization 　　　　　　Explicit 　　　　　　Implicit 　　　　　　Mixed Implicit-Explicit 　　　　Matrix Solvers 　　　　　　ADIP 　　　　　　Direct Solution 　　　　　　Iterative ADIP 　　　　　　SOR/LSOR/SSOR 　　　　　　SIP

when the contaminants are entering the aquifer over areas where the length of the source greatly exceeds its width, such as leaking pipes or unlined trenches. Areal sources are often associated with agricultural applications of fertilizers and pesticides. Uranium mill tailings would also frequently be treated as an areal source for modeling purposes.

In some instances, it may be desirable to model multiple contaminant source areas. This would be particularly important if cumulative health effects are to be determined or if the extent and nature (e.g., commingling of various contaminant plumes) of contamination will have a significant impact on the remedial design. It is possible, however, to perform multiple-source modeling with codes that do not inherently allow the incorporation of multiple sources. The most common approach to accomplishing this objective is to perform a series of simulations in which each model run assumes only one source. The output from each of the successive model runs is subsequently cumulated into a representative multiple-source site model.

The number of dimensions (i.e., one, two, or three) that will be explicitly modeled will tend to impose limitations on how a contaminant source can be modeled.

A point source can be simulated with either a one-, two-, or three-dimensional model, whereas a line or areal source must be modeled with either a two- or three-dimensional model. One-dimensional codes are constrained to simulating contaminant sources as points. The following four factors will determine whether the source should be modeled as a point, line, or area source:

    !   Modeling objectives

    !   History of waste disposal activities

    !   Distribution of contaminants

    !   Fate and transport processes

The modeling objectives are probably the single most important factor in determining the way in which the source term should be modeled. One-dimensional simulations of point sources will yield generally conservative approximations of contaminant concentrations because of limited dispersion.

Therefore, if the modeling objective is to determine maximum peak concentrations arriving at downgradient receptors, area and line sources could be simulated as point sources comprised of average or peak concentrations. However, if more realistic values of concentrations and plume geometry are required, it will generally be necessary to simulate the source term characteristics more accurately.

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 dispersed over a larger area and discarded in many different forms. The presence of product and waste lines immediately suggests that line 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 the nature of their source. Contaminants that are wide-spread and of similar concentrations suggest an area source, while narrowly defined areas of contamina-tion indicate a more localized or point source.

Dominating fate and transport processes should also be considered when assigning source term characteristics. If flow and transport properties are strongly confined to one or two dimensions, as in the unsaturated zone (i.e., liquids flow down vertically due to gravity in the unsaturated zone), it may be possible to use a more simplified approximation of the source geometry (e.g., point).

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.

It is generally preferable to pose the source-term release in terms of contaminant mass flux, rather than specified concentrations. This is true even if the concentration at the source is known. The primary problem with specifying the concentration of the contaminants entering the system is that care must be taken to ensure that the total mass that enters the system does not exceed that which would actually be available from the source. Furthermore, specified concentrations tend to over-predict contaminant concentrations near the source because the effects of dilution and dispersion are not properly accounted for. However, it is not uncommon for specified concentrations to be used if the release of the contaminant is controlled by its solubility limit; that is, if the contaminant is relatively insoluble. The rationale for this approach is that specified concentrations would tend to describe leaching rates that are solubility controlled.

Not all computer codes allow the concentration or mass of a continuous release to change with time. This quality is particularly important if it is suspected that conditions in the past or future are not approximated by those of the present. A specific example would be modeling the performance of an engineered barrier whose performance is expected to change with time.

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

Computer codes have been developed that can simulate single or multiple aquifers which may behave as confined, unconfined, or change from one condition to another. Intrinsic characteristics of the aquifers and aquitards, which control flow and transport, are also simulated to various degrees by computer codes. The most common code selection criteria with regard to aquifers and their characteristics include the following:

- ! Confined aquifers

- ! Water-table (unconfined) aquifers

- ! Multiple aquifers/aquitards

- ! Heterogeneous

- ! Anisotropic

- ! Fractures/macropores

- ! Layered soils/rocks

<u>Water-Table and Confined Aquifers</u>

The ground water flowing within a water-table aquifer is in immediate contact with the atmosphere and is directly recharged through the overlying unsaturated zone. This water-table surface is equal to atmospheric pressure and 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 (Figure 4-6).

A confined aquifer is one in which the ground water is isolated from the atmosphere by some geologic feature (e.g., confining unit). As a result, the ground water is under pressure greater than that of atmospheric, and, if a well penetrates a confined aquifer, the water in the well will rise above the top of the aquifer.

In most circumstances, the water first encountered beneath the site will be under water-table conditions. However, this does not always mean that water levels measured in wells are indicative of the water-table

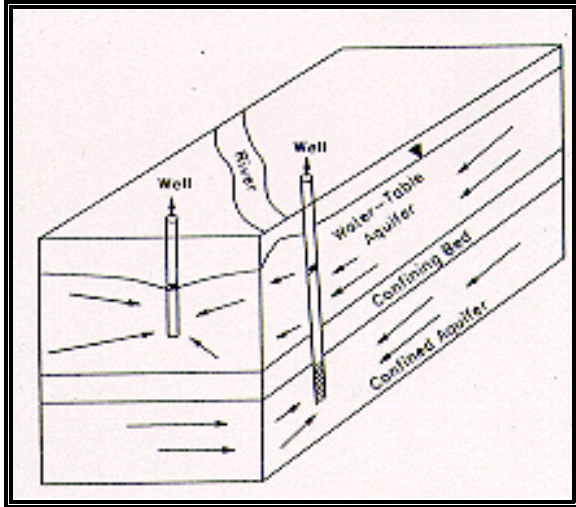**4.3.1.2 Aquifer and Soil/Rock Characteristics**

Figure 4-6.   Water Table and Confined Aquifers

surface. This discrepancy may occur when a well is screened below the water table in an unconfined aquifer with large vertical gradients (or a well with a very long screen in an unconfined aquifer with large vertical gradients). In many instances, particularly with domestic wells, water in the shallow water-table aquifer has been cased off and a deeper unit, that may be under confined conditions, is supplying water to the well. The importance of this is that the water in a well that taps a confined aquifer can rise significantly higher in the well than the true water-table surface. If this is the case, the thickness of the unsaturated zone may be significantly underestimated.

The mathematical description for ground-water flow in a water-table aquifer is more complex than that for flow in a confined aquifer. This is largely because the saturated thickness of a water-table aquifer will vary with time and, therefore, the transmissivity (which is the quantity of volume of water flowing through the aquifer, mathematically calculated as the product of the hydraulic conductivity and the vertical thickness of the aquifer) is also time dependent. Confined aquifers always remain saturated and, therefore, the mathematics do not have to account for a varying transmissivity.

Computer codes that simulate confined aquifers can also be used to simulate water-table conditions if the saturated thickness of the aquifer is not expected to vary by more than ten percent over the time of interest. This assumption would generally be appropriate if the

modeling objectives can be met by assuming steady-state conditions. If significant changes (greater than ten percent) in the water-table elevation are expected over the time of interest, not only would a steady-state modeling approach be of uncertain value, but the validity of applying a computer code designed to simulate confined flow to problems that involve unconfined flow would be questionable.

The importance of whether the system is under steady state or transient conditions dictates that the length of the time of interest needs to be carefully considered in context of the code applicability. In general, the shorter the time of interest the more likely it is that fluctuations of the water table will exceed ten percent of the saturated thickness. As the length of the time of interest increases, long-term averages tend to dampen out the extremes within the water-table fluctuations.

Examples of conditions where a code developed for confined conditions would probably not be applicable to simulate ground-water flow in water-table aquifers include:

!   Highly variable recharge rates

!   Ephemeral effects of surface-water bodies

!   Remediation activities

!   Physical properties of the contaminants

Shallow ground-water flow systems that are recharged primarily from percolating precipitation tend to be strongly influenced by seasonal fluctuations of the local climate. Summer droughts and spring snow melts can cause dramatic shifts in the water-table elevation. For reliable seasonal predictions, computer codes would have to be able to simulate changes in the aquifer transmissivity through time. Such is not the case if the use of long-term recharge averages could be justified, as when estimating average annual radiation doses associated with the drinking water pathway.

In many cases, water-table aquifers are closely tied to surface-water bodies which are ephemeral in nature. These surface-water bodies may include intermittent and ephemeral streams, waste lagoons, and tidal marshes. It is important that the transient effect of these features on the water table be considered when selecting an appropriate computer code.

Remediation activities may also create large oscillations of the water table. Activities that include active remediation, such as pump and treat, artificial recharge, and ground-water injection will generally have the greatest impact on the ground-water table. Relatively passive remediation activities, such as ceasing the disposal of liquids into lagoons or streams, may also affect the shallow aquifer by causing the water table to find a new equilibrium which may or may not be significantly different from the initial position.

A special consideration for modeling water-table aquifers, particularly when the aquifer is being significantly dewatered, as in pump and treat operations, is that not all computer codes with the capability to simulate water-table aquifers have the capacity to resaturate the aquifer if it becomes completely dewatered. This could pose a serious limitation if one of the objectives is to evaluate the effectiveness of a pump and treat system that is operated intermittently.

In determining whether a computer code that does not simulate water-table conditions is appropriate, some consideration needs to be given to the nature of the contaminants. For example, the flow of LNAPL (contaminants less dense than water, such as oil) is complicated by the rise and fall of the water table within the seasons. As the water table falls, the layer of mobile contaminant also falls. When the water table rises, the contaminant also rises. However, residual contamination is left behind in the saturated zone. If the water table rises faster than the contaminant can rise, "pockets" of free contaminants might become left below the water table. The flow of water and contaminants is controlled by Darcy's law and depends upon the effects of density, viscosity, and relative permeability. Depending upon these factors, either the contaminant or the water could have a greater velocity as the water table rises and falls. Therefore, in order to predict remediation times accurately, the volume of the contaminant remaining in the unsaturated zone needs to be estimated. If the code does not allow the water table to rise freely within the aquifer, the interaction between the contaminant and the water table cannot be simulated.

Relatively few computer codes have been developed that will simulate conditions within an aquifer that are changing from confined conditions to water-table conditions. This capability is particularly useful for simulating a ground-water system where a confined aquifer will be heavily pumped and potentially dewatered.

Multiple Aquifers/Aquitards

Computer codes have been developed that can simulate either single or multiple hydrogeologic layers (Figure 4-6). Generally, a single-layer code is used if the bulk of the contamination is confined to that layer or if the difference of the flow and transport parameters between the various layers is not significant enough to warrant the incorporation of various layers.

In deciding whether there is a significant difference in the flow and transport properties between various layers, the investigator should keep in mind that the parameter values that could vary from layer to layer include: hydraulic conductivity, effective porosity, distribution coefficients, and bulk densities. In most instances, effective porosities, distribution coefficients, and bulk densities are estimated from the literature and could have a large associated error. Hydraulic conductivities, which are typically measured in the field, also may be off by an order of magnitude. Therefore, it generally does not make much sense to model discrete layers if estimated parameter values, separating different layers, fall within probable error ranges. Furthermore, unless the discrete hydrogeologic units are continuous over the majority of the flow path, it is often possible to model the system as one layer using average flow and transport properties.

The greater the depth to which the system is modeled, the more likely it will be that aquifers of varying characteristics will be encountered. Ideally, the depth to which the system should be modeled is the depth at which ground-water gradients become consistently vertically upward. This depth will define the basement flow of the shallow system, and most contamination would be confined to shallower depths unless contaminants are being driven downward against the ambient ground-water flow by density gradients.

If very little information is available on the distribution of vertical gradients, a general rule that is often useful in estimating the relative base of the flow system is that discharge areas (e.g., perennial streams, lakes, and swamps) are associated with upward gradients, while recharge areas (e.g., mountains and uplands) are typified by downward gradients. Thus, it is more

likely that the vertical extent of contamination is greater when the contaminant source is located in a recharge area than in a discharge area.

Layered Soils/Rocks in the Vadose Zone

Rarely would soils and rocks within the vadose zone not exhibit some form of natural layering. The first consideration as to how this natural layering should be treated in the modeling analysis is related to whether the various soil layers have significantly different flow and transport properties. If these properties do not vary from layer to layer, then there would be little need for the code to have multiple-layer capability. On the other hand, if the layers have distinctive properties that would affect flow and transport, a decision needs to be made how best to achieve the modeling objectives; i.e., should each layer be discretely treated or should all of the layers be combined into a single layer?

In most instances, it would be appropriate to combine the layers into a single layer for all phases of the remedial program with the following notable exceptions:

> ! Vapor-phase transport

> ! Model calibration

> ! Conceptual model development

Vapor-phase transport within the vadose zone, which can occur with tritiated water vapor, will be largely controlled by the various flow properties of the soils within the unsaturated zone. Vapors will tend to congregate beneath layers with low air permeabilities and freely move through more permeable layers. The direction of movement of the vapor is often governed by the dip and orientation of the soil beds above the water table and are independent of the ground-water gradients.

Percolating rainwater may induce a phase-transformation of radionuclide vapor back to a liquid phase, thus allowing transport to the saturated zone. If this process occurs in beds through which radionuclide vapors have migrated, both away from the source and up the ground-water gradient, it is possible that significant amounts of radioactivity may be detected in the ground-water upgradient of the source area.

This phenomenon is particularly important to consider when determining how far upgradient background monitoring wells should be placed to ensure that the ambient ground water has not been contaminated via vapor transport from the contaminant source. In many systems, with relatively thin vadose zones (< 10 m), it may be more practical to approach this problem empirically and simply measure radionuclide vapor concentrations in the unsaturated zone. However, the expense of investigating relatively thick vadose zones (> 50 m) is often significant, and modeling could be very useful in estimating the likely distance that vapor may have moved.

An evaluation of expected vapor movement and concentrations could also be of considerable value depending upon remedial measure alternatives. For instance, it may be desirable to predict the potential movement of vapor out from under a remedial cap or the movement of water vapor under a capped area. Without the ability of the code to accommodate discrete layers, the effect that a low permeability cap would have on vapor transport could not be simulated. Under other circumstances, maintenance- related issues could be addressed, such as the build- up of hydrogen gas within landfills that contain pyrophoric uranium (i.e., spontaneously combustible). In landfills where pyrophoric forms of uranium metal were placed in drums and submerged in petroleum-based or synthetic oils to prevent rapid oxidation, there is the potential for the uranium and petroleum to react to form hydrogen gas which, at high enough concentrations, is an explosion hazard.

Models are generally calibrated against measured field values. However, unless the field characteri-zation program was designed to characterize the unsaturated zone, data are frequently insufficient to calibrate a vadose zone model. Soil sampling would have had to provide vertical, and in many instances horizontal, profiles of radionuclide concentrations, soil permeability, and moisture content data. Therefore, it is important to decide prior to site characterization whether a fully calibrated vadose zone transport model will be required to meet the modeling objectives. After the characterization is completed, it can be determined, from the data, whether a code is needed that will allow the simulation of discrete layers.

Calibration of flow and transport through the unsaturated zone generally becomes important in areas with relatively thick unsaturated zones (> 100 m). In

these areas, deep boreholes are both very expensive to install and difficult to instrument. Under these circumstances, a calibrated model may be useful in performing mass-balance calculations to determine the depth that contaminants could have potentially migrated, and to provide an estimate of contaminant volumes requiring remediation.

An accurate portrayal of the site-conceptual model is essential for all phases of the remedial program. A computer code with the capability to allow layering may facilitate the evaluation of various aspects of the conceptual model. For example, infiltration through the vadose zone may move laterally over significant distances, particularly when there are soil layers of low permeability which impede vertical migration and allow saturated flow to occur in perched-water zones (Figure 4-7). This transport process is particularly important in areas where a relatively thick unsaturated zone is bisected by deep-cut streams, and the perched water movement in the unsaturated zone is predominantly horizontal rather than vertical infiltration to the water table. Under these circumstances, the radionuclides may short-circuit the ground-water pathway and discharge to seeps and springs along the river wall. Therefore, it could be important to evaluate the potential for horizontal movement in the unsaturated zone to ensure that all exposure pathways are properly accounted for in the conceptual model.

Anisotropic/Isotropic

In a porous medium made of spheres of the same diameter packed uniformly, the geometry of the voids is the same in all directions. Thus, the intrinsic permeability of the unit is the same in all directions, and the unit is said to be isotropic. On the other hand, if the geometry of the voids is not uniform, and the physical properties of the medium are
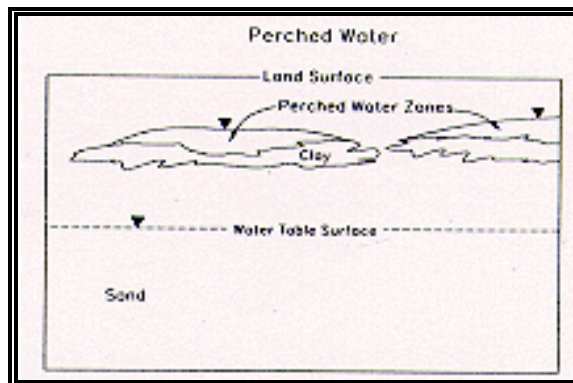

Figure 4-7.   Perched Water

dependent on direction, the medium is said to be anisotropic.

Anisotropy can play a major role in the movement of ground water and contaminants. In most sedimentary environments, clays and silts are deposited as horizontal layers. This preferential orientation of the mineral particles allows the horizontal hydraulic conductivities to greatly exceed those in the vertical direction. As a general rule, for sedimentary environments, it is assumed that horizontal hydraulic conductivities are 10 to 100 times greater than those in the vertical direction.

If the modeling analysis does not account for anisotropy, the contaminants will be predicted to be more dispersed in the vertical direction than would probably be occurring in the real world. One of the primary drawbacks to this taking place is that the predicted concentrations would be significantly reduced due to this artificial vertical dispersion and resulting dilution.

Macropores/Fractures

Modeling flow through the unsaturated zone is 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 (Figure 4-8). 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.
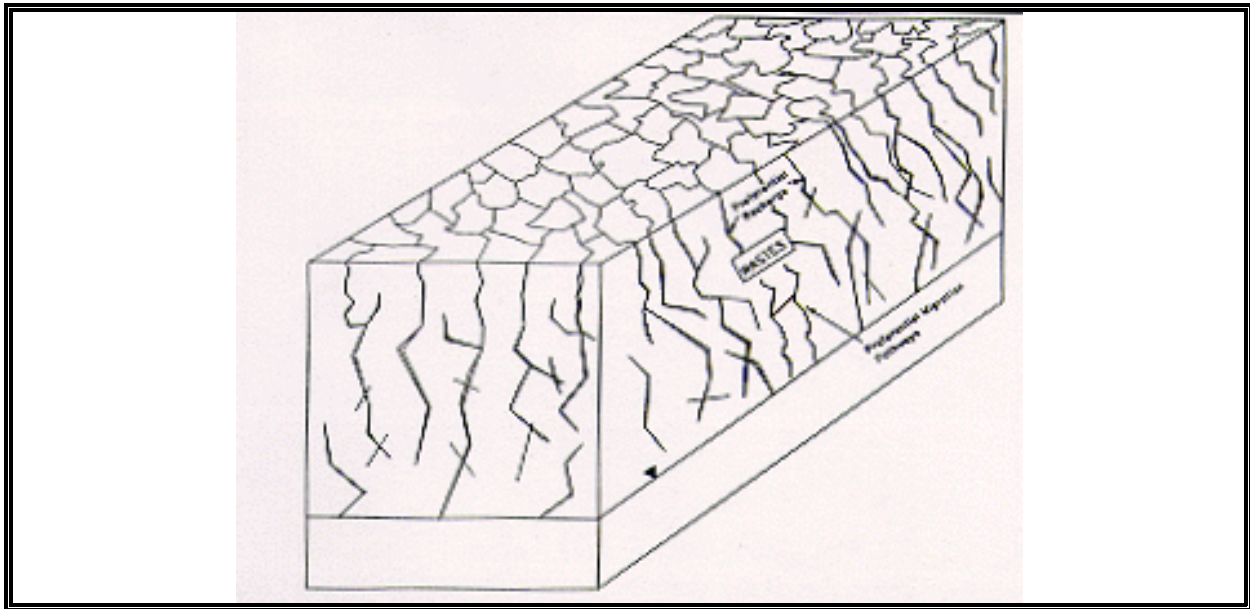
Figure 4-8.   Macropores and Fractures

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.

Many water flow processes of interest, such as ground-water recharge, are concerned only with areally averaged water input. Therefore, preferential flow of water through structural voids does not necessarily invalidate the code formulations that assume uniform flow and do not directly account for macropores. However, preferential flow is of critical importance in solute transport because it enhances contaminant mobility and can significantly increase pollution hazards.

Since codes do not exist that directly simulate flow through macropores, it is important to select a code with features that will allow an indirect simulation of the effects of macropores on flow and transport. A number of factors should be considered when determining whether macropores are important in the modeling analysis, including:

! Presence, geometry, and spatial distribution of macropores
! Location of the waste relative to macropores
! Rainfall duration, intensity, and runoff

Determining the presence of macropores may sound relatively straightforward; however, in many instances, the formation of macropores is an ephemeral process where the desiccation and shrinkage of clays will occur only during the summer months or after long periods of drought. Therefore, if it is suspected that conditions are suitable for the formation of macropores, a special effort should be made to tour the site during the periods when macropores are most likely to be present. After establishing the existence of macropores, the next step would be to gain some understanding of their geometry and spatial distribution. If macropores are relatively shallow (< 1 m), it is highly unlikely that they would have a significant effect on the flow and transport even if they are closely spaced. However, if the macropores are relatively deep compared to the thickness of the unsaturated zone, on the order of ten percent, their effect on flow and transport should be considered in the modeling exercise.

The location of the wastes relative to any macropores plays a significant role in determining their importance. Obviously, if the contaminated area is dissected by numerous relatively deep macropores extending well below the wastes, it would raise concerns that flow and radionuclide transport may be facilitated due to their presence. On the other hand, if the wastes are buried below the maximum depth of the macropores, or if the site has been capped or covered with a material that is not prone to macropore development, their presence would play a lesser role. The direct effect that the macropores will have on the mobility of the wastes is closely tied to whether the macropores are located beneath the waste. If so, they may be providing an avenue for radionuclide transport or, if they terminate above the waste, they may be indirectly enhancing transport by allowing greater amounts of recharge to come in contact with the contaminants.

The rainfall duration, intensity, and runoff also play a major role in evaluating the relative importance of macropores on radionuclide transport. If an area is prone to high-intensity, short-duration storms (convective precipitation) with low runoff, the rainfall rates may exceed matrix infiltration rates, and it is not necessary for the soil to become saturated before water can flow within the macropores. In this manner, water and/or contaminants can move well in advance of the wetting front and be carried beyond the maximum saturation extent of the soil matrix. In contrast, in an area which is typically subjected to long-duration rainfall events with low intensities, it is more likely that flow will not occur in the macropores but will be confined to the soil matrix. This is because the soil matrix infiltration rate will exceed the rainfall rates characteristic of this cyclonic precipitation.

As mentioned previously, there are no codes that directly simulate flow and transport through macropores in the unsaturated zone. Therefore, if it is determined that macropores are present and may potentially have an important effect on flow and transport, several approaches could be used to account indirectly for the flow and transport within the macropores. These approaches are based upon the geometry of the macropores, location of the wastes, and rainfall characteristics. Each of the approaches will require a code with the proper attributes, as outlined below.

If the maximum depth of the macropores is above the top of the wastes and rainfall occurs at such an intensity that flow will take place within the macropores, it will be necessary to evaluate the effect that additional water reaching the wastes will have on contaminant transport. To account for this phenomenon, the code will need the ability to regulate recharge as well as infiltration rates. More precisely, the code must be very stable numerically and able to accommodate areally variable and transient recharge, anisotropy, and heterogeneity. In essence, higher recharge rates are applied over short time intervals to areas of the site with known macropores. However, in order to enable the soil to absorb the additional water and to simulate greater infiltration rates, the soil in this area must also be assigned larger hydraulic conductivities with high vertical to horizontal ratios. To handle these sharp soil material contrasts, the code must be well formulated and not be plagued with convergence problems (see Appendix C).

In instances where macropores extend beneath the bottom of the buried wastes, several alternatives exist for modeling their potential effect on flow and transport. The most straightforward approach is to simulate the portion of the macropores that extend below the wastes by removing an equivalent thickness from the modeled unsaturated zone. This essentially assumes instantaneous transport through the macropores and would result in very conservative values. This approach has a number of advantages, the greatest of which is that the computer code does not need any additional features than it would have otherwise needed without the macropores. However, if this approach is thought to be overly conservative, which would probably be the case if more than half the thickness of the unsaturated zone would need to be removed, an alternative could be employed which involves methods that are used to simulate deep fractured networks in the vadose zone.

Determining the importance of fractures within the unsaturated zone generally presents more of a problem than making the same determination for macropores because: (1) fractures are usually not visible from the surface and are difficult to characterize in the subsurface; (2) if fractures are present, they will often extend through the entire unsaturated zone and into the saturated zone; and (3) fractures may serve as either conduits or barriers to flow. All of these issues must be addressed in the site characterization program to determine whether the fractures need to be

considered in the modeling. In general, fractures that can be traced through the waste area are important and should be considered, at least conceptually, in the analysis.

Fracture modeling of the unsaturated zone can generally use computer codes with attributes very similar to those used for modeling macropores with a few notable exceptions. For the purposes of this discussion, it is assumed that the fractures are found to extend through the unsaturated zone into the saturated zone, and that an assumption of instantaneous flow through the entire vadose zone thickness would not be acceptable for the analysis. Unlike macropores, which will probably not extend to depths greater than 5 meters, fractures may reach depths on the order of hundreds of meters. This factor has a number of implications for both the flow of water and transport of radionuclides.

Rainfall percolating through a fracture will slowly diffuse into the soil matrix. Thus, eventually the water moving in the fracture will become so depleted that fracture flow will no longer develop unless other sources of water are intercepted (e.g., perched). The depth at which fracture flow would cease depends on a number of factors including fracture properties, rainfall characteristics, and soil matrix qualities, all of which are closely interrelated and are difficult to quantify. Conceptually, this process of diffusion into the matrix at depth suggests a direct correlation between the importance of the fractures and the depth of the unsaturated zone. That is, at some depth, fracture flow will no longer be important.

There will always be a large degree of subjectivity associated with deciding the importance of fractures' effects on flow and transport within the vadose zone. However, it would probably be safe to assume that in most unsaturated systems, fracture flow below 200 meters is insignificant unless a continuous source of water is available (e.g., overlying adsorption beds).

The features of computer codes that would be necessary to describe fracture flow would be similar to those required to simulate macropores, except that now, because the pulse-like nature of the recharge would be dampened at greater depths, it would probably not be necessary for the code to accommodate transient recharge, particularly if the depths of interest are greater than 50 meters. However, the codes must still be very stable numerically and able to incorporate

anisotropy and heterogeneity, which are discussed in greater detail in the following sections.

Almost all of the discussion to this point has focused upon modeling flow and transport in porous media. It is important to realize, however, that a number of radioactively contaminated sites overlie areas where fractures and solution channels are probably dominant mechanisms for flow and transport. The uncertainty associated with fracture zone modeling is generally high, and if fracture modeling is to be successful, a concentrated effort needs to go into the design of the field investigation. Therefore, the benefits associated with modeling fractured flow and transport processes have to be carefully weighed against a number of deterrents which include:

- ! An expanded field program is needed;
- ! Significant uncertainties are associated with fracture characterization methods;
- ! High degree of expertise is required of the modeler;
- ! Codes available to simulate fracture flow are difficult to use.

A number of analytical models are available that do simulate ground-water flow and radionuclide transport through fractures. However, it is unlikely that analytical models could adequately describe flow and transport processes in most fractured systems because these processes are much more complex than those in unfractured granular porous media. This is due to the extreme heterogeneities, as well as anisotropies, in the fractured systems. 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 also diffuses 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 contamin-ant in the porous matrix will be

removed very slowly via diffusion back to the fracture openings.

In general, data limitations and narrow objectives would preclude the modeling of fractured systems until at least the Site Characterization phase. If it is determined that numerical modeling of a fractured system will be performed during the Site Characterization, it becomes necessary to evaluate the data needed to support fracture flow and transport numerical modeling. In order to adequately understand the potential data requirements for fracture flow and transport modeling, the following text provides a very basic understanding of modeling fractured systems.

At present there are two general numerical methods for solving flow and transport in a fractured medium: modeling of the flow, accounting for the fractures one by one, or modeling with an equivalent continuous medium approach.

Flow and transport modeling in a fracture system by a continuous porous medium approach is performed by assigning each family of fractures a directional conductivity, thus constituting a hydraulic conductivity tensor. As the frequency and direction of these conductivities are defined, the principal axes of anisotropy of the tensor and the conductivities in these directions can be calculated. It is thus assumed that the fracture spacings are frequent enough that, when viewed from the perspective of the entire physical system, flow and transport processes would be consistent with those associated with porous media. Therefore, computer codes developed for porous media may sometimes be used to simulate multiple fracture families. This approach relies heavily upon the presence of multiple fractures. However, if there are a relatively limited number of fractures, as is often the case with solution channel(s) or faults, an alternative approach is necessary. This alternative approach consists of three general methods, which are termed dual-porosity, dual-permeability, and discrete fracture. All of these methods need a computer code that is specifically developed for modeling fracture flow. The code will have separate equations which are developed for flow and transport in the rock matrix and are coupled to equations describing flow and transport in the fractures. This allows fractures to be assigned flow and transport properties which are discrete from the matrix properties. The dual-porosity method assumes that fractures are relatively uniformly spaced and does not allow flow to occur among matrix blocks. Contaminants leave and enter the fractures only through diffusion. The dual-permeability approach also assumes that fracture networks are well developed although this method does allow advective and dispersive flow through the matrix blocks and is conducive to simulating highly fractured systems in which both the matrix and the fractures are relatively permeable. The discrete fracture approach is similar to the dual-permeability method although the discrete fracture method allows single fractures to be modeled separately as line elements.

In most instances, it is very difficult to obtain the field data necessary to perform detailed fracture flow and transport modeling. Such modeling could require a substantial dedication of resources, and any commitment should be carefully weighed against that which may be gained from the modeling. Circumstances that could lead to a decision to perform fracture-flow modeling may include:

- Future risks cannot be assessed without explicitly accounting for flow and transport in a fractured system;
- Sensitivity or bounding analyses cannot be designed to meet objectives; and
- Empirical data are either not available or can not be effectively used to estimate risks, capture zones, influent concentrations, etc.

Homogeneous/Heterogeneous

A homogeneous unit is one that has the same properties at all locations. For a sandstone, this would indicate that the grain-size distribution, porosity, degree of cementation, and thickness are variable only within small limits. The values of the transmissivity and storativity of the unit would be about the same at all locations. A plutonic or metamorphic rock would have the same amount of fracturing everywhere, including the strike and dip of the joint sets. A limestone would have the same amount of jointing and solution openings at all locations.

In heterogeneous formations, hydraulic properties change spatially. One example would be a change in thickness. A sandstone that thickens as a wedge is nonhomogeneous, even if porosity, hydraulic conductivity, and specific storage remain constant.

Most numerical computer codes have the ability to assign varying hydraulic conductivities and storage properties to the hydrostratigraphic units being simulated. Furthermore, computer codes have also been developed that have the ability to simulate constant or variable thicknesses.

Analytical methods are constrained to modeling aquifers that do not change significantly in thickness or other aquifer characteristics. Numerical codes may or may not have been developed for problems involving an aquifer of variable thickness. Numerical codes that do not allow the thickness of the aquifer to vary significantly use transmissivity as the model input parameter which indirectly describes aquifer thickness (hydraulic conductivity multiplied by thickness). However, numerical codes that specify hydraulic conductivity and aquifer thickness as input parameters independently calculate aquifer transmissivity throughout the model domain and, therefore, allow aquifer thickness to vary. If advective-dispersive contaminant transport calculations are expected to be performed at some time in the analysis, it is important that hydraulic conductivities and aquifer thicknesses are known even when their product (i.e., transmissivity) is only required as model input. This is because the quantity of ground-water flow through aquifers of identical transmissivity will be the same under equal gradients. Therefore, an aquifer which is very thick and has a low hydraulic conductivity can have an identical transmissivity to that of another aquifer which is thin but has a high hydraulic conductivity. As far as the bulk movement of groundwater is concerned, the two systems will behave in a similar fashion when comparative boundary conditions are applied. However, the transport of radionuclides would behave very differently within the two systems, in that velocities would generally be much greater in systems with higher hydraulic conductivities.

A few finite-element computer codes use what are termed curvilinear elements. These are specialized elements that can be spatially deformed to mimic the elevations of the upper and lower surfaces of the hydrogeologic units. Curvilinear elements are particularly useful when aquifers and aquitards have highly variable thicknesses.

In general, if it is expected that the aquifer thickness will vary by more than ten percent, it is recom-mended that the computer code be capable of simulating variable thicknesses. If a code does not properly simulate the aquifer thicknesses, the contaminant velocities will be too large in areas where the simulated aquifer is thinner than the true aquifer thickness and too small in those regions that have too great a simulated thickness.

The ability to simulate aquifer heterogeneities may also be very important during the remedial design phase of the investigation. If engineered barriers of low permeability are evaluated as potential remedial options, it would be necessary to determine their overall effectiveness. In this scenario, it would be important not only to select a computer code that can simulate highly variable hydraulic conductivities, but also to ensure that the sharp contrasts in hydraulic conductivities do not cause instabilities in the mathematical solutions.

4.3.1.3 Transport and Fate Processes

The transport of radionuclides by flow through either a porous matrix or a fractured system will, in each case, be affected by various geochemical and mechanical processes. Among the chemical processes are adsorption on mineral surfaces (both internal and external to the crystal structure), including the kinetics of adsorption, and processes leading to precipitation. The mechanical processes are advection, dispersive effects (hydrodynamic dispersion, channeling), and diffusion. Radioactive compounds can also decay. As a result of sorption processes, some solutes will move more slowly than the ground water that is transporting them; this effect is called retardation. Biological transformation, radioactive decay, and precipitation will decrease the concentration of the solute in the plume but may not necessarily slow the rate of plume movement. The following are the primary processes that affect the mobility and concentrations of radionuclides being transported by ground water:

! Advection

! Dispersion

! Matrix Diffusion

! Retardation

! Radioactive Decay

Advection

The process by which solutes are transported by the bulk movement of water is known as advection. The amount of solute that is being transported is a function of its concentration in the ground water and the quantity of the ground water flowing.

Computer codes that account only for advective transport and ignore dispersion and diffusion processes generally take one of two approaches. The first approach uses a semi-analytical method (Appendix C) to solve the ground-water flow and transport equations, whereas the second approach uses fully numerical methods to determine the ground-water velocity field from which directions and rates of solute movement are calculated by the code.

The semi-analytical method frequently fails when aquifers are of complicated shape and nonhomogeneous. In these instances, it is better to use the second option which utilizes a fully numerical code for determining the velocity distributions and particle (i.e., solute) paths. This may be accomplished with either finite-differences or finite-elements (Appendix C).

Computer codes that consider only advection are ideal for designing remedial systems (e.g., pump and treat) because the model output is in the form of solute pathlines (i.e., particle tracks) which delineate the actual paths that a contaminant would follow. Therefore, capture zones created by pumping wells are based solely on hydraulic gradients and are not subject to typical problems that occur when solving contaminant transport equations which include dispersion and diffusion in the aquifer. These problems are numerical dispersion and artificial oscillation. Numerical dispersion arises because computers have a limited accuracy, thus some round-off error will occur in the computations. This error results in the artificial spreading of contaminants due

to the amplification of the dispersivity. Hence, the contaminant will disperse farther than it should with a given physical, or "real" dispersivity. This extra dispersion will result in lower peak concentrations and more spreading of the contaminant. Methods exist to control numerical dispersion, but the methods themselves may introduce artificial oscillation. Artificial oscillation is the over- or under-shooting of the true solution by the model and results in inaccurate solutions and may give erroneously high and low concentrations.

There are other ground-water solute modeling situations where the phenomenon of dispersion, together with its many uncertainties, is only a minor factor in describing the transport of radionuclides in ground water and can be ignored. For example, the flux of contaminants entering a river that is recharged from a contaminated aquifer is much less sensitive to dispersion than the concentration in a particular well. In the former case, the contaminated ground water would enter over a wide area, which would tend to smear out the effects of dispersion. For similar reasons, the transport from nonpoint sources of con-tamination, such as mill tailings and large landfills, would diminish the sensitivity of the modeled results to dispersion. In these instances, computer codes that consider only advection may be appropriate.

As mentioned previously, advective codes are also excellent in the remedial design stage for determining the number and placement of extraction or injection wells and in evaluating the effect that low permeability barriers may have on the flow system. However, there are a number of drawbacks that must be carefully considered when selecting a code that ignores dispersion and diffusion. The most significant of these is that matrix diffusion, which is discussed below, can be one of the most important processes that will determine the length of time that a pump and treat system must operate before clean-up goals will be met. Without the ability to evaluate the effects of diffusion on solute transport, it would be very difficult to estimate remediation times accurately.

A second potential problem with advection-based codes is that dispersion will tend to spread contaminants over a much wider area than would be predicted if only advective processes are considered, thereby underestimating the extent of contamination. However, because dilution is under-accounted for, unrealistically high peak concentrations are generally obtained, which

may be appropriate if conservative estimates are desired.

Advective codes also tend to yield more accurate travel-time determinations of unretarded contaminants because the solution techniques are inherently more stable, and numerical oscillations, which artificially advance the contaminant front, are minimized.

Another important advantage of advective codes is that the output (i.e., particle tracks) is a very effective means of ensuring that ground-water gradients, both vertical and horizontal, are consistent with the conceptual model.

Hydrodynamic Dispersion

In the previous discussion, advective processes of transport in porous media were presented. In reality, the transport of contaminants is also influenced by dispersion and molecular diffusion, which is caused by the tendency of the solute to spread out from the path that it would be expected to follow if only transported by advection (Figure 4-9). 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 particles 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.

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 as will be discussed under the topic of matrix diffusion.

There is concern as to how adequately dispersion can be represented in computer codes because it is related to spatial scale and variations in aquifer properties which are generally not explicitly simulated in the code (e.g., tortuosity). Furthermore, dispersion coefficients are very difficult to measure in the field
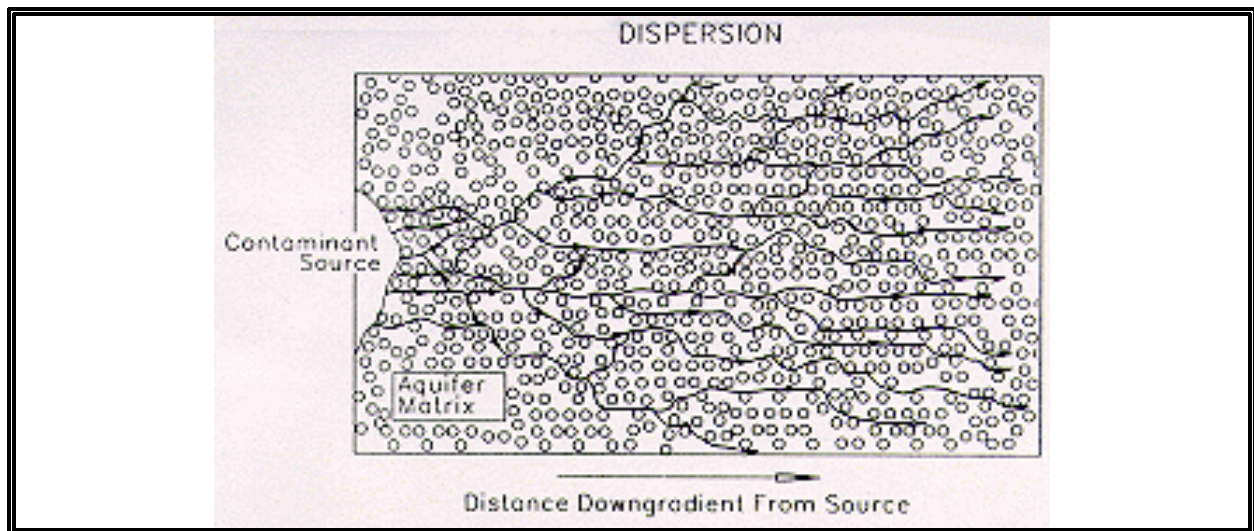

Figure 4-9. Hydrodynamic Dispersion

and are usually obtained during the model calibration process.

These limitations suggest that not too much confidence be placed in dispersion values, and that it is generally best to use advection-dispersion-based codes to bound the maximum probable extent that contamination may have spread. However, as mentioned previously, peak concentrations will tend to be underestimated.

Matrix 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 (Figure 4-10). The diffusion of radionuclides from water moving within fractures, or coarse-grained material, into the rock matrix or finer-grained clays 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., mobility) as well as properties of the rocks (such as porosity, tortuosity, and sorption ratios).

As stated previously, matrix diffusion is frequently insignificant and is often neglected in many of the contaminant-transport codes. However, potential problems arise when matrix diffusion is ignored and contaminant distributions are based solely on advective-dispersive principles. For example, ground-water pump and treat remediation systems work on the premise that a capture zone is created by the pumping well and all of the contaminants within the capture zone will eventually flow to the well. The rate at which the contaminants flow to the well may, however, be very dependent on the degree to which the contaminants have diffused into the fine-grained matrix (e.g., clays). This is because the rate at which they will diffuse back out of the fine-grained materials may be strongly controlled by concentration gradients, rather than the hydraulic gradient created by the pumping well. Therefore, matrix diffusion can significantly retard the movement of contaminants, and, if the computer code does not explicitly account for this process, the overall effectiveness of the remediation system (i.e., clean-up times) could be grossly underestimated.

Other instances where matrix diffusion processes can lead to erroneous model predictions is in the determination of travel times, peak concentrations, and flushing volumes. The fact that diffusion can play a significant role in slowing the transport of radionuclides suggests that, if it is ignored, travel rates, as well as peak concentrations, will be overestimated. Frequently, clean-up times are estimated based on the flushing of a certain number of pore volumes. However, matrix diffusion
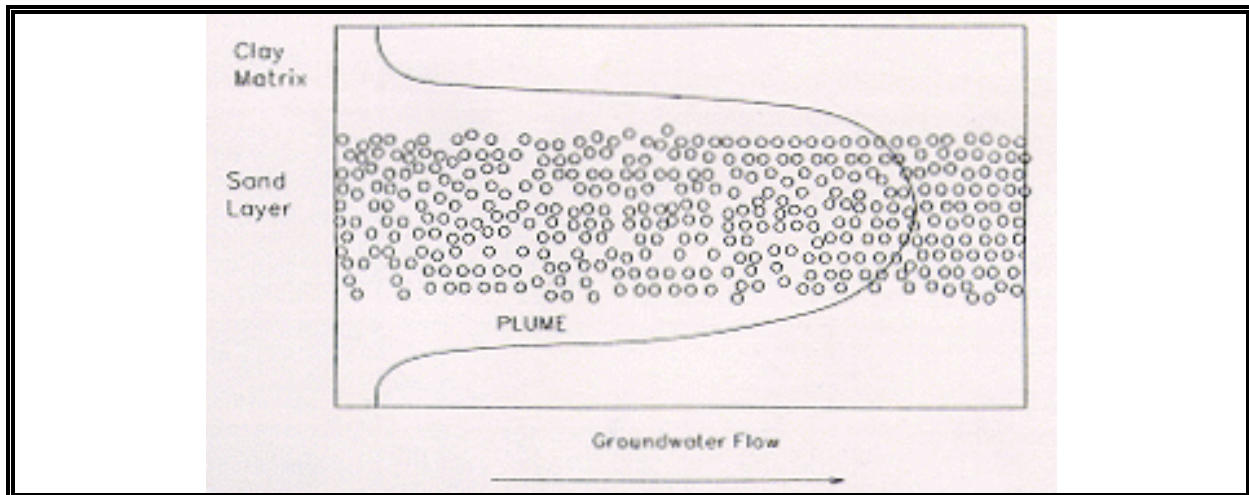

Figure 4-10. Matrix Dispersion

processes, if unaccounted for, can cause the number of required pore volumes to be greatly underestimated. This is because pore volume calculations generally assume that water moves freely through all of the pores and does not account for the relatively stagnant conditions of fine-grained rocks in which contaminants may have diffused.

Retardation

In addition to the physical processes, the transport of radionuclides is affected by chemical processes. The following summary of geochemical processes that could potentially play a role in the transport of radionuclides has been provided in order to offer an appreciation of their wide variety and complexity:

- Sorption -- the attachment of chemical species on mineral surfaces, such as ion exchange, chemisorption, van der Waals attraction, etc., or ion exchange within the crystal structure.

- Ion exchange phenomena -- that type of sorption restricted to interactions between ionic contaminants and geologic materials with charged surfaces which can retard the migration of radionuclides.

- Speciation -- the distribution of a given constituent among its possible chemical forms of the radionuclide which can influence its solubility and therefore its rate of transport by limiting the maximum concentration of the element dissolved in the aqueous phase.

- Precipitation -- the process by which dissolved species exceed solubility limits, resulting in a portion precipitating out of solution.

- Natural colloidal formation -- the attachment of radionuclides to colloids resulting in a mode of radionuclide transport or retardation which involves the movement or mechanical retardation of radionuclides attached to large colloidal particulate matter suspended in the ground water or the formation of colloidal clusters of radionuclide molecules.

- Radiolysis -- the change in speciation due to radiation or recoil during radioactive decay, which can affect the solubility of radionuclides.

- Biofixation -- the binding of radionuclides to the soil/organic matrix due to the action of some types of microorganisms and plants, thus affecting mobility of the radionuclide.

- Natural organic matter interactions -- soil organic matter can play a significant role in mobilizing, transporting, sorbing, and concentrating certain radionuclides.

- Anion exclusion -- negatively charged rock surfaces can affect the movement of anions, by either retarding the movement of anions by not allowing negatively charged radionuclides to pass through the pore opening, or by enhancing the transport of ions by restricting the anion movement to the center of the pore channel where ground-water velocities are higher.

Obviously, a wide range of complex geochemical reactions can affect the transport of radionuclides. Many of these reactions are poorly understood and are primarily research topics. 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) 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 to the soil. Because the distribution coefficient is strongly affected by site-specific conditions, it is frequently obtained from batch or column studies in which aliquots of the solute, in varying concentrations, are well mixed with representative solid from the site, and the amount of solute removed is determined.

If the sorptive process is rapid compared with the flow velocity, the solute will reach an equilibrium condition with the sorbed phase, and there is a greater likelihood that the distribution coefficient approach will yield reasonable values. However, if the sorptive process is slow compared with the rate of fluid flow, the solute may not come to equilibrium with the sorbed phase and geochemical (i.e., based on thermodynamics and kinetics) models are generally required.

Most computer codes assume that the distribution coefficient is constant over all solute concentration ranges (i.e., linear isotherm). However, this assumption may place a serious limitation on the predictive capability of the code, in that a linear relationship between the concentration of solute in solution and the mass of solute sorbed on the solid does not limit the amount of solute that can be sorbed onto the solid. In actuality, this is not the case; there must be an upper limit to the mass of solute that can be sorbed, due to a finite number of sorption sites on the solid matrix. This upper bound on sorption suggests that, in a natural system, retardation would decrease as contaminant concentrations in the ground-water increase. This discrepancy between computer codes assuming linear sorption behavior when, in fact, non-linear sorption is more accurate, can have important implications when predicting the migration of the center of mass versus the leading edge of a contaminant plume, or when predicting required pumping times for a pump and treat remedial action. At high concentrations, the linear assumption will over-predict retardation and under-predict radionuclide travel rates and contaminant concentrations.

A basic assumption in code development is that at dilute concentrations the errors associated with using linear sorption isotherms to predict non-linear relationships will be minimal. However, radionuclides present a special problem in that frequently the releases may be at dilute concentrations but over extended durations. These long time frames may allow all of the sorption sites to be filled, even at low release concentrations, and model results will diverge from actual values by under-predicting radionuclide travel rates and concentrations.

The ability of a code to accommodate retardation effects is essential for evaluating radionuclide transport rates unless a special case is being considered, such as one involving tritium which moves unretarded or if the primary objective is to determine the absolute minimum travel times and maximum travel distances. It is possible to back out travel rates and distances from computer codes that do not accommodate distribution coefficients; however, if the species are decaying, the calculations can become very tedious.

Radioactive Decay

Radionuclides decay to stable products or to other radioactive species called daughters. For some radionuclides, 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 health risk than the parent. Accounting for the chain-decay process is particularly important for predicting the potential impacts of uranium, thorium, 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. However, not all computer codes that simulate radioactive decay allow for ingrowth of the daughters, which may not cause a problem if the daughter half-lives are very long (i.e., they take a very long time to grow in) or if the daughter products are of little interest. In addition, it is computationally difficult to account for ingrowth of daughters during transport. Codes that do address daughter ingrowth generally account for ingrowth in the contaminated zone only. The difficulty arises in the need to use the Kd of the daughter and changes in the travel distance as the daughters grow during transport through the unsaturated and saturated zones.

4.3.1.4 Multiphase Fluid Conditions

The movement of contaminants that are immiscible in water (i.e., non-aqueous phase liquids - NAPL) through the vadose zone and below the water table results in systems which have multiple phases (i.e., air, water, NAPL). This coexistence of multiple phases can be an important facet in many contaminant-transport analyses. However, only the water and the vapor phase are of concern when evaluating the transport of radionuclides. A limited number of radionuclides can form volatile species that are capable of being transported in a moving vapor or gas. Among these are tritium, carbon-14, and iodine-129. Over a large scale, factors that affect transport in flowing ground water also affect transport in flow-ing 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 consi-dered when assessing the impact of vapor transport.

Currently a number of analytical and numerical codes allow the investigation of vapor transport in the unsaturated zone; however, almost all of these codes assume an immobile water phase. The limitation of this assumption is that one of the principal concerns regarding gaseous transport is its role in transporting gas-phase radionuclides through the unsaturated zone to the water table where they may be dissolved and transported by the ground water. Without the capability to simulate the percolation of water through the unsaturated zone, tritium concentrations reaching the water table will be greatly underestimated. Furthermore, remediation strategies cannot be fully developed if the residual water held in the unsaturated zone is assumed to remain stagnant. For instance, a method that has been proposed to remediate tritium involves pumping the tritiated water from withdrawal wells located downgradient from the source area. The contaminated water is subsequently reinjected into wells upgradient from the withdrawal wells. In this manner, tritium is recycled continuously until it decays to levels below the remedial criteria (e.g., the drinking water standards). Two aspects of this system that could not be evaluated without having the ability to simulate mobile water and vapor in the unsaturated zone are, first, whether vapor transport will carry tritium beyond the limits of the hydraulic capture zone created by the pumping wells, and second, what the expected loading rates will be from the source term.

4.3.1.5 Flow Conditions

The ground-water environment can be divided into a variably saturated (vadose zone) and saturated regimes. The irregular surface that forms the boundary between these two regimes is known as the water table. Below the water table, pressures are equal to or greater than atmospheric and the pores and spaces within and between individual soil particles are filled with water. Above the water table, in the partially saturated zone, water is generally under negative pressure or tension (less than atmospheric). Some of the pore space is usually occupied by gases derived primarily from the atmosphere as well as pore water.

Radionuclide releases to the ground water may result from a number of mechanisms. These mechanisms can affect ground water directly or indirectly, and they include the following:

! Direct discharge (e.g., on-site release from treatment processes)

! Leachate generation (e.g., from buried wastes, surface impoundments, and absorption beds)

! Overland flow (e.g., from impoundment overflow or failure, drum leakage)

! Contaminated stream interaction with aquifers

The decision as to whether the vadose zone and/or saturated zone will be modeled is directly related to the mechanism by which the contamination was released. That is, if radionuclides are being released directly to the water table, little would probably be gained by modeling the vadose zone. However, if the risk assessment is based only on radionuclide concentrations reaching the water table, it may not be necessary to model the saturated zone.

After a determination is made as to whether the vadose zone and/or saturated zone are to be modeled, it becomes necessary to address a much more difficult question, i.e., the complexity at which each zone should be modeled. This question can be answered only by attaining a thorough understanding of the modeling objectives, as well as an appreciation of the advantages and disadvantages of each prospective approach.

The sophistication of the unsaturated zone modeling approach will be based primarily on the overall modeling objectives, although the complexity of the hydrogeology may also play a significant role. For instance, accurate predictions of radionuclide flow and transport through a very complex unsaturated zone may be irrelevant and unnecessary if credit is not taken for it in the baseline risk assessment. On the other hand, if the risk assessment is based solely upon arrival times and peak concentrations of radionuclides arriving at the ground-water table, then a detailed analysis of flow and transport through even a thin, uncomplicated unsaturated zone may be significant and require complex modeling.

Relative to saturated zone modeling, vadose zone modeling is characterized (plagued) by significant numerical difficulties and greater uncertainty regarding conceptualization and parameter estimation. In many vadose zone modeling situations, it may be advisable to use simple models and conservative assumptions to estimate exposure concentrations. The

appropriate level of modeling and data collection for risk assessment at individual sites should be determined during the remedial process.

Situations may arise where reliable simulations of flow and transport of radionuclides through the unsaturated zone may not be possible even with complex ground-water models. In particular, if the unsaturated zone is indurated with fractures or macropores with high permeability, the flow and transport processes become so involved that mathematical formulations of porous media transport are poor representations of the physical phenomena. Furthermore, localized zones of higher permeability may cause the wetting front to advance at highly variable rates, which may introduce significant disparities between the actual and predicted contaminant concentrations.

Under single-phase flow conditions, an option to select a vadose zone code which simulates hysteresis is provided. Hysteresis is simply a term which describes the fact that wetting and drying curves for a certain soil (pressure head versus volumetric water content), under partially saturated conditions, are not the same. That is, the pressure head is not only dependent upon the water content but also on whether water is being removed or added to the system. The effect is due to both the geometric shapes of the pores and the contact angle between the water and the mineral surface, which is different depending on whether the water is advancing and retreating. Of particular relevance in considering hysteric effects as a code-selection criteria is that hysteresis will have little effect on the flow and transport of contaminants. The primary utility of including hysteresis is to account for this process during model validations studies. Therefore, if model validation will not be performed, which will be the case in the vast majority of modeling studies, the capability of a code to simulate hysteresis will be of little importance.

4.3.1.6 Time Dependence

The most frequently performed ground-water modeling is that of the saturated zone. The parameter needs are well defined and the field data collection activities are relatively straightforward. The major factors that provide immediate insight into whether sophisticated ground-water modeling will be necessary are the complexity of the:

!   Source term

!   Dominant flow and transport processes
!   Hydrogeology (e.g., layers, heterogeneity)
!   Hydraulic boundaries

Previous discussions have addressed the relative importance of these issues in the code selection process. However, one aspect that has not been fully considered is the temporal nature of flow and transport within the system. As discussed previously, simulations can be performed in either a steady or a transient state. At steady-state, it is assumed that the flow field and contaminant releases remain constant with time, whereas a transient system simply means one that fluctuates with time. This fluctuation may be induced by both natural (e.g., tides, rainfall) and manmade influences (e.g., wells, hydraulic barriers). In many instances, transient systems, if observed over the long term, will approach relatively steady-state conditions.

As far as code selection is concerned, relative to the temporal behavior of the system, it is a fairly straightforward decision. Namely, most analytical models do not simulate a transient flow system; therefore, if a transient flow system needs to be modeled, analytical and semi-analytical methods are generally not available. Furthermore, if a steady-state flow system is acceptable, but a transient transport capability is required, both analytical and numerical codes are readily available for these conditions and the selection criteria should be deferred to other considerations.

4.3.2 Code-Related Characteristics

In addition to the site-related characteristics presented in the previous section, the code selection process must also consider attributes that are integral components of the computer code(s), including:

!   Geometry

!   Source Code Availability

!   Code Accessibility/Ease of Use

!   Code Verification and Validation

!   Code Output

!   Solution Methodology (Appendix C)

4.3.2.1 Geometry

The decision to model a site in a particular number of dimensions should be based primarily upon both the modeling objectives and the availability of field data. Other considerations include whether a computer code exists that can simulate the dominant processes in the desired number of dimensions, and whether hardware requirements are compatible with those available.

In determining how many dimensions are necessary to meet the objectives, it becomes necessary to gain a basic understanding of how ground-water flow and contaminant concentrations are affected by the exclusion or inclusion of an additional dimension. It should be kept in mind that the movement of ground water and contaminants is usually controlled by advective and dispersive processes which are inherently three-dimensional. Advection is more responsible for the length of time (i.e., travel time) it takes for a contaminant to travel from the source term to a downgradient receptor, while dispersion directly influences the concentration of the contaminant along its travel path. This fact is very important in that it provides an intuitive sense for what effect dimensionality has on contaminant migration rates and concentrations. As a general rule, the fewer the dimensions, the more the model results will over-predict concentrations and under- predict travel times. Concentrations will be over- predicted because dispersion, which is a three-dimensional process, will be dimension limited and will not occur to the same degree as it actually would in the field. Travel times will be under-predicted, not because of a change in the contaminant velocities, but because a more direct travel path is assumed. Therefore, the lower dimensionality models tend to be more conservative in their predictions and are frequently used for screening analyses.

One-dimensional simulations of contaminant transport usually ignore dispersion altogether, and contamination is assumed to migrate solely by advection, which results in a highly conservative approximation. Vertical analyses in one dimension are generally reserved for evaluating flow and transport in the unsaturated zone.

Two-dimensional analyses of an aquifer flow system can be performed as either a planar representation, where flow and transport are assumed to be horizontal (i.e., longitudinal and transverse components), or as a cross section where flow and transport components are confined to vertical and horizontal components. In most instances, two-dimensional analyses are performed in an areal orientation, with the exception of the unsaturated zone, and are based on the assumption that most contaminants enter the saturated system from above and that little vertical dispersion occurs. However, two-dimensional planar simulations have a number of limitations. These include the inability to simulate multiple layers (e.g., aquifers and aquitards) as well as any partial penetration effects. That is, the contaminant source, wells, rivers, lagoons, and lakes are all assumed to penetrate the entire thickness of the aquifer. Furthermore, because vertical components of flow are ignored, a potentially artificial lower boundary on contaminant migration has been automatically assumed which may or may not be the case.

A two-dimensional formulation of the flow system is frequently sufficient for the purposes of risk assessment, provided that flow and transport in the contaminated aquifer are essentially horizontal. The added complexities of a site-wide, three-dimensional flow and transport simulation are often believed to outweigh the expected improvement in the evaluation of risk. Complexities include limited site-wide hydraulic head and lithologic data with depth and significantly increased computational demands.

Quasi-three-dimensional analyses remove some of the limitations that are inherent within two-dimensional analyses. Most notably, quasi-three-dimensional simulations allow for the incorporation of multiple layers; however, flow and transport in the aquifers are still restrained to longitudinal and transverse horizontal components, whereas flow and transport in the aquitards are even further restricted to vertical flow components only. Although partial penetration effects still cannot be accommodated in quasi-three-dimensional analyses, this method can sometimes provide a good compromise between the relatively simplistic two-dimensional analysis and the complex, fully three-dimensional analysis. This is the case, particularly if movement of contaminants from the shallow aquifer through a confining unit and into a deeper aquifer is suspected.

Fully three-dimensional modeling generally allows both the geology and all of the dominant flow and transport processes to be described in three dimensions. This approach usually affords the most

reliable means of predicting ground-water flow and contaminant transport characteristics, provided that sufficient representative data are available for the site. Fully three-dimensional analyses are often the only defensible means to evaluate the effectiveness of many potential remedial scenarios. For example, extraction and injection wells may create strong vertical gradients, as well as three-dimensional capture zones. Without the ability to accommodate these gradients and capture zones, dilution effects and capture zones could be over- or underestimated. The ground-water flow and contaminant transport beneath a barrier wall would also be subject to serious predictive limitations without a three-dimensional analysis, again because of the strong vertical gradients that generally accompany these features.

4.3.2.2 Source Code Availability

As a general rule, an effort should be made to use publicly available computer codes, provided they have been well documented and tested and can meet all of the major requirements of the modeling objectives. In certain instances, however, it may be necessary to purchase a proprietary code. A proprietary code may be needed for a number of reasons, but, most commonly, proprietary codes are selected either because the user is familiar with the code or because the publicly available codes would not meet the modeling objectives.

The following is a list of factors that need to be considered during the selection process of both proprietary and non-proprietary computer codes:

> ! Whether the code has been widely used and is generally accepted by the technical community;
>
> ! How well the code is documented and verified;

> ! Whether the code has been independently peer reviewed;
>
> ! Whether the purchase price of the code provides any technical support, and, if additional support is required, what it will cost;
>
> ! Whether the source code is provided, and, if not, under what conditions could it be obtained if necessary;
>
> ! Whether the code has ever been applied to a similar problem with consistent objectives;
>
> ! Whether the code has been field tested on problems directly relevant to the subject site;
>
> ! Whether the code has ever been used to support a case in litigation or regulatory enforcement action;
>
> ! Whether any additional enhancements or modifications to the code are planned in the future.

4.3.2.3 Code Testing and Processing

The verification process is generally undertaken during the developmental stages of the computer code. It is a procedure in which analytical equations of known solutions are used to ensure that there is an agreement between the formulations and solutions of the same basic equations, which are solved with more complex numerical methods. In some instances, numerical methods, which have been verified with analytical solutions, are used to check other newly formulated or even more complex numerical solutions. The purpose of verification is to show only that the numerical techniques work and that no errors exist in either the mathematical formulation or in the actual coding of the formulation.

One important aspect of code verification is that it can usually be performed independently of the code development process. This allows the accuracy of codes to be checked even without access to the source-code documentation. It is not recommended, however, that codes be selected that were not verified during the development process and are not well documented.

Calibration and validation are activities designed to test the realism of the ground-water flow and transport model. From a philosophical perspective, calibration and validation are very different. When addressing the subject of calibration, it is generally assumed that both the conceptual model and numerical models are reasonably correct or adequate. Therefore, to calibrate a model, model parameters are simply adjusted within an acceptable range, based on site-specific measurements, to arrive at a best fit of the dependent variable, which is usually hydraulic head or solute concentrations. Validation, on the other hand, examines in more detail the realism of both the conceptual model and the numerical model.

Model calibration of vadose zone models is very difficult and rarely attempted primarily due to data limitations, whereas calibration of saturated flow and transport models is relatively straightforward, provided there are sufficient field measurements of hydraulic head or solute-concentration data. One potential problem with calibration of saturated flow models is that a unique solution for the hydraulic head distribution is not available if all of the boundary conditions are either no-flow or fixed head. In other words, if the model does not contain a flux condition of significant magnitude (relative to total flux through the model), increasing or decreasing all the hydraulic conductivities in equal proportion will result in the exact same hydraulic head distribution. The only difference is that the amount of flux through the model will be increased or decreased in proportion to the change in hydraulic conductivities. This is why it becomes very important to not only narrow the probable ranges of hydraulic conductivities through methods such as aquifer tests but also to use mass balance information to check the calibration results.

Model validation is, in general, a comparison of the solutions of the mathematical equations from which the model is formulated with field-measured data. Compelling arguments have been made that ground-water models cannot be validated, only invalidated (KON92). Accordingly, validation is best thought of as a process for determining the degree to which a model can be relied upon to support a specific modeling objective at a specific site. Validation, at best, may consist of reasonable agreement between simulated results and actual field data at two or more time periods.

Attempts to validate models must address the issue of spatial 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 fall within the bounds of field-measured values.

Regardless of whether the solution is obtained by analytical or numerical techniques, true validation or history matching can be done only through comparison with field measurements and, in some cases, laboratory data. Furthermore, given the lack of comprehensive field data sets that adequately describe the spatial parameter distributions, and our inability to directly measure water and solute fluxes which are more logical variables for model validation, it is highly unlikely that complete validation of any simulation model can be possible.

Such complete validation, however, is not necessary for most modeling approaches if model limitations are adequately recognized. It should also be kept in mind that validation is site-specific and consequently its utility, if achieved at one location, is limited when considering application of the model at another location.

The need for the overall validation or history matching outlined above is directed at the creation of reasonably reliable computational and forecast capabilities for studies that would generally go beyond the baseline-risk assessment. It is acknowledged that the field testing efforts outlined here usually occur concurrently with the remedial process; however, validation or field testing is not simply applying models within the remedial investigation context. This is because the remedial investigation of a waste site may strongly focus on the calculation of risk. For example, if all contaminants released at a waste site are immobile, the remedial investigation activities in support of the baseline risk assessment may concentrate on the quantification of partitioning between the water and the solid phase. As such, simplified flow and transport models may be used to support the baseline risk assessment under this situation. Within this context, it is recognized that flow and transport modeling is only one component of the risk calculation, and those

responsible for the quantification of the baseline risk assessment may employ a relatively unsophisticated modeling approach for the baseline and perhaps very conservative simulations. On the other hand, for other situations, detailed flow and transport analyses may be required. Under these conditions, resolution of the flow and transport model validation issue will require examination of the waste site with models of some complexity or sophistication with regard to the geologic structure and dominant processes.

4.3.2.4 Model Output

One aspect of the computer code that is frequently ignored in the selection process is the form that the model output will take. It is true, however, that in most instances the actual output can be fashioned into the desired format, provided the model itself is consistent with required output. That is, output in three dimensions cannot be obtained with a two-dimensional model.

In general, the model output is expressed in terms of hydraulic head, pressure, or solute concentrations. The spatial coverage of parameter output values is either dependent on the frequency of nodal spacing (numerical) or on the number of specified x and y coordinates (analytical) which are included in the model input files. Code output will also vary due to the inherent nature of the code itself. For example, codes that simulate movement in the unsaturated zone produce what are termed saturation profiles. These profiles indicate what percentage of the pore space is filled with water, whereas saturated zone codes have no need for this capability because all of the pores below the water table are assumed to be filled.

Some codes provide output in a format which is very useful and saves time during the post-processing of the data. The best example of this is where the user can specify nodes where concentration profiles are desired with time (i.e., breakthrough curves). These profiles allow arrival times, peak concentrations, and contaminant mass changes to be easily evaluated.

The single most important code selection criteria, relative to the model output, would be that the code provides mass-balance information. A mass-balance determination is a check to ensure that at steady-state, the amount of water or contaminant mass entering the system equals the amount exiting the system. If inflow does not equal outflow for a steady-state simulation, there may be something wrong with the numerical solution, although errors in the mass balance may also indicate that there are problems with the mass balance formulation itself. Therefore, mass-balance information not only provides a check on the mathematical formulations within the code, but it also assists in ensuring that input parameter conversions and other errors have not been made.

It is not uncommon for codes that do include mass-balance output to provide information (e.g., fluxes, heads) on specific boundaries as well as the source term, all of which can be used in the interpretation and evaluation of the predicted flow and solute transport directions and rates.

4.4 MODELING DILEMMAS

The previous sections have described how site- and code-related features affect the model selection process. What is not presented, however, is a discussion of the processes that are very difficult, if not impossible, to model with currently available models. Complex flow and transport processes present another difficulty in that computer codes currently do not exist that explicitly accommodate a number of these processes including:

!　　Turbulent Ground-Water Flow

!　　Facilitative Transport

!　　Unsaturated Fracture Flow

!　　Complex Geochemical Reactions

Although these processes are very complex, it is important that at least a basic understanding of these mechanisms and concepts be grasped prior to initiating field or modeling investigations in which they may be important. The subsequent discussion will introduce the difficulties associated with modeling these complex processes. Of particular relevance is that the processes are not fully understood and are, therefore, not well described mathematically. If modeling is not possible

because of the overall complexity of the site characteristics, it is common for a greater emphasis to be placed on empirical rather than predicted data. This may involve establishing long-term monitoring programs, which in effect, have objectives similar to those of ground-water modeling.

Turbulent Ground-Water Flow. As ground-water velocities increase, flow diverges from the laminar-type which is characteristic of low velocities and becomes more turbulent. At the point in which turbulent flow is reached, a basic law describing the relationship between hydraulic gradient and specific discharge (i.e., Darcy's) breaks down and is no longer valid. Most ground-water flow, however, is not turbulent, except in the very close proximity of large pumping or recharging wells. In practice, however, turbulent flow over relatively small areas is generally ignored without introducing any severe limitations in the modeling. On the other hand, in cases where turbulent flow is observed over relatively large areas, such as cavernous limestone aquifers, Darcy's law may be significantly violated and results from flow and transport modeling would be of questionable value.

Facilitative Transport of Radionuclides. Field and laboratory investigations have indicated that under certain conditions contaminants are more mobile than would be predicted based on properties such as solubility, ion exchange, speciation, sorption-desorption and ground-water velocities. These predictions, however, have not accounted for the potential interactions between the inorganic contaminants and mobile colloids. Colloidal-size particles include humic substances, clay minerals, iron oxides and microorganisms. Colloids not only have a high surface area per unit mass and volume, but many types of colloids are also extremely reactive sorbants for radionuclides. Therefore, radionuclides 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.

A number of actinides, plutonium in particular, can form natural colloids under conditions of near-neutral solutions of low ionic strength. It is also suspected that americium may form colloids under similar conditions. 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. At this time it is believed that plutonium and americium are most likely to be transported as colloids, although other radionuclides might be subject to this transport process under certain conditions. 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), and neutralization of the repulsive charges on the colloids, thus allowing them to coagulate.

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 ground water may also adsorb radionuclides.

The degree to which facilitative transport can be modeled is largely dependent upon the objectives of the modeling and the extent of understanding of the transport mechanisms active at the site. A site-specific evaluation may be required to determine the possible importance of colloidal transport on the mobility of the radionuclides. To estimate the amount of radionuclides that could 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 could 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.

An alternative approach to detailed site investigations to characterize the potential for colloidal transport would be to undertake a conservative approach and set all of the distribution coefficients to zero. This approach, however, may not always be conservative in that it is possible that under certain circumstances colloids may have a velocity greater than the average linear ground-water velocity. This may be due to both size-exclusion and charge-repulsion. Size-exclusion

occurs when molecules or ions are so large that they cannot be transported through the smaller pores. As a result, they are restricted to the larger pores, in which the ground-water velocity is greater than average. The charge-repulsion phenomenon occurs when the colloids have a negatively charged surface which is repelled by the negatively charged clays which line the pore channels. This process may confine the colloid to the central part of the channel where the velocities are highest and the ground-water velocity is greater than average.

Attempts have also been made to model the transport of colloids which are more mobile than water by setting the distribution coefficient to less than zero. This approach, however, has a number of problems. One of the most significant of these is that all of the waste released from the source term would be assumed to be transported as colloids which may result in overly conservative solutions.

Currently, ground-water models do not exist that describe the constitutive relationships involved with colloidal transport and explicitly account for the dominant geochemical interactions responsible for colloidal transport.

Unsaturated Fracture Flow. As previously discussed, ground-water modeling of the unsaturated zone is based upon developing sets of moisture-characteristic curves, that is the functional dependence of liquid-water saturation and relative hydraulic conductivity on the liquid-water potential within the rock matrix and fractures for each hydrogeologic unit. In unfractured rocks, these relations refer to the storage and movement of liquid water within and through the interstitial pore space. In fractured rocks, allowance must be made for the storage and movement of water within the interconnected fracture openings as well as for the movement of water between the fracture openings and the rock-matrix pore space. Standard field and laboratory methods are not yet available by which to determine the moisture-characteristic relations for fractures within the unsaturated zone.

Liquid-water storage within fractures probably is insignificant, but the flow of liquid water within and across fractures is not yet well understood. Theoretical models for liquid-water flow in single unsaturated fractures have been developed but have not yet been field tested. Fractures may or may not impede liquid-water flow at low matrix saturations, and longitudinal

flow within the fractures may dominate liquid-water flow above some critical matrix saturation. Consequently, at high matrix saturations, fracture systems and fault zones may become highly efficient pathways for liquid-water flow. Liquid-water flow within fractures may or may not be Darcian (i.e., laminar) and will be dependent on the gradient and hydraulic conductivity.

At low matrix saturations, little or no water moves longitudinally within the fracture openings, and the effective hydraulic conductivity is controlled by that of the fracture-bounded matrix blocks. As the matrix approaches complete saturation, however, the movement of water within and along the fracture aperture rapidly becomes more efficient so that at complete saturation the fractures may be dominant contributors to the net hydraulic conductivity. The relative contributions of fractures and matrix to the net effective hydraulic conductivity depend on the fracture frequency, aperture-size distribution, and degree of interconnectivity. However, there is currently no way to generate a complete set of fracture location and geometry data.

In essence, a generally poor understanding of the physics controlling fluid flow in fractured-unsaturated systems, in conjunction with an inability to characterize the fracture properties and locations, makes it nearly impossible to model these systems reliably.

Complex Geochemical Reactions. Radionuclides are undergoing geochemical reactions. The principal geochemical properties and processes of the radionuclides, which may be site-specific and important to understand, include the following:

- ! Complexation

- ! Phase transformations

- ! Adsorption and desorption

- ! Precipitation

As stated previously, if it is desired to model these processes explicitly, as opposed to using simplifying assumptions such as default or aggregate retardation coefficients, geochemical rather than flow and transport models may be required. As indicated, some of the more common radionuclides, such as uranium

and plutonium, can exist in a number of chemical states, which can significantly affect their rate of transport. Other radionuclides, such as tritium, are relatively insensitive to the site geochemical conditions but undergo phase transformations which are difficult to simulate with existing codes. Explicit geochemical models can be applied to assist in evaluating the general effect that the geochemical environment will have on the radionuclide fate and transport, but even these methods are often unreliable and the results must be interpreted carefully.

SECTION 5

THE CODE SELECTION PROCESS

Section 4 described the various waste and site characteristics and processes and the code-related characteristics pertinent to the code selection process. The emphasis was placed on recognizing when specific waste, site, and code characteristics are important and therefore must be considered in order to meet the modeling needs of each phase of the remedial process. This section presents the basic procedure that should be followed in evaluating ground-water flow and transport code(s) prior to making a final selection among two or more potential codes.

5.1 OVERVIEW OF THE CODE REVIEW AND SELECTION PROCESS

Given that an investigator understands the various waste and site characteristics that need to be modeled in order to meet specific modeling objectives, there will often be several suitable computer codes which could potentially be chosen from a large number of codes published in the scientific literature (BAC80, EPA91, and MOS92). As mentioned in Section 1, IMES "Integrated Model Evaluation System" provides an excellent computerized means by which codes may be screened automatically for their respective capabilities. The user simply checks off the desired code capabilities within a screening module of IMES, and the program eliminates all of the codes without the specified capabilities from an extensive internal database. Furthermore, IMES will provide some information on the code itself although these descriptions are, in many instances, somewhat limited. Ideally, a detailed evaluation of each candidate code should be performed to identify the one most appropriate for the particular site and modeling objectives. The resources to complete a detailed study are seldom available, and usually only one to two codes are selected based upon a cursory review of code capabilities. Regardless of whether a detailed or more cursory review is performed, it is important for the reviewer to be cognizant of the following factors and how they will affect final code selection:

1. Code Capabilities Consistent with:
    User needs
    Modeling objectives
    Site characteristics
    Contaminant characteristics
    Quality and quantity of data

2. Code Testing
    Documentation

Verification
Validation

3. History of Use Acceptance

The first aspect of the review concentrates on the appropriateness of the particular code to meet the modeling needs of the project. This subject is discussed in depth in Sections 3 and 4. The reviewer must also determine whether the data requirements of the code are consistent with the quantity and quality of data available from the site. Next, the review must determine whether the code has been properly tested for its intended use. Finally, the code should have some history of use on similar projects, be generally accepted within the modeling community, and be readily available to the public.

Evaluating a code in each of the three categories would take a significant effort, especially with respect to code testing. Theoretically, the reviewer should obtain a copy of the computer code, learn to use the code, select verification problem sets with known answers, and compare the results of the model to the benchmark problems. This task is complicated, largely because no standard set of benchmark problems exists, and the mathematical formulation for each process described within the code has to be verified through the benchmarking process. Primarily for this reason, selection of codes that are already widely tested and accepted is recommended. Code validation, which involves checking the model predictions against actual field investigations designed specifically to test the accuracy of the model, would almost never be practical during the code evaluation and selection process.

The selection and evaluation process presented in this section takes an approach which is consistent with industry standards by relying on published reports and user interviews as a substitute for actual hands-on testing. The result is a code selection and evaluation

process that provides a reasonable technical review that is relatively straightforward and takes a relatively short time to complete (Figure 5-1).

The model evaluation process presented in subsequent sections involves the following steps:

1. Contact the author or curator of the code and obtain the following:

   Documentation and other model-related publications

   List of users

   Information related to code testing

2. Read all publications related to the model, including documentation, technical papers, and testing reports.

3. Contact code users to find out their opinions.

4. Complete the written evaluation using the criteria shown in Table 5-1.

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

Most of the items in Table 5-1 should be described in the code documentation, although excessive use of modeling jargon may make some items difficult to find. For this reason, some assistance from an experienced modeler may be required to complete the evaluation. Detailed conversations with users can also be used to decipher cryptic aspects of the documentation.

The evaluation process recommended in the following sections relies on user opinions and published information to take the place of hands-on experience and testing. User opinions are especially valuable in determining whether the code functions as documented or has significant errors (bugs). In some instances, users have performed extensive testing and benchmarking or are familiar with published papers

documenting the use of the code. In essence, the proposed evaluation process substitutes second-hand experience for first-hand knowledge (user opinions) to shorten the time it takes to perform the review. It is also important to keep in mind that code selection is a very dynamic process, and multiple codes may need to be selected over the remedial lifetime of the site in order not only to reflect the remedial phase of the project, but also to remain current with existing technology.

Models attempt to simulate natural processes through a series of mathematical expressions. Because of the simplifications and assumptions needed to simulate these processes, all models will be inexact and imprecise. Thus, it is important to understand the magnitude of these deficiencies prior to the selection and/or application of any model. As a first step in this process, available documentation on the model must be reviewed and evaluated to determine if the documented capabilities of the model correspond with the objectives of the study. Code documentation is, however, often biased and in many cases incomplete. Furthermore, major inherent weaknesses of the code (e.g., omission of a process such as daughter in-growth) may not be highlighted. For this reason, it is important to secure or prepare independent reviews of any code before it is selected. These reviews can be obtained from the literature and supplemented with code-specific evaluations similar to those presented in this report. To the extent possible, the code should be exercised with representative data prior to its final selection. Failure to conduct such audits and benchmark testing may result in the inappropriate selection of a code and in a waste of time and resources.

As the user friendliness of the codes increase, the practical expertise of the user typically decreases. This is a potentially dangerous situation because of the large potential for code misuse. In prior years when codes were available only in mainframe-type environments, they were almost always used by "experts" who had knowledge of the capabilities of a selected code. Based on this knowledge, appropriate inputs would be used in a modeling effort. Now,
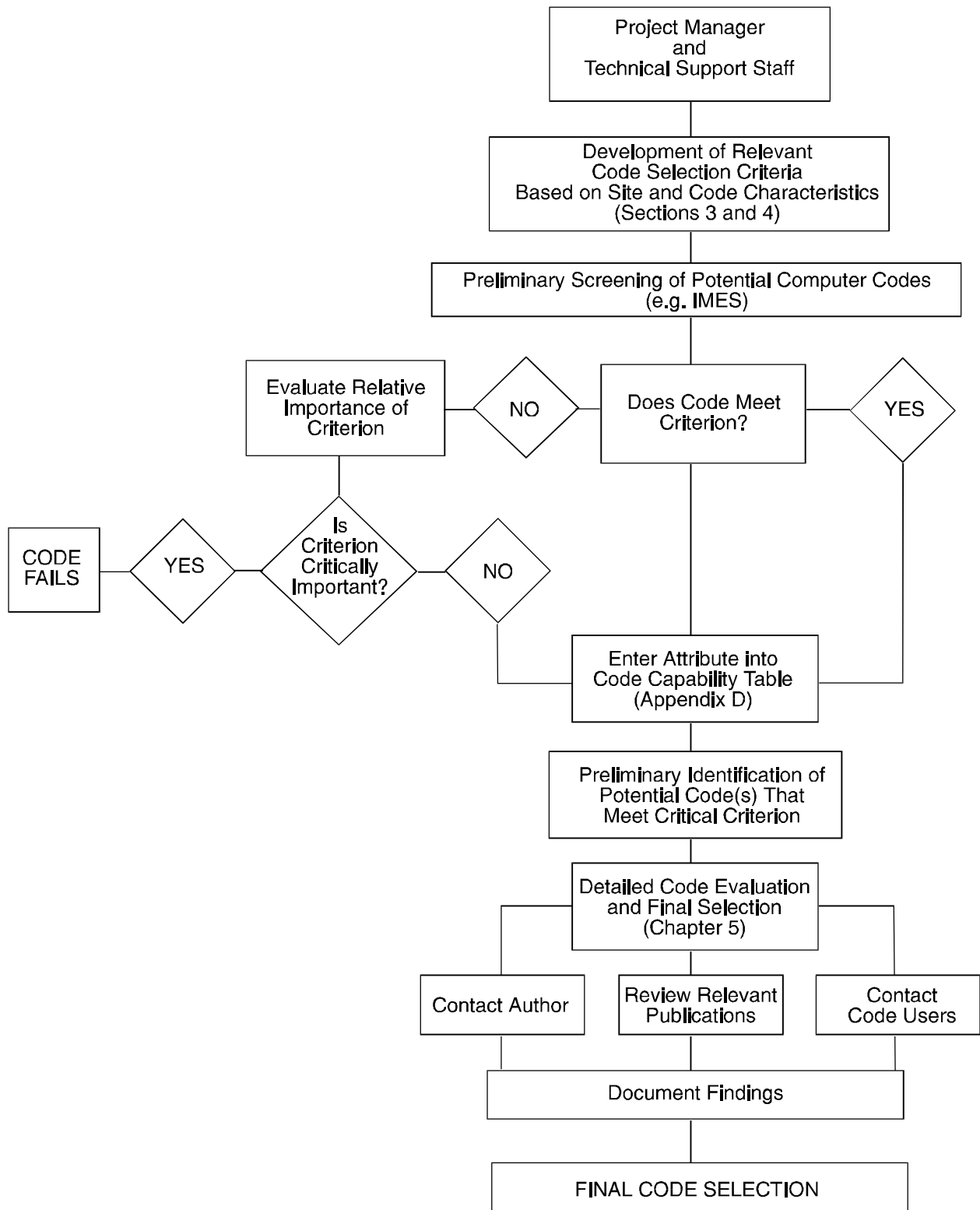
```
                    ┌─────────────────────┐
                    │   Project Manager   │
                    │         and         │
                    │ Technical Support   │
                    │       Staff         │
                    └─────────────────────┘
                              │
                    ┌─────────────────────────────┐
                    │  Development of Relevant     │
                    │  Code Selection Criteria     │
                    │  Based on Site and Code      │
                    │  Characteristics             │
                    │  (Sections 3 and 4)          │
                    └─────────────────────────────┘
                              │
                    ┌─────────────────────────────────────┐
                    │ Preliminary Screening of Potential   │
                    │ Computer Codes (e.g. IMES)           │
                    └─────────────────────────────────────┘
```

Figure 5-1. Code Selection Review Process

Table 5-1. Model Selection Criteria

CRITERIA
Section 5.2.1 Administrative Data
Author(s)
Development Objective (research, general use, education)
Organization(s) Distributing the Code
Organization(s) Supporting the Code
Date of First Release
Current Version Number
References (e.g., documentation)
Hardware Requirements
Accessibility of Source Code
Cost
Installed User Base
Computer Language (e.g., FORTRAN)
Section 5.2.2 Remedial Process
Scoping
Characterization
Remediation
Section 5.2.3 Site-Related Criteria
Boundary/Source Characteristics
Source Characteristics
Multiple Sources
Geometry
line
point
area
Release type
constant
variable
Aquifer System Characteristics
confined aquifers
unconfined aquifers (water-table)
aquitards
multiple aquifers
convertible
Soil/Rock Characteristics
heterogeneity in properties
anisotropy in properties
fractured
macropores
layered soils
Transport and Fate Processes
dispersion
advection
diffusion
density dependent
partitioning between phases
solid-gas
solid-liquid

Table 5-1. (Continued)

CRITERIA
equilibrium isotherm:
linear (simple retardation)
Langmuir
Freundlich
nonequilibrium isotherm
radioactive decay and chain decay
speciation
Multiphase Fluid Conditions
two-phase water/NAPL
two-phase water/air
three-phase water/NAPL/air
Flow conditions
fully saturated
variably saturated
Temporal discretization (steady-state or transient)

5.2.4	**Code-Related Criteria**
	Source Code Availability
	History of Use
	Code Usability
	Quality Assurance
	code documentation
	code testing
	Hardware Requirements
	Solution Methodology
	Code Output
	Code Dimensionality

default values are available, and it is possible for a user with only limited knowledge to produce a result. This result may, however, be highly inaccurate, and the user may be unaware of potential errors.

5.2 EVALUATION CRITERIA

The code(s) to be used for a particular application will satisfy a combination of needs defined by the intersection of regulatory requirements, site characteristics, and attributes of the code (Figure 5-2). The code review process outlined within the next sections is based upon a complete and consistent set of evaluation criteria. The evaluation process follows a scheme which groups evaluation criteria based on their similarity to one another. That grouping is reflected in the organization of Table 5-1. Yet the selection process must also account for the interrelationships between evaluation criteria. For example, certain groups of criteria will influence model selection and evaluation in different ways. Some criteria are important in choosing among codes, others in

controlling the way the code operates, and still others in how the results can be interpreted and applied. In the discussion that follows, these criteria are described in terms of the way in which they influence the code selection process.

5.2.1 Administrative Data

Few administrative data are, in fact, discriminatory criteria, yet some administrative data may be indicative of factors that exert overwhelming control over the use of codes. Thus, codes must be available and obtainable if they are to be used. The pedigree of a code, while it does not prevent the use of older versions, may imply that newer versions should be used. Undocumented codes would impose different emphasis on some of the other criteria used in the evaluation. These and other similar data will often control whether or not a code is used at all rather than how a code is applied to model a given problem.
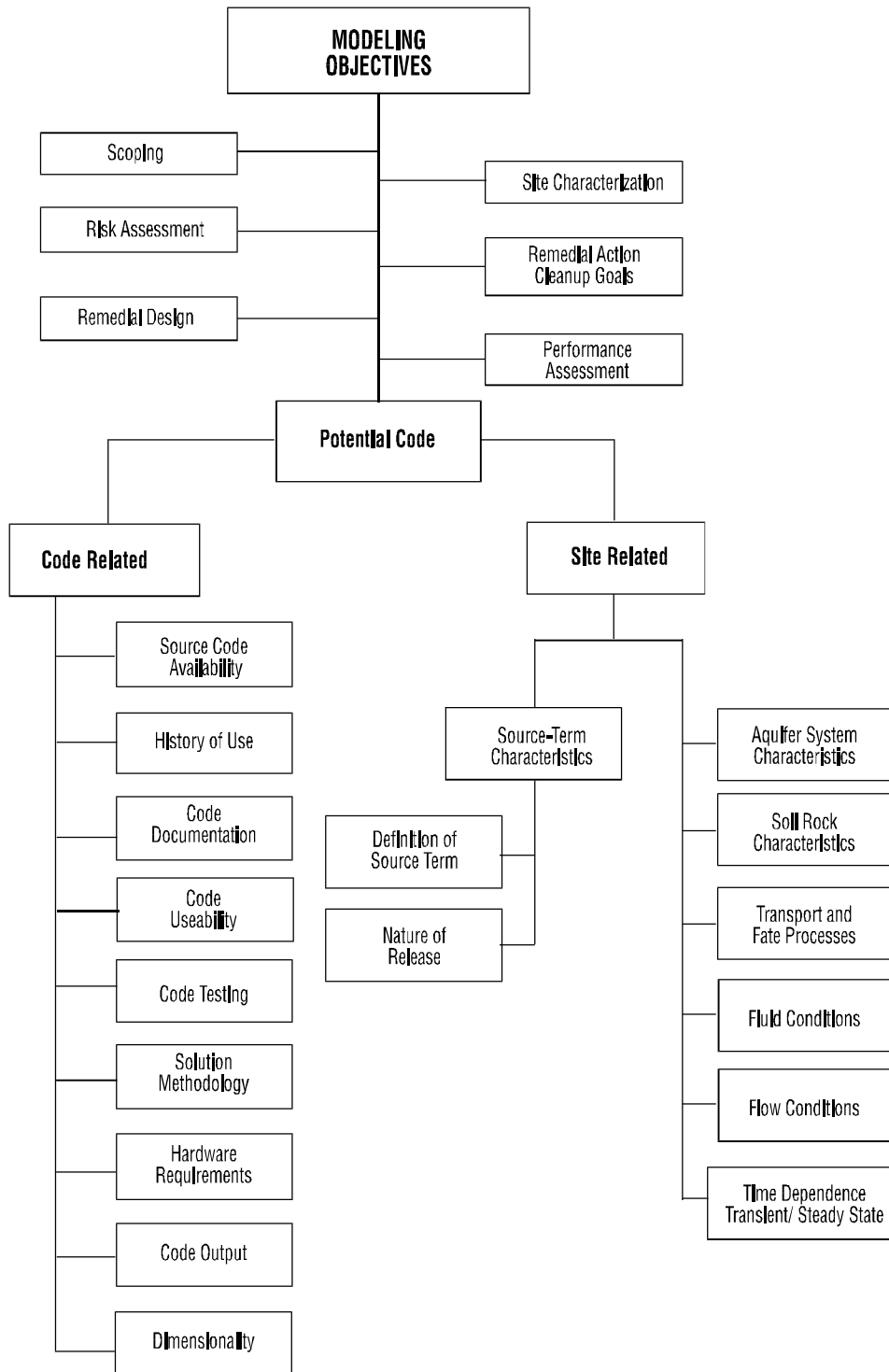
Figure 5-2. General Classification of Selection Criteria

5.2.2 Criteria Based on Phase in the Remedial Process

In general, regardless of the nature of the on-site contamination or the regulations being followed, the remedial process for contaminated sites may generally be divided into three discrete phases: the scoping phase, the site characterization phase, and the remediation phase.

The overall remedial process begins with the scoping phase, which is designed to assess the existing and potential risks that the contaminated site poses to human health and to the environment, and to develop site characterization plans. The objectives of the site characterization phase are to obtain sufficient information to support dose and risk assessment and to provide specific-site data required to identify feasible remedies and remedial action goals. The final phase of the remedial process is the selection, implementation, and evaluation of a remedy. In each phase of the remedial process, some information is available to assist in code selection. In the early stages, only broad-based decisions can be supported by the available data. However, as the process continues, the available information becomes more detailed, and the code selection can be based upon very specific criteria dictated by the following factors:

- **!** Modeling objectives
- **!** Waste characteristics
- **!** Hydrogeological characteristics
- **!** Fate and transport processes
- **!** Fluid and flow conditions
- **!** Local land use and demography

The influence that these criteria have on code selection is fully described in Sections 3 and 4.

5.2.3 Criteria Based on Waste and Site Characteristics

Section 4 presents a detailed description of how specific waste and site characteristics influence code selection. This section summarizes these points within the context of completing Table 5-1.

Transport of radionuclides through subsurface materials is influenced by the physical and chemical nature of both the transporting media (usually water) and the medium through which flow occurs (usually soil or rock). Criteria used to select or evaluate models

will be related to those processes that control the rate of flow of water through earth materials and those processes that either remove or deliver materials to water as it flows through earth materials. Subsurface flow is controlled by two master variables, hydraulic conductivity and driving force, and modified by the variability or continuity among those two variables. The hydraulic conductivity of porous or fractured subsurface materials is determined by the volumetric extent of voids or porosity within the material and the ease or rate with which fluids can move from one void to another. Flow within and between void spaces is a function of the properties of the fluid and the interaction of that fluid with the walls of the pore spaces. Since most ground-water flow consists of the movement of dilute water solutions at very low velocity, changes in fluid properties generally can be ignored.

The properties of the media through which the water flows and which are of overwhelming significance in controlling the velocity, direction, and quantity of flow are the relative degree of saturation of the materials, and the relative importance of fractured versus porous media flow. These site characteristics can generally be determined from a study of the type of soil and rock underlying a site.

The driving force, summed up within the concept of hydraulic head, for moving a fluid through subsurface materials is a combination of gravity and any external force applied to the ground-water flow system, such as areal recharge.

The factors that control flow through subsurface materials can be either uniformly or non-uniformly distributed. When they are uniformly distributed, a number of simplifying assumptions can be made about the nature of flow and transport. These simplifying assumptions have a great influence on the application of a mathematical model. When subsurface material properties are anisotropic and/or inhomogeneous, the direction and rate of flow will vary with position. These site characteristics alone have a marked effect on differentiating among codes which tend to be relatively simple and generalized and those that tend to be relatively complex and focused.

As solutions move through the spaces within subsurface materials, solutes may either be added to or removed from that solution. Which solutes are removed or added, and the quantity and rate at which

they are added or removed, is controlled by the geochemical nature of the solution and subsurface matrix. These geochemical process may be very complex, and their understanding may require an extensive base of physical and chemical data which are rarely available. Because of their complexity, geochemical models are generally developed as stand-alone modules that assume equilibrium (i.e., instantaneous reactions) and run independently of flow and transport models. The site characteristics that will trigger the requirement to utilize geochemical modeling are unusual subsurface chemistry such as sharp variations in chemical conditions (e.g., redox, pH) within soils and rocks.

Most subsurface transport models lump the effects of all geochemical reactions into the concept of the distribution coefficient (K_d) or related retardation factors because, without assuming any retardation, there would be a tendency to over-estimate the mobility of certain highly reactive radionuclides. There is, however, a very wide range of experimental- and field-determined values for distribution and retardation coefficients, and, in practice, as with so many other characteristics, these parameters are usually best determined on a site-specific basis. At many sites, it may be unknown whether predicted changes in the concentration of radionuclides in ground water can be adequately explained by the simplifying assumptions that underlay the K_d concept. As the assumption of a K_d to calculate radionuclide partitioning is theoretically valid only if: (1) chemical equilibrium exists among all aqueous species containing the solute; (2) reversible, linear sorption is the dominant process controlling exchange of the solute between the groundwater and the rock; and (3) transport of the solute by particulates (colloids) is insignificant. The site characterization program would need to determine if these assumptions are valid for radioelement transport in the ground water or if deviations from these conditions will produce significant errors. Consequently, focused geochemical modeling and laboratory studies may be needed to address these uncertainties.

The conceptual model is the set of hypotheses and assumptions about the physical characteristics (e.g., aquifer properties and boundary type) and the phenomena (e.g., model of fluid flow) that describes and postulates the behavior of the actual system. The approach to formulating an appropriate conceptual model(s) of the site integrates the generalized knowledge of physical processes with the available information. Therefore, a conceptual model provides a simplifying framework in which information can be organized and linked to processes that can be simulated with predictive models.

The mathematical model is the mathematical representation of the conceptual model. A mathematical model might include coupled algebraic, ordinary or partial differential, or integral equations that approximate the physical processes for a specified portion of the site conceptual model. The process by which the input and output of various mathematical models may be linked to support the conceptual model in order to meet the modeling objectives also plays an important role in the selection of a computer code(s). For example, the conceptual model may include flow and transport processes in both the unsaturated and saturated zones, in which case it would be possible to select one code that would simulate the flow and transport processes in the unsaturated zone at the desired level of detail and to use this model output as input into a second code which is capable of simulating flow and transport within the saturated zone. Therefore, the code selection and evaluation process has to reflect this availability to potentially dissect the conceptual model into discrete components.

The overall application of this approach will essentially be reduced to two considerations: (1) each component of the conceptual model is adequately described by the mathematical model; and (2) each of the separate mathematical models has been successfully integrated to where the sum of the parts is equal to the whole. The second consideration is more applicable to the application of the code and will be far more difficult to evaluate than the first.

Each code, however, should individually meet the basic criteria which are related to the site characteristics and which have been outlined as general components of the conceptual model that need to be considered when assessing the appropriateness of a computer code (Figure 5-3).
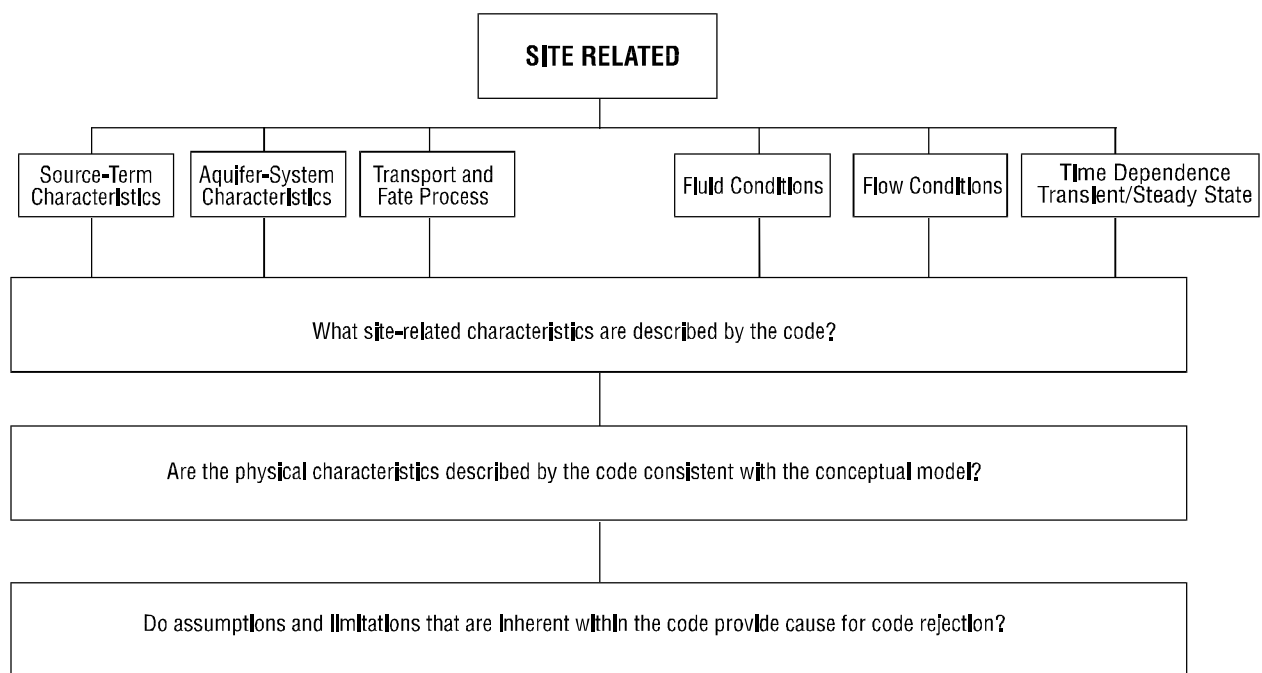
Figure 5-3. Physical, Chemical, and Temporal Site-Related Selection Criteria

These broad subjects are further broken down into their individual components both in the table presented as Appendix D and in the discussion presented in Sections 3 and 4.

5.2.4 Criteria Based on Code Characteristics

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. Therefore, 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
- Code Output
- Solution Methodology
- Code Dimensionality

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 (Figure 5-4). 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 for use by 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 (Figure 5-4). In fact, inability to obtain the necessary publications can be an indication 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

It is recommended that code selection criteria be closely tied to the quality assurance criteria which were followed during the development of the computer code. These criteria will be associated with the adequacy of the code testing and documentation (Figure 5-5).

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
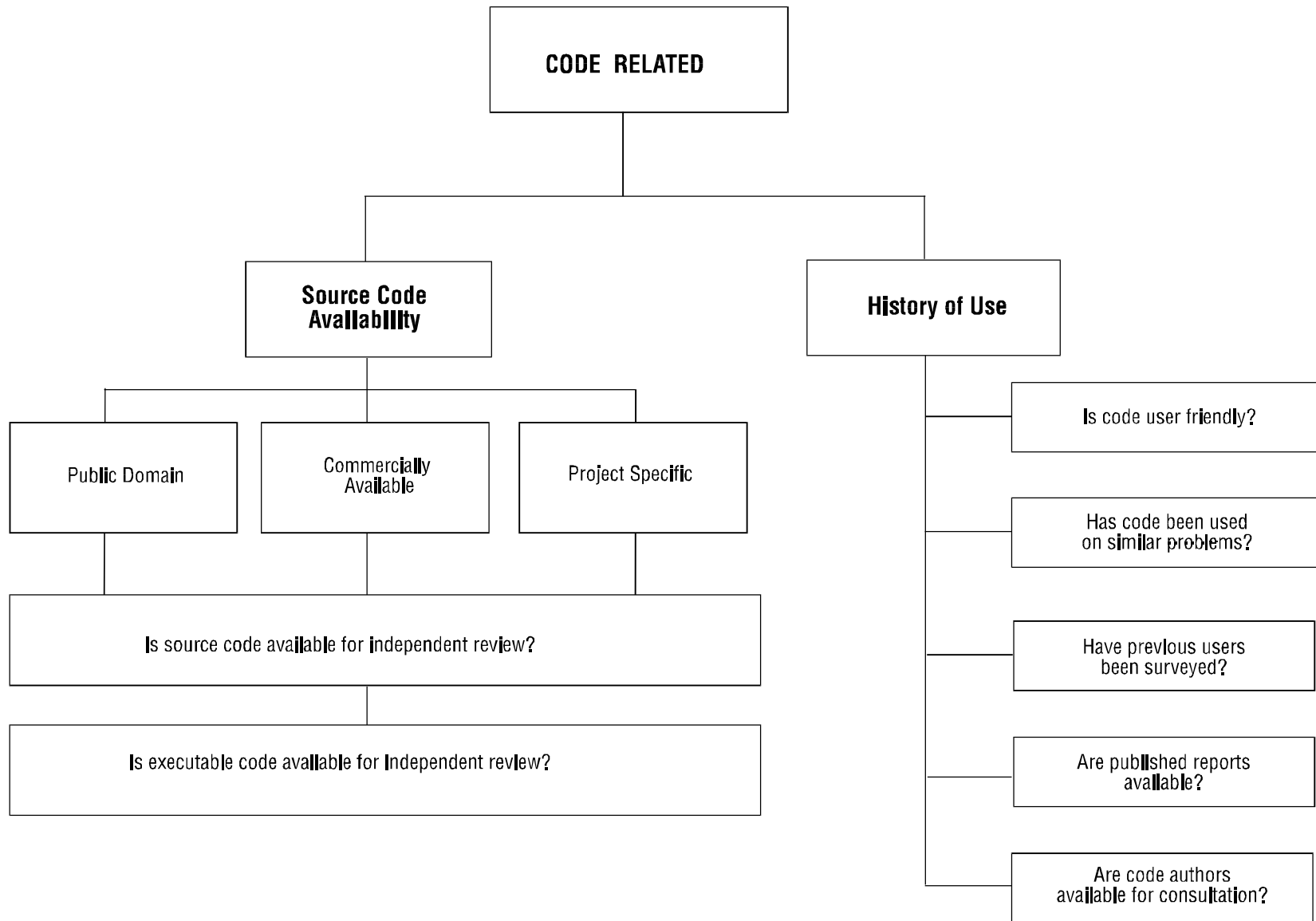
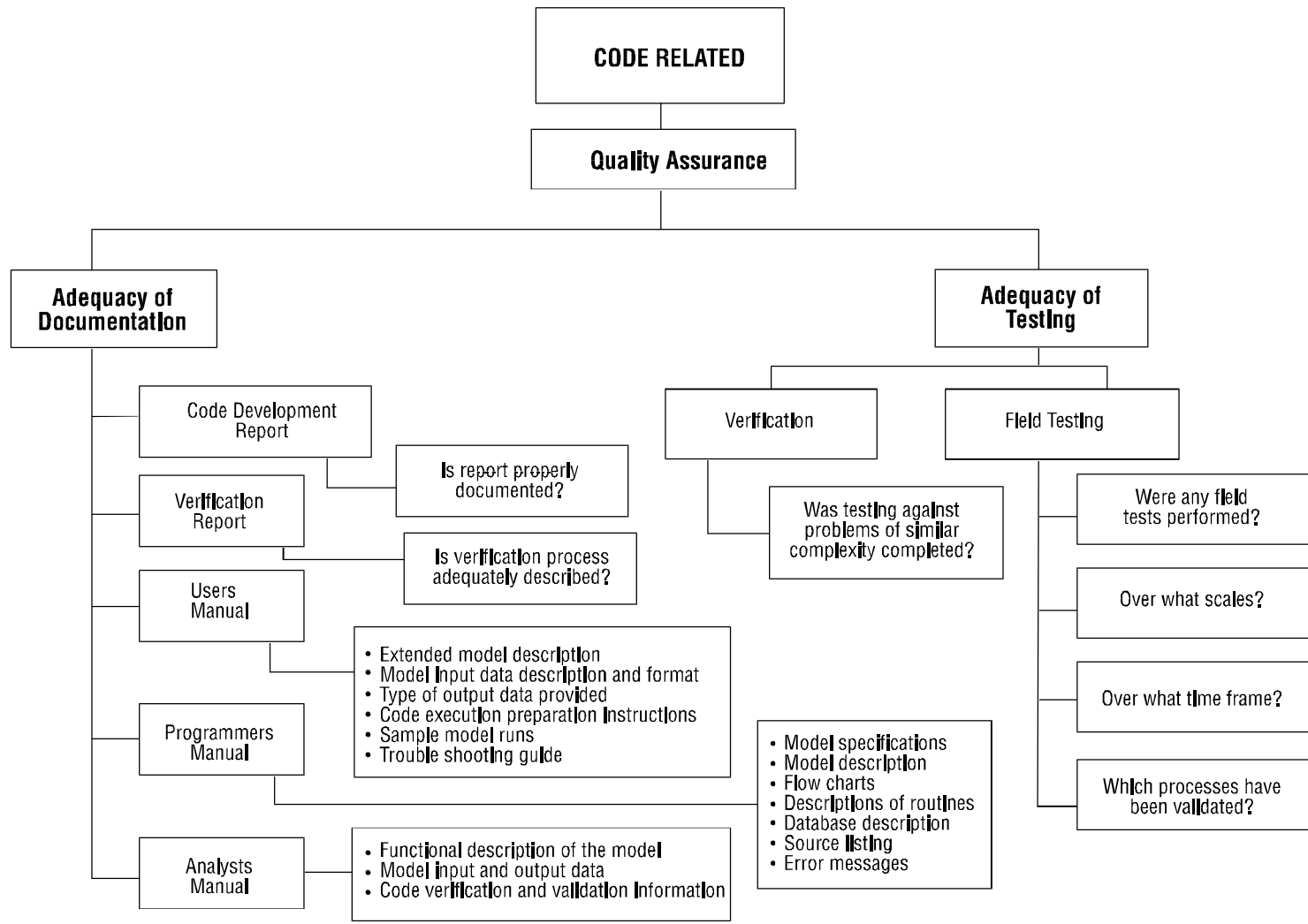Figure 5-4. Source Code Availability and History of Use Selection Criteria

Figure 5-5. Quality Assurance Selection Criteria

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 among the codes' numerical solutions with either 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 (FED81). This publication discusses the structure recommended for four types of manuals providing model information for managers, users, analysts and programmers. According to FEDSIM (1981), 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 (1992), 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. Furthermore, 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-orientated 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, programmers 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 (HEI89). Of the two major approaches available, the evaluation or review process is rather 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 with obtaining a correct solution.

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) present a compelling argument 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 (Figure 5-6). 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.

Mathematical Solution Methodology

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

Mathematical methods can be broadly classified as either deterministic or stochastic (Figure 5-7). 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. Stochastic methods pre-suppose 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 (i.e., Monte Carlo). 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.

Deterministic methods may 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 models are simpler to use than numerical models and can generally be solved with the aid of a calculator, although computers are also used. Analytical models 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 numerical models.

Analytical solutions are used in modeling investigations to solve many different kinds of problems. For example, aquifer parameters are obtained from aquifer pumping and tracer tests through the use of analytical models, and ground-water flow and contaminant transport rates can also be estimated with the use of analytical models.

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

The validity of the results from mathematical models depends strongly on the quality and quantity of the input data. Stochastic, numerical, and analytical codes have strengths and weaknesses inherent within their formulations, all of which need to be considered prior to their selection.

Code Output

One aspect of the computer code that is frequently ignored in the selection process is the form of the model output (Figure 5-8). It is true, however, that in most instances the actual output can be fashioned into the desired format, provided the model itself is consistent with required output (e.g., output in three dimensions cannot be obtained with a two-dimensional model).
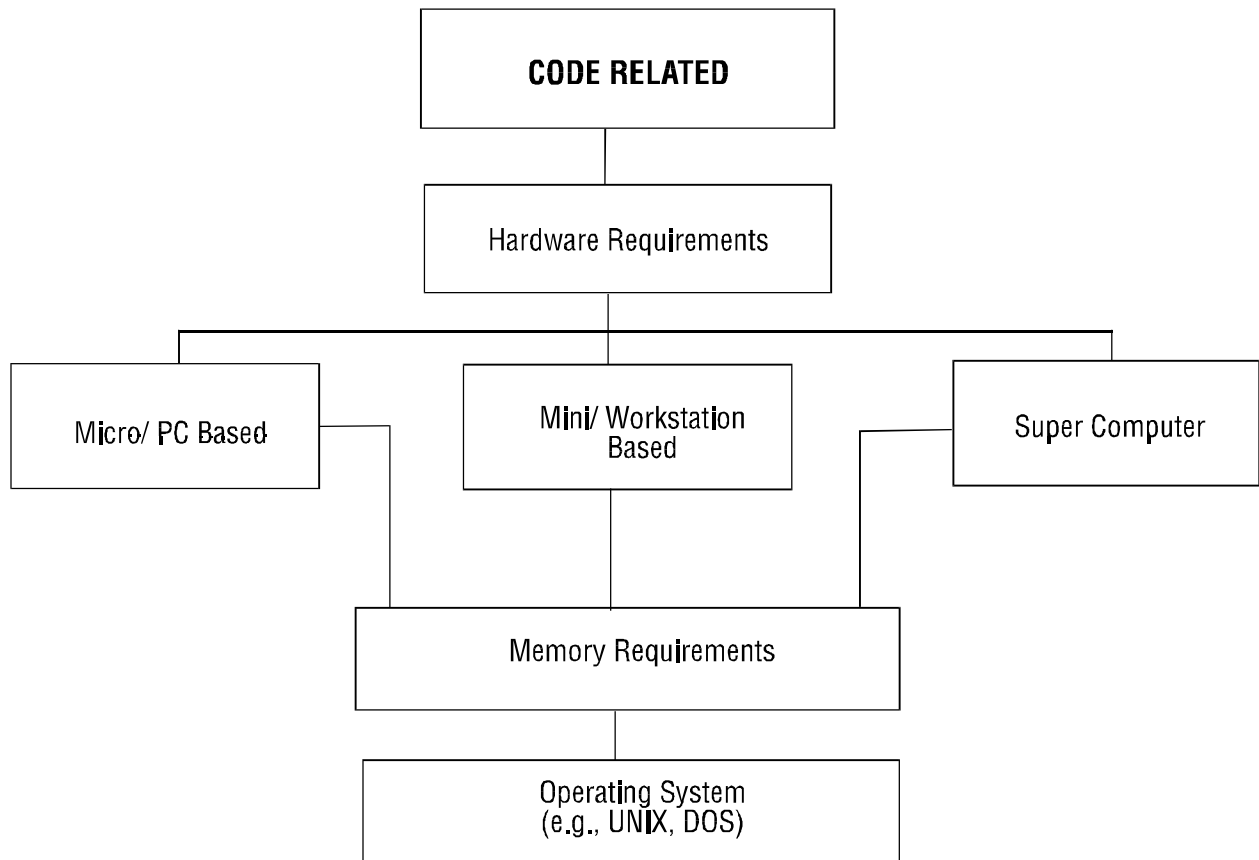
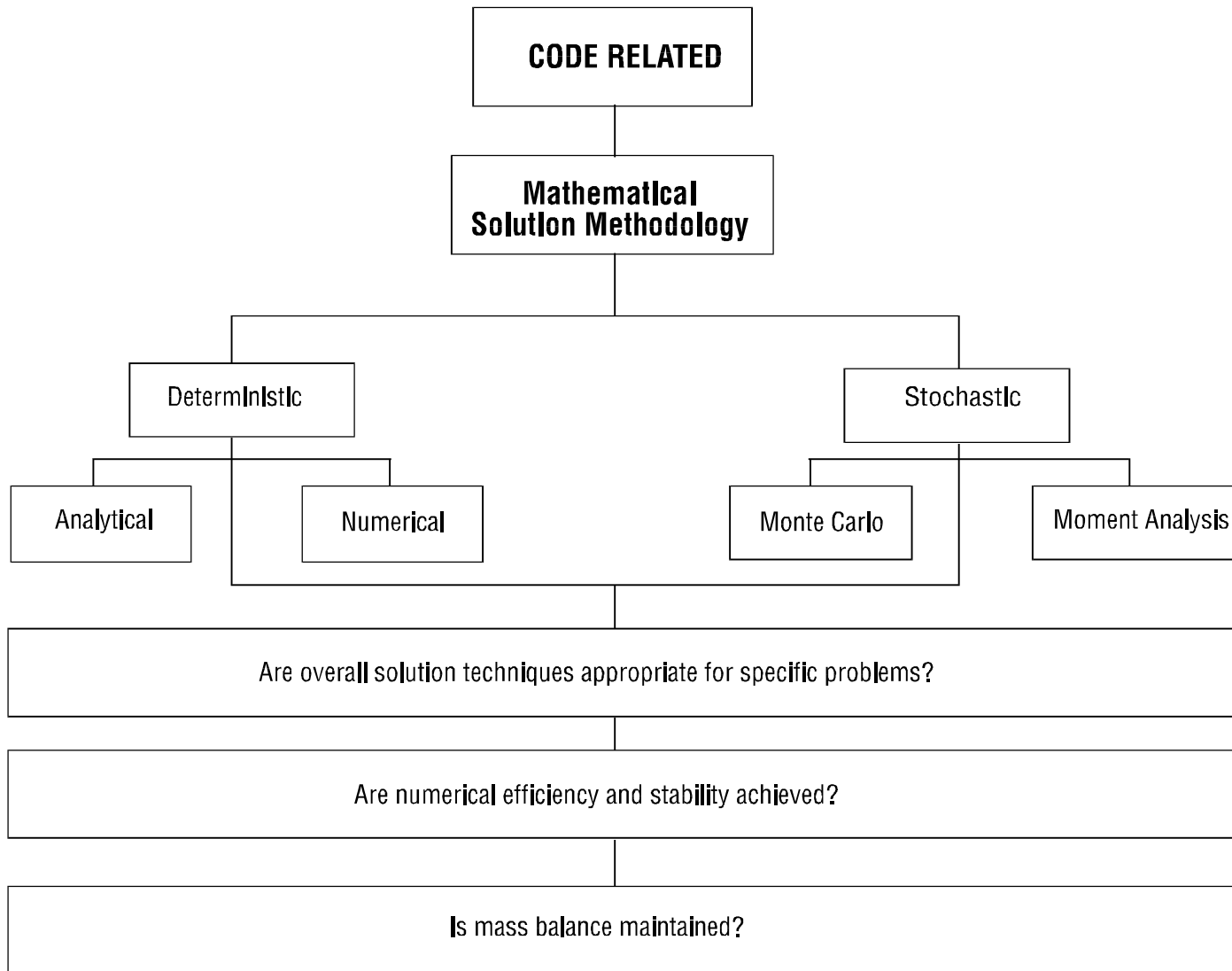Figure 5-6. Hardware Requirements Selection Criteria

Figure 5-7. Mathematical Solution Methodology Acceptance Criteria

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                    ┌─────────────────────────┐
                    │     CODE RELATED        │
                    └─────────────────────────┘
                                 │
                    ┌─────────────────────────┐
                    │      Code Output        │
                    └─────────────────────────┘
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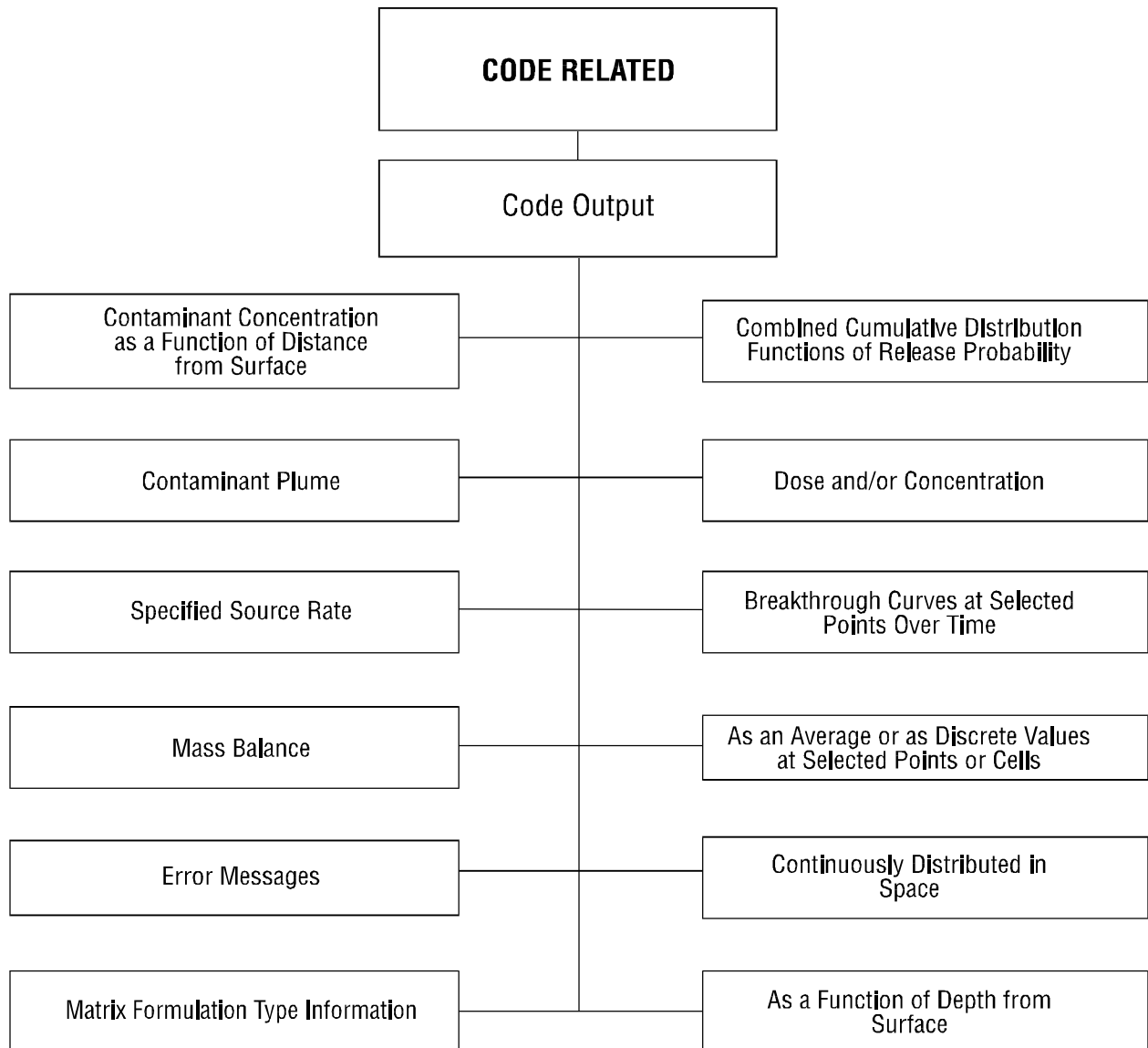| Contaminant Concentration as a Function of Distance from Surface	Combined Cumulative Distribution Functions of Release Probability
Contaminant Plume	Dose and/or Concentration
Specified Source Rate	Breakthrough Curves at Selected Points Over Time
Mass Balance	As an Average or as Discrete Values at Selected Points or Cells
Error Messages	Continuously Distributed in Space
Matrix Formulation Type Information	As a Function of Depth from Surface

Figure 5-8. Code Output Selection Criteria

In general, the model output is expressed in terms of hydraulic head, pressure, velocities, or solute concentrations. The spatial coverage of parameter output values is either dependent on the frequency of nodal spacing (numerical) or on the number of specified x and y coordinates (analytical) which are included in the model input files. Model output will also vary due to the inherent nature of the code itself. For example, codes that simulate movement in the unsaturated zone generally produce saturation profiles. These profiles indicate the percentage of the pore space that is filled with water, whereas saturated zone codes have no need for this capability because all of the pores below the water table are assumed to be filled completely with water. The single most important code selection criteria, relative to the model output, would be that the code provides mass-balance information. A mass-balance determination is a check to ensure that the amount of water or contaminant mass entering the system equals the amount exiting the system plus the change in the quantity stored in the system. If there is a significant discrepancy in the model's mass balance, something may be wrong with the numerical solution, although errors in the mass balance may also indicate problems with the mass-balance formulation itself. Therefore, mass-balance information not only provides a check on the mathematical formulations within the code, but also assists in ensuring that input parameter conversions and other errors have not been made. It is not uncommon for codes that do include mass-balance output to provide information (e.g., fluxes, heads) on specific boundaries as well as the source term, all of which can be used in the interpretation and evaluation of the predicted flow and solute transport directions and rates.

Code Dimensionality

The determination as to the number of dimensions that a code should be capable of simulating is based primarily upon the modeling objectives and the dimensionality of the processes the code is designed to simulate (Figure 5-9).

In determining how many dimensions are necessary to meet the objectives, it becomes necessary to gain a basic understanding of how the physical processes (e.g., ground-water flow and transport) are affected by the exclusion or inclusion of an additional dimension. It should be kept in mind that the movement of ground water and contaminants is usually controlled by advective and dispersive processes which are inherently three-dimensional. Advection is more responsible for the length of time (i.e., travel time) it takes for a contaminant to travel from the source term to a downgradient receptor, while dispersion directly influences the concentration of the contaminant along its travel path. This fact is very important in that it provides an intuitive sense for the effect dimensionality has on contaminant migration rates and concentrations.

As a general rule, the fewer the dimensions, the more the model results will over-estimate concentrations and under-estimate travel times. In a model with fewer dimensions, predicted concentrations will generally be greater because dispersion, which is a three-dimensional process, will be dimension limited and will not occur to the same degree as it actually would in the field. Similarly, predicted travel times will be shorter than the actual travel time, not because of a change in the contaminant velocities but because a more direct travel path is assumed. Therefore, the lower dimensionality models tend to be more conservative in their predictions and are frequently used for screening analyses.

One-dimensional simulations of contaminant transport usually ignore dispersion altogether, and contamination is assumed to migrate solely by advection, which may result in a highly conservative approximation. Vertical analyses in one dimension are generally reserved for evaluating flow and transport in the unsaturated zone. Two-dimensional analyses of an aquifer flow system can be performed as either a planar representation, where flow and transport are assumed to be horizontal (i.e., longitudinal and transverse components), or as a cross section where flow and transport components are confined to vertical and horizontal components.

In most instances, two-dimensional analyses are performed in an areal orientation, with the exception of the unsaturated zone, and are based on the assumption that most contaminants enter the saturated system from above and that little vertical dispersion occurs. However, a number of limitations accompany two-dimensional planar simulations. These include the inability to simulate multiple layers (e.g., aquifers and aquitards) as well as any partial penetration effects. Furthermore, because vertical
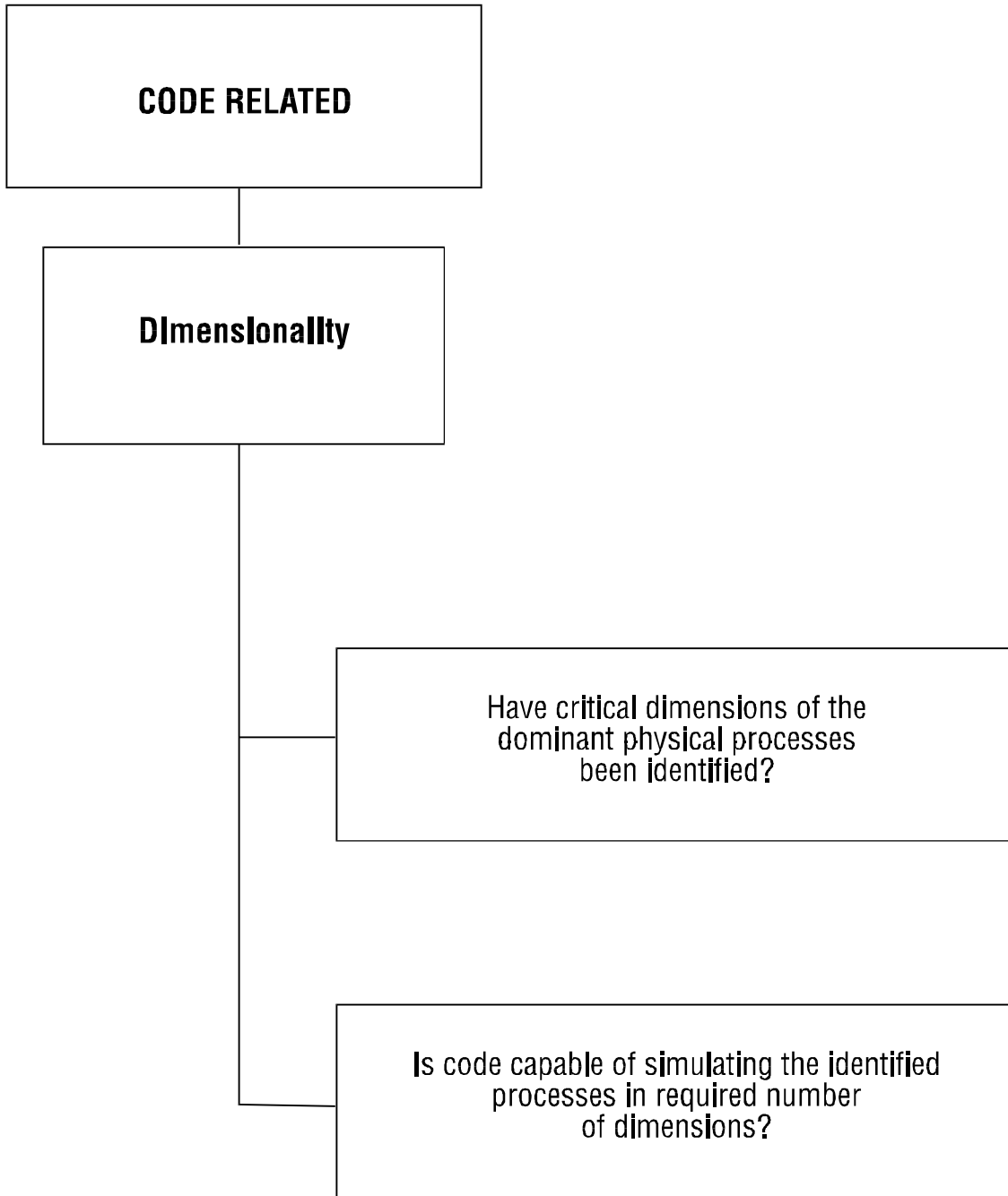
Figure 5-9. Code Dimensionality Selection Criteria

components of flow are ignored, an artificial lower boundary on contaminant migration has been automatically assumed which may or may not be the case.

A two-dimensional formulation of the flow system is frequently sufficient for the purposes of risk assessment provided that flow and transport in the contaminated aquifer are essentially horizontal. The added complexities of a site-wide, three-dimensional flow and transport simulation are often believed to outweigh the expected improvement in the evaluation of risk. Complexities include limited site-wide hydraulic head and lithologic data with depth and significantly increased computational demands.

Quasi-three-dimensional analyses remove some of the limitations inherent in two-dimensional analyses. Most notably, quasi-three-dimensional simulations allow for the incorporation of multiple layers; however, flow and transport in the aquifers are still restrained to longitudinal and transverse horizontal components, whereas flow and transport in the aquitards are even further restricted to vertical flow components only. Although partial penetration effects still cannot be accommodated in quasi-three-dimensional analyses, this method can sometimes provide a good compromise between the relatively simplistic two-dimensional analysis and the complex, fully three-dimensional analysis. This is the case, particularly if vertical movement of contaminants or recharge from the shallow aquifer through a confining unit and into a deeper aquifer is suspected.

Fully three-dimensional modeling generally allows both the geology and all of the dominant flow and transport processes to be described in three dimensions. This approach usually affords the most reliable means of predicting ground-water flow and contaminant transport characteristics, provided that sufficient representative data are available for the site.

Although the intrinsic dimensionality of the code should be an important consideration relative to the acceptance or rejection of the code, this determination will also be closely tied to the code application and modeling objectives.

REFERENCES

AND92   Anderson, M.P., and W.W. Woessner, 1992. Applied Groundwater Modeling: Simulation of Flow and Advective Transport. Academic Press, Inc., San Diego, California.

ASTM84   Am. Soc. for Testing and Materials (ASTM), 1984. Standard Practices for Evaluating Environmental Fate Models of Chemicals. Annual Book of ASTM Standards, E 978-84, Am. Soc. for Testing and Materials, Philadelphia, Pennsylvania.

BAE83   Baes, C.F., and R.D. Sharp, 1983. "A Proposal for Estimation of Soil Leaching Constants for Use in Assessment Models," Journal of Environmental Quality, 12 (1):17, January - March 1983.

BAC80   Bachmat, Y., J. Bredehoeft, B. Andrews, D. Holtz, and S. Sebastian, 1980. Ground-Water Management: The use of numerical models, Water Resources Monograph 5, American Geophysical Union, Washington, D.C., 127 pp.

BRY87   Bryant, J.L., and N.P. Wilburn, 1987. Handbook of Software Quality Assurance Techniques Applicable to the Nuclear Industry. NUREG/CR-4640, Off. of Nuclear Reactor Regulation, U.S. Nuclear Regulatory Commission, Washington, D.C.

DOE91   Department of Energy, 1991. Ground-Water Model Development Plan in Support of Risk Assessment, Decisional Draft, RL-91-62.

EPA88   Environmental Protection Agency, 1988. "Guidance for Conducting Remedial Investigations and Feasibility Studies Under CERCLA," EPA/540/G-89/004, OSWER Directive 9355.3-01, October 1988.

EPA90   Environmental Protection Agency, OSWER, 1990. OSWER Models Management Initiative: report on the usage of computer models in hazardous waste/superfund programs, Phase II Final Report, December 1990.

EPA91   Environmental Protection Agency, 1991. Integrated Model Evaluation System (IMES), prepared for Office of Health and Environmental Assessment, Exposure Assessment Group, Washington, D.C.

EPA93   Environmental Protection Agency, "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.

FED81   Federal Computer Performance Evaluation and Simulation Center (FEDSIM), 1981. Computer Model Documentation Guide. NBS Special Publ. 500-73, Inst. for Computer Science and Technology, Nat. Bur. of Standards, U.S. Dept. of Commerce, Washington, D.C.

GAS79   Gass, S.I., 1979. Computer Model Documentation: A Review and an Approach. NBS Special Publ. 500-39, Inst. for Computer Science and Technology, Nat. Bur. of Standards, U.S. Dept. of Commerce, Washington, D.C.

GIL88   Gilbert, T.L., M.J. Jusko, K.F. Eckerman, W.R. Hansen, W.E. Kennedy, Jr., B.A. Napier, and J.K. Soldat. "A Manual for Implementing Residual Radioactive Material Guidelines" (RES-RAD), U.S. Department of Energy, 1988, 217 pp.

GRA6-1   Environmental Protection Agency, 1992. Ground-Water Modeling Compendium, EPA/540/G-88/003.

GRA6-1   Environmental Protection Agency. Basics of Pump and Treat Ground-Water Remediation Technology, EPA/600/9-90/003.

GRA6-1   Environmental Protection Agency, 1988. Guidance on Remedial Actions for Contaminated Ground Water at Superfund Sites, EPA/540/G-88/003.

GRA6-1   EPA, 1988. Superfund Exposure Assessment Manual, EPA/540/1-88/001.

HAW88   Hawking, S.W., 1988. A Brief History of Time: From the Big Bank to Black Holes. Bantam Books, New York, 1988.

HEI92   van der Heijde, P.K.M., and O.A. Elnawawy, 1992. Compilation of Ground-water Models. GWMI 91-06. International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado.

HEI89   van der Heijde, P.K.M., 1989. Quality Assurance and Quality Control in Groundwater Modeling. GWMI 89-04. Internat. Ground Water Modeling Center, Holcomb Research Inst., Indianapolis, Indiana.

HEI88   van der Heijde, P.K.M., and M.S. Beljin, 1988. Model Assessment for Delineating Wellhead Protection Areas. EPA 440/6-88-002, Office of Ground-Water Protection, U.S. Environmental Protection Agency, Washington, D.C.

HUY91   Huyakorn, P.S., J.B. Kool and Y.S. Wu, October 1991. VAM2D - Variability Saturated Analysis Model in Two Dimensions, Version 5.2 with Hysteresis and Chain Decay Transport. NUREG/CR-5352, Rev. 1. U.S. Nuclear Regulatory Commission, Washington, D.C.

KON78   Konikow, L., and J. Bredehoeft, 1978. Computer model of two-dimensional solute transport and dispersion in ground water, U. S. Geological Survey Water Resources Investigation, Book 7, Chapter C2.

KON92   Konikow, L.F., and J.D. Bredehoeft, 1992. Ground-Water Models Cannot be Validated. Advances in Water Resources SWRENI 15(1): 75-83.

MCD88   McDonald, M.G., and A.W. Harbaugh, 1988. A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model. U. S. Geological Survey TWRI, Book 6, Chapter A1.

MER81   Mercer, J.W., and C.R. Faust, 1981. Ground Water Modeling, Nat. Water Well Assoc., Dublin, Ohio.

MOS92   Moskowitz, P., R. Pardi, M. DePhillips, and A. Meinhold, 1992. Computer models used to support cleanup decision making at hazardous waste sites, Brookhaven National Laboratory.

NRC86   Nuclear Regulatory Commission, 1986. "Update of Part 61 Impacts Analysis Methodology," Prepared by O.I. Oztunali, W.D. Pon, R. Eng, and G.W. Roles, NUREG/CR-4370, January 1986.

NRC90   Nuclear Regulatory Commission, 1990. "Background Information for the Development of a Low-Level Waste Performance Assessment Methodology. Computer Code Implementation and Assessment," Prepared by Sandia National Laboratory, NUREG/CR-5453, August 1990.

NRC90a   Nuclear Regulatory Commission, 1990. "Performance Assessment Methodologies for Low-Level Waste Facilities," Prepared by Sandia National Laboratory, NUREG/CR-5532, July 1990.

PAR92   Pardi, R.R., Daum, M.L., and Moskowitz, P.D., 1992. Environmental Characteristics of EPA, NRC, and DOE Sites Contaminated with Radioactive Substances. U. S. Environmental Protection Agency, Office of Radiation Programs, Washington, D.C.

SHE90   Sheppard, M.I., and E.L. Gershey, 1990. "Default Solid Soil/Liquid Partition Coefficients, Kds, for Four Major Soil Types: A Compendium," Health Physics, 59 (4):471, October 1990.

TAY85   Taylor, J.K., 1985. What is Quality Assurance? In: J.K. Taylor and T.W. Stanley (eds.), Quality Assurance for Environmental Measurements, pp. 5-11. ASTM Special Technical Publication 867, Am. Soc. for Testing and Materials, Philadelphia, Pennsylvania.

ZHE90   Zheng, C., 1990. A Modular Three-Dimensional Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Ground-Water Systems, Prepared for the United States Environmental Protection Agency, Robert S. Kerr Environmental Research Laboratory, Ada, Oklahoma.

BIBLIOGRAPHY

Barney, G.S., J.D. Navratil, and W.W. Schultz, 1984. Geochemical Behavior of Disposed Radioactive Waste, American Chemical Society, Washington, D.C.

Bear, J., 1979. Hydraulics of Ground Water. McGraw-Hill Book Company.

Boonstra, J. and N.A. de Ridder, 1981. Numerical Modeling of Ground-Water Basins. ILRI Publication 29.

de Marsily, G., 1986. Quantitative Hydrogeology. Ground-Water Hydrology for Engineers, Academic Press, Inc.

Drever, J.I., 1982. The Geochemistry of Natural Waters. Prentice-Hall Inc., Englewood Cliffs, N.J.

Environmental Protection Agency, 1985. "Modeling Remedial Actions at Uncontrolled Hazardous Waste Sites," EPA/540/2-85/001, Office of Solid Waste and Emergency Response and Office of Research and Development.

Environmental Protection Agency, 1987. "The Use of Models in Managing Ground-Water Protection Programs," EPA/600/8-87/003, Robert S. Kerr Environmental Research Laboratory.

Environmental Protection Agency, 1988. "Groundwater Modeling: An Overview and Status Report," EPA/600/2-89/028, Robert S. Kerr Environmental Research Laboratory.

Environmental Protection Agency, 1989. "Predicting Subsurface Contaminant Transport and Transformation: Considerations for Model Selection and Field Validation," EPA/600/2-89/045, Robert S. Kerr Environmental Research Laboratory.

Environmental Protection Agency, 1992. "Quality Assurance and Quality Control in the Development and Application of Ground-Water Models," EPA/600/R-93/011, Office of Research and Development.

Environmental Protection Agency, 1992. "Ground-water Modeling Compendium," EPA-500-B-92-006, Office of Solid Waste and Emergency Response.

Environmental Protection Agency, 1993. "Compilation of Ground-Water Models," EPA/600/R-93/118, Office of Research and Development.

Fetter, C.W., 1993. Contaminant Hydrogeology. Macmillan Publishing Company.

Freeze, R.A. and J.A. Cherry, 1979. Ground Water. Prentice-Hall, Inc.

Hern, S.C. and S.M. Melancon, 1986. Vadose Zone Modeling of Organic Pollutants. Lewis Publishers, Inc. Chelsea, Michigan.

Istok, J., 1989. Ground-Water Modeling by the Finite Element Method, Water Resources Monograph 13, American Geophysical Union.

Jorgensen, S.E., 1984. Modelling the Fate and Effect of Toxic Substances in the Environment, Developments in Environmental Modelling, 6.

Jury, W.A., W.R. Gardner and W.H. Gardner, 1991. Soil Physics, Fifth Edition. John Wiley & Sons, Inc.

Liggett, J.A., and P.L-F. Liu, 1983. The Boundary Integral Equation Method for Porous Media Flow. School of Civil and Environmental Engineering, Cornell University, N.Y.

Matthess G., 1982. The Properties of Ground Water. John Wiley & Sons, Inc.

Resources Management and Information Staff, 1992. Ground-Water Modeling Compendium OSWER Models Management Initiative: Pilot Project on Ground-Water Modeling. Office of Solid Waste and Emergency Response.

Thomas, R.G., 1973. "Groundwater Models," Food and Agriculture Organization of the United Nations, Rome, FAO Irrigation and Drainage Paper.

Wang, H.F. and M.P. Anderson, 1982. Introduction to Ground-Water Modeling, Finite Difference and Finite Element Methods. W.H. Freeman and Company.

APPENDIX A

GLOSSARY

GLOSSARY

ACTINIDES - Elements 90 through 103.

ADSORPTION - Physical attraction and adhesion of gas, vapor, or dissolved molecules to the surface of solids without chemical reaction.

ADVECTION - The process by which solutes are transported by the bulk motion of flowing ground water.

ALLUVIAL FLOODPLAIN - The lowland adjacent to a river, usually dry but subject to flooding when the river overflows its banks. It is that flat area constructed by the present river in the present climate. It is built of **alluvium** carried by the river during floods and deposited in the sluggish water beyond the influence of the swiftest current.

ANALYTICAL MODEL - A model based on known initial and boundary conditions which incorporates a continuous exact solution of a simple flow or solute transport equation such as Darcy's Law. Analytical models are ordinarily restricted to conditions of homogeneous, isotropic flow, and transport.

ANION EXCLUSION - Negatively charged rock surfaces can affect the movement of anions, by either retarding the movement of anions by not allowing negatively charged radionuclides to pass through the pore opening or by enhancing the transport of ions by restricting the anion movement to the center of the pore channel where ground-water velocities are higher.

ANISOTROPIC - Having some physical property that varies with direction of flow.

AQUIFER - A unit of porous material capable of storing and transmitting appreciable quantities of water to wells.

AQUITARD - A saturated, but poorly permeable bed, formation, or group of formations that can store ground water and also transmit it slowly from one aquifer to another.

ARTESIAN WELL - A well deriving its water from a confined aquifer in which the water level in the casing stands above the top of the confined aquifer.

BASALT - A general term for dark-colored iron- and magnesium-rich igneous rocks, commonly extrusive, but locally intrusive. It is the principal rock type making up the ocean floor.

BEDROCK - A general term for the rock, usually solid, that underlies soil or other unconsolidated material.

BIOFIXATION - The binding of radionuclides to the soil/organic matrix due to the action of some types of microorganisms and plants, thus affecting mobility of the radionuclide.

BULK DENSITY - The mass or weight of oven-dry soil per unit bulk volume, including air space.

CALIBRATION - The process by which a set of values for aquifer parameters and stresses is found that approximates field-measured heads and flows. It is performed by trial-and-error adjustment of parameters and boundary conditions or by using an automated parameter estimation code.

CAPTURE ZONE - The portion of the flow system that contributes water to a well or a surface water body such as a river, ditch, or lake.

CHAIN DECAY - Form of radioactive decay in which several daughter products may be produced before the parent species decays to a stable element.

CLAY - (Clay particles are mineral particles < 0.002 mm. in diameter). In the grading of soils by texture, clay is the extreme of fineness.

CONFINED AQUIFER - An **aquifer** which is overlain by a unit of porous material that retards the movement of water.

CURVILINEAR ELEMENTS - Specialized elements used by finite-element computer codes that can be spatially deformed to mimic the elevations of the upper and lower surfaces of the hydrogeologic units.

DARCY'S LAW - A derived equation that can be used to compute the quantity of water flowing through an aquifer assuming that the flow is laminar and inertia can be neglected.

DETERMINISTIC MODEL - A model whose output is fixed by the mathematical form of its equations and the selection of a single value for each input parameter.

DIP - The angle to the horizontal (slope) that a geologic unit may have.

DISCHARGE - The volume of water flowing in a stream or through an aquifer past a specific point in a given period of time.

DISPERSION - A mixing phenomenon linked primarily to the heterogeneity of the microscopic velocities inside the porous medium.

DISTRIBUTION COEFFICIENT - The slope of a linear **Freundlich isotherm**.

EFFECTIVE POROSITY - The volume of the void spaces through which water or other fluids can travel in a rock or sediment divided by the total volume of the rock or sediment.

FACILITATIVE TRANSPORT - 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 be predicted by their respective distribution coefficients.

FAULT - A fracture or a zone of fractures along which there has been displacement of the sides relative to one another parallel to the fracture.

FINITE DIFFERENCE - A particular kind of a digital computer model based upon a rectangular grid that sets the boundaries of the model and the nodes where the model will be solved.

FINITE ELEMENT - A digital ground-water flow model where the aquifer is divided into a mesh formed of a number of polygonal cells.

FLOCCULATION - The agglomeration of finely divided suspended solids into larger, usually gelatinous, particles; the development of a "floc" after treatment with a coagulant by gentle stirring or mixing.

FRACTURED LITHOLOGY - Porous media which is dissected by fractures.

FREUNDLICH ISOTHERM - An empirical equation that describes the amount of solute adsorbed onto a soil surface.

GEOCHEMICAL FACIES - A unit of material of similar physical properties that was deposited in the same geologic environment.

GROUT CURTAIN - An underground wall designed to stop ground-water flow; can be created by injecting grout into the ground, which subsequently hardens to become impermeable.

GROUTING - The operation by which grout is placed between the casing and the sides of the well bore to a predetermined height above the bottom of the well. This secures the casing in place and excludes water and other fluids from the well bore.

HETEROGENOUS - Pertaining to a substance having different characteristics in different locations.

HYDRAULIC CONDUCTIVITY - A coefficient of proportionality describing the rate at which water can move through a permeable medium. The density and kinematic viscosity of the water must be considered in determining hydraulic conductivity. The rate of flow of water in unit volume per unit of time through a unit cross section of area of geologic material under a unit **hydraulic gradient**, at the prevailing temperature.

HYDRAULIC GRADIENT - The change in total head with a change in distance in a given direction. The direction is that which yields a maximum rate of decrease in head.

HYDRODYNAMIC DISPERSION - The process by which ground water containing a solute is diluted with uncontaminated ground water as it moves through an **aquifer**.

HYDROFRACTURING - The process in which fluid is added to an aquifer at sufficient pressures to where the pore pressure in the rock causes the rocks to fracture.

HYDROSTATIGRAPHIC UNIT - A formation, part of a formation, or group of formations in which there are similar hydrologic characteristics allowing for grouping into **aquifers** or confining layers.

HYSTERESIS - A term which describes the fact that wetting and drying curves for a certain soil (pressure head versus volumetric water content) under partially saturated conditions, are not the same.

IMMISCIBLE - Substances that do not mix or combine readily.

IN-SITU VITRIFICATION - Process by which electrodes are used to heat the soil-waste matrix to temperatures high enough to melt soils and destroy organics by pyrolysis.

INTRINSIC PERMEABILITY - Pertaining to the relative ease with which a porous medium can transmit a liquid under a hydraulic or potential gradient. It is a property of the porous medium and is independent of the nature of the liquid or the potential field.

INVERSE MODEL - The model in which values of the parameters and the hydrologic stresses are determined from the information about heads.

ION EXCHANGE - A process by which an ion in a mineral lattice is replaced by another ion that was present in an aqueous solution.

LANGMUIR ISOTHERM - An empirical equation that describes the amount of solute adsorbed onto a soil surface.

LAYERED LITHOLOGY - Interbedded geologic units (e.g., sand, clay, gravel).

LEACH - The removal of soluble chemical elements or compounds by the passage of water through the soil.

LEACHATE - Water that contains a high amount of dissolved solids and is created by liquid seeping from a landfill.

LIMESTONE - A sedimentary rock consisting chiefly of calcium carbonate, primarily in the form of the mineral calcite.

LITTORAL - Pertaining to the ocean environment between the high tide and the low tide.

LOADING RATES - The rate at which contaminants and/or water enters the model domain.

LOW PERMEABILITY BARRIERS - Vertical or horizontal obstructions that are of sufficiently low permeability to retard significantly the migration of water and/or contaminants.

MACROPORES - Large or noncapillary pores. The pores, or voids, in a soil from which water usually drains by gravity. Is differentiated from a micropore, or capillary pore space, which consists of voids small enough that water is held against gravity by capillarity. Sandy soils have a large macropore, or noncapillary pore space and a small micropore, or capillary, pore space. Non-granular clayey soils are just the reverse.

MATRIX DIFFUSION - The diffusion of radionuclides from water moving within fractures, or coarse-grained material, into the rock matrix or finer grained clays.

METAMORPHIC ROCK - Any rock derived from preexisting rocks by mineralogical, chemical, and/or structural changes, essentially in the solid state, in response to marked changes in temperature, pressure, shearing stress, and chemical environment, generally at depth in the Earth's crust.

MOLECULAR DIFFUSION - Dispersion of a chemical caused by the kinetic activity of the ionic or molecular constituents.

NON-AQUEOUS PHASE LIQUIDS (NAPL) - Liquids that are **immiscible** in water.

NUMERICAL MODEL - One of five methods (finite-difference, finite element, integrated finite difference, boundary integral equation method, and analytical elements) used to approximate by means of algebraic equations the solution of the partial differential equations (governing equation, boundary, and initial conditions) that comprise the mathematical model. Numerical models can be used to describe flow under complex boundary conditions and where **aquifer** parameters vary within the model area.

ORGANIC COMPLEXATION - The formation of organic complexes by the combination of organic material or radionuclides.

PARTICLE TRACK - The movement of infinitely small imaginary particles placed in the flow field.

PARTITIONING - The process by which a contaminant, which was originally in solution, becomes distributed between the solution and the solid phase.

PERCHED WATER - Unconfined ground water separated from an underlying main body of ground water by an unsaturated zone.

POROUS MEDIA - Rocks that are not dissected by discrete features (e.g., macropores, fractures).

PROPRIETARY - A code in which the ownership rights are held by a company or organization.

RADIAL FLOW - The flow of water in an aquifer toward a vertically oriented well.

RADIOACTIVE DECAY - The change of a nucleus into another nucleus (or a more stable form of the same nucleus) by the loss of a small particle or a gamma ray photon.

RECHARGE - The addition of water to the zone of saturation; also, the amount of water added.

RETARDATION FACTOR/COEFFICIENT - A measure of the capability of adsorption within the porous media to impede the movement of a particular radionuclide being carried by the fluid.

SANDSTONE - A sedimentary rock composed of abundant rounded or angular fragments of sand set in a fine-grained matrix (silt or clay) and more or less firmly united by a cementing material.

SATURATED ZONE - The zone in which the voids in the rock or soil are filled with water at a pressure greater than atmospheric. The water table is the top of the saturated zone in an unconfined aquifer.

SECONDAY MINERALIZATION - Mineralization that occurred later than the rock enclosing it.

SEDIMENTARY ENVIRONMENT - An environment in which the rocks are formed by the accumulation and cementation of mineral grains transported by wind, water, or ice to the site of deposition or chemically precipitated at the site of deposition.

SHALE - A fine-grained sedimentary rock, formed by the consolidation of clay, silt, or mud. It is characterized by finely laminated structure and is sufficiently indurated so that it will not fall apart on wetting.

SILT - Soil particles between 1/256 and 1/2 mm in diameter, smaller than sand and larger than clay.

SOLUTION FEATURES - An opening resulting from the decomposition of less soluble rocks by water penetrating pre-existing interstices, followed by the removal of the decomposition products.

SOURCE TERM - The quantity of radioactive material released to the biosphere, usually expressed as activity per unit time. Source terms should be characterized by the identification of specific radionuclides and their physical and chemical forms.

SPECIATION - The chemical form of the radionuclide, which can influence its solubility and therefore its rate of transport by limiting the maximum concentration of the element dissolved in the aqueous phase.

APPENDIX B

GROUND-WATER MODELING RESOURCES

ELECTRONIC MEDIA-BASED SOURCES OF ASSISTANCE

Bulletin Boards

Access to bulletin boards is made via modem either by direct dialing or through a communication system like TELNET or TYMNET. Access to most systems is controlled by the use of login protocols and passwords obtained from the system operator. Examples of existing systems include:

Name:	**ORB-BBS**
Purpose:	Information about ORD operations and software available through ORD
Maintained by:	U. S. Environmental Protection Agency
	Office of Research and Development
	Cincinnati, Ohio
System Operator:	Charles W. Gulon
Modem Phone(s):	(513) 569-7610 (1200-2400 bps)
	(800) 258-9605 (1200-9600 bps)
	(513) 569-7700 (1200-9600 bps)
	(513) 569-7272
Communication Parameters:	1200, 2400, 4800, 9600 - N-8-1
Hours/Cost:	24 hours/7 days - Free

Name:	**CEAM**
Purpose:	Supports the use of exposure assessment models, especially those used to model the transport of agricultural chemicals.
Maintained by:	U. S. EPA
	Office of Research and Development
	Athens, Georgia
System Operator:	David Disney
Modem Phone(s):	(706) 546-3402
	(FTS) 250-3549
Voice Phone(s):	(706) 546-3590
	(706) 546-3136
Communication Parameters:	1200, 2400 - N-8-1
Hours/Cost:	24 hours/7 days - Free

Name:	**CSMoS**
Purpose:	The Center for Subsurface Modeling Support (CSMoS) provides ground-water modeling software and services to public agencies and private companies throughout the nation.
Maintained by:	U.S. Environmental Protection Agency
	Center for Subsurface Modeling Support
	R.S. Kerr Environmental Research Laboratory
System Operator:	Dr. David S. Burden
Voice Phone(s):	(405) 332-8800

Bulletin Boards (Continued)

Name: **CLU-IN**
Purpose: Current events information for hazardous waste cleanup professionals,
                               innovative technologies, and access to databases.
Maintained by: U. S. EPA
                               Office of Solid Waste and Emergency Response
                               Technology Innovation Office
                               Washington, D.C.
System Operator: Dan Powell
Modem Phone(s):   (301) 589-8366
Voice Phone(s):   (301) 589-8368
Communication Parameters: 1200, 2400 - N-8-1
Hours/Cost: 24 hours/7 days - Free

Name: **USGS BBS**
Purpose: General information from USGS
Maintained by: U. S. Geological Survey
System Operator:
Modem Phone(s):   (703) 648-7127
                               (703) 648-4168
Voice Phone(s):   (703) 648-7000
Communication Parameters:
Hours/Cost: CD-ROM conference is Free

Name: **ESDD**
Purpose: Earth Science Data Directory - list of nationwide databases of earth
                               science data
Maintained by: U. S. Geological Survey
                               Reston, Virginia
System Operator: Joe Kemper
Modem Phone(s):   (703) 648-4100
                               (703) 648-4200
Voice Phone(s):   (703) 648-7112\
Communication Parameters: 300, 1200, 2400, 9600 - 7-M-1
Hours/Cost: Free (call voice phone for ID number)

Networks

In order to join a network conference, you must have access to a computer system that is a node in that network. Access to the network can then be made by subscribing to a LISTSERV or joining a newsgroup. Subscribing to a LISTSERV is accomplished using the e-mail facility of a local node. A simple mail message is sent, SUB **name**, where **name** is one of the address names below. Mail from that network conference will then appear in the user's e-mailbox. Unsubscribing is accomplished by sending the message UNSUB **name**.

In addition, if the remote system permits, the user can access the remote node of the network via software like **f**ile **t**ransfer **p**rotocol (FTP). Within a system like ftp, the user has direct access to the remote node as if it were a local computer, and in some cases, software on the remote system can be run and the results later transferred to the local node.

To FTP a remote site, the user types ftp **node** from the local node where **node** is one of the address names below. In most cases, the remote node will require a login name and password if the ftp process is successful. The login name is often **anonymous** and the password **guest**, although other login strings are often called for and can only be determined by contacting the individual in charge of the remote system.

Name: **AQUIFER@BACSATA**
Network: BITNET
Purpose: Discussion group on various ground-water protection issues.
Access: LISTSERV

Expert Systems

Name: **Integrated Model Evaluation System**
Source: Environmental Protection Agency
                        Office of Solid Waste and Emergency Response
                        Versar, Inc.
                        Ecological Sciences and Analysis Division
                        9200 Runsey Road
                        Columbia, Maryland 21045
System Requirements: MSDOS
Cost: Not yet determined

Name: **GMSYS**
Purpose: Estimate leach rates from landfills
Source: **ORD-BBS**
Cost: Free

APPENDIX C

SOLUTION METHODOLOGY

APPENDIX C

Solution Methodology

Every ground-water model is based upon a set of mathematical equations. Solution methodology refers to the strategy and techniques used to solve these 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 of the 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 that has occurred as a result of the growing awareness of the importance of intrinsic variability of the hydrogeologic environment. Stochastic methods are still primarily research tools; however, as computer speeds continue to increase, stochastic methods will be able to move further away from the research- oriented community and more into mainstream management applications. The more widespread use of deterministic methods suggests a more immediate need for code-selection guidance. Therefore, this section focuses primarily on deterministic methods.

Deterministic methods may 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 models are simpler to use than numerical models and can generally be solved with the aid of a calculator, although computers are also used. Analytical models 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 numerical models.

Analytical models are used in ground-water investigations to solve many different kinds of problems. For example, aquifer parameters are obtained from aquifer tests through the use of analytical models, and ground-water flow and contaminant transport rates can also be estimated with the use of analytical models. To avoid confusion, only analytical models designed to estimate ground-water flow and radionuclide transport rates are discussed in this section.

Numerical models provide solutions to the differential equations describing water movement and solute transport using numerical methods such as finite differences and finite elements. Numerical methods can account for complex geometry and heterogenous media, as well as 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-hydrogeologist.

The validity of the results from numerical models depends strongly on the quality and quantity of the input data. Numerical and analytical codes have their respective strengths and weaknesses which are inherent within their formulations. The fundamental characteristics of both analytical and numerical methods are presented below and are discussed in more detail in the following sections:

Analytical

- Provides a solution at any location and point in time;

- Exact, closed-form solutions or well-documented, convergent solutions (approximate analytical);

- Requires regular geometry of the domain;

- Generally requires uniform material properties;

- 1-, 2-, or 3-D capability;

- Transient effects can be considered;

- Less prone to computational errors than numerical methods;

- Usually requires that problems are linear;

- Low computer storage requirements;

- Data can be easily input.

Numerical

- Provides a solution only at prespecified locations and moments in time;

- Approximate solutions;

- Irregular domain and boundaries can be simulated;

- Nonuniform material properties can be simulated;

- Can simulate non-linear problems;

- 1-, 2-, or 3-D capability;

- Transient effects can be considered;

- Computational errors can be a problem;

- Can require large computer storage;

- Large amount of data input.

Analytical Methods

Analytical methods that solve ground-water flow and contaminant transport in porous media are comparatively easy to use. However, because the governing equations are relatively simple, analytical solutions are generally restricted to either 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 belong to systems having a uniform and steady flow. This means that the magnitude and direction of the velocity throughout the system are invariable with respect to time and space, which requires the system to be homogeneous and isotropic with respect to the hydraulic conductivity. The three most general types of analytical methods include the following:

- Approximate analytical

- Exact analytical

- Semi-analytical

Typical analytical solutions, which are termed approximate, are in the form of an infinite series of algebraic terms, or a double infinite series, or even an infinite series of definite integrals. Because an infinite series of numbers cannot be solved for exact solutions, each one of these expressions must be approximated by truncating the series after considering a predetermined number of terms. If, on the other hand, the analytical solution can be expressed by equations which take a closed form (finite number of terms), the solution is said to be exact. Even though the solution may contain errors due to rounding.

In general, exact analytical equations tend to require infinite domains and boundaries. These constraints typically result in solutions that are more appropriate for solving problems of well hydraulics than those associated with ground-water flow and contaminant transport.

An obvious problem with approximate analytical equations is that they are of an open form and may not converge if they are inherently unstable. Therefore, it is very important that care has been taken during the code development process to ensure that the equations used do converge properly and that the code documentation provides the methods by which the convergence was examined. It is also important to

recognize that just because a code is written using analytical techniques it does not mean that convergence may not still be a problem even if the formulation is correct.

Semi-analytical methods are more complex than analytical methods and more simplistic than most numerical methods. These techniques use the concepts from fluid mechanics and velocity potentials which are extended using numerical tools to construct flow and contaminant patterns. Advantages of semi-analytical methods include the following:

! Require only simple computer input data and do not require the design of a mesh as with fully numerical methods;

! May be used where complex boundaries (e.g., multiple pumping wells) do not allow analytical equations to be written;

! Techniques can be used to easily estimate travel times of a conservative, retarded, or decaying contaminant to a downgradient receptor;

! Can provide screening information to judge the need for more sophisticated modeling.

Limitations of semi-analytical methods include the following:

! Mass transport by dispersion and diffusion is generally not considered, which in many cases may lead to predictions of travel times that are longer than actual values and may underestimate the true impact of a contaminant source;

! Usually are formulated in two dimensions and three-dimensional effects are ignored;

! Heterogeneous properties of the media cannot be simulated although some semi-analytical methods do allow for anisotropy;

! Most semi-analytical formulations are for steady-state problems; however, in some cases they can be extended to handle transient problems.

Numerical Methods

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, boundary and initial conditions, then analytical methods are generally abandoned and more approximate numerical methods are used to solve the set of equations. The most common of these methods include the following:

! Finite Difference

! Integrated Finite Difference

! Finite Element

! Method of Characteristics

Of particular importance to the following discussion is the understanding that the flow and transport equations, which describe the movement of ground water and contaminants, are composed of both spatial and temporal terms both of which require discretization within the model domain. These terms simply describe the concentration or head (i.e., water elevations) 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 the time-stepping methods, discussed later in this section, are used to discretize or describe the temporal term.

Finite Difference

The basic idea of finite-difference methods is to replace derivatives at a point by ratios of the changes in appropriate variables over small but finite intervals. Unlike analytical methods, where values can be calculated at any point in the problem domain, numerical methods (e.g., finite differences) make approximations at a predetermined finite number of points and reduce a continuous boundary-value problem to a set of algebraic equations. Once the partial differential equations have been converted into a set of algebraic equations involving a number of unknowns, the unknowns may be found by what are termed matrix solvers.

In practice, the problem domain is divided into a rectangular grid in which either the x and y

intersections, called nodes, are designated as solution points (i.e., mesh centered) or the solution points are at the center of the grid cell (i.e., block centered). Time step sizes are specified over the simulated time of interest, and the mathematical expressions are successively solved for each individual time step until the solution converges upon a value which satisfies the predesignated convergence criteria (i.e., error tolerance).

The form of the system of equations is that the values of head at each nodal point are a function of x and y grid coordinates, as well as the size of specified time steps. The values of head are related to the values in the surrounding nodal points and those at the beginning and at the end of a time step. If the values at the beginning of a time step are known (which is usually the case), the values at the end of the time step are the unknowns, and the resulting system of equations is a system of N linear equations with N unknowns. The value N indicates the total number of mesh points. Thus, the mathematical problem to be solved is the solution of a linear system of equations.

The system of equations may turn out to be rather large. For example, a grid with 50 mesh points in the x-direction and 50 mesh points in the y-direction will have 2,500 unknowns as well as equations to be solved.

Relevant considerations related to the finite-difference method include:

- Uses a direct Taylor Series approximation of the derivative terms of the partial differential equations at nodal points;

- Formulation is based on a rectangular (block-centered or mesh-centered) grid;

- Relatively simple to formulate as compared to other numerical methods;

- Conducive to efficient matrix solving techniques;

- May be sensitive to grid orientation effects in solving 2-D and 3-D flow and transport problems;

- Use of rectangular grid necessitates staircase (or stepwise) approximation of irregular boundary and/or aquifer material zoning;

- May be prone to numerical dispersion or oscillation in solving transport problems.

A closely related alternative to the conventional finite difference is the integrated finite-difference method which uses integral approximations of the partial differential equations of nodal subdomains. The primary advantage of this method is that it will accommodate non-rectangular grid elements, which allow irregular boundaries to be efficiently modeled. The following, however, are the disadvantages associated with this method:

- Necessitates more complex grid generation scheme than the traditional finite-difference method;

- Subdomain boundaries surrounding individual nodes must satisfy certain orthogonality constraints to ensure that mass is conserved;

- Method leads to less efficient matrix solution techniques than the conventional finite-difference method.
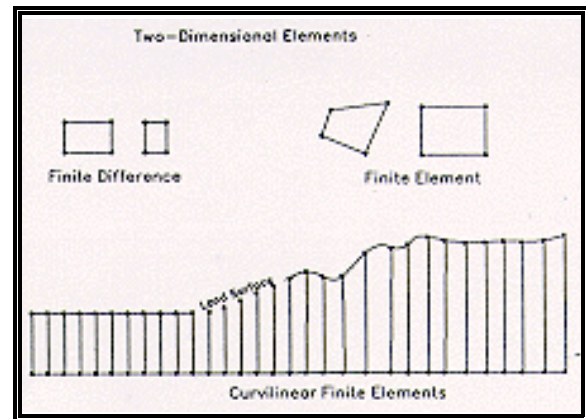

Figure C.1   Finite Two-Dimensional Elements

Finite Element

While approximations to a continuous solution are defined at isolated points by finite differences, with finite elements, the approximate solution (i.e., heads or

concentration) is defined over the entire domain by interpolation functions, although solutions to the functions are calculated only at the element nodes. This integral formulation for the governing ground-water flow or solute transport equation leads to a system of algebraic equations that can be solved for the unknown(s) (i.e., hydraulic head, pressure head or solute concentration) at each node in the mesh. The method of weighted residuals is the commonly used general approach that defines an approximate solution to the boundary or initial value problem. When this approximate solution is substituted into the governing differential equation, an error or residual occurs at each point (node) in the problem domain. The weighted average of the residuals for each node in the finite-element mesh is then forced to equal zero, thus minimizing the error between the approxi-mate solution and the actual solution. Relevant characteristics of the finite-element method as compared with the finite-difference method include:

!   Allows a much greater flexibility in handling irregular domain geometry, material heterogeneity, and/or anisotropy;

!   Less prone to numerical dispersion; however, it is necessary to be more careful to limit potential oscillation in solving the transport problem;

!   The elements do not have to be rectangular, but can also be other simple polygons (commonly triangles or quadrilaterals);

!   Matrix solutions generally require substantially greater computational effort and computer storage capability;

!   Finite-element solutions are less sensitive to grid orientation.

Two typical problems that arise when solving the contaminant transport equations are numerical dispersion and artificial oscillation. Numerical dispersion arises from grid size, time-step size, and the fact that computers have a limited accuracy, thus some of the round-off error will occur in computations. This error results in the artificial spreading of contaminant due to amplification of dispersivity. Hence, the contaminant will disperse farther than it should with a given physical, or "real" dispersivity. This extra dispersion will result in lower peak concentrations and

more spreading of the contaminant. Methods exist to control numerical dispersion, but the methods themselves may introduce artificial oscillation. Artificial oscillation is the over or undershooting of the true solution by the model, and results in "waves" in the solution. Usually numerical dispersion is associated with the finite-difference method; however, numerical oscillation is associated with the finite-element method. Depending upon the method employed to solve the advection term, both methods can exhibit both types of behavior. Special techniques have been developed to deal with these problems, one of which is the Method of Characteristics (MOC).

This method has been widely used and can be applied to finite differences as well as finite elements, in two or three dimensions. The basic idea is to decouple the advective part and the dispersive part of the transport equation and to solve them successively. However, all MOC methods are not strictly based on the principle of mass conservation, hence large contaminant mass balance errors may arise. While it is recognized that these errors may be an artifact of the technique, the quality of the results of a numerical model are judged, in part, by the degree that mass is conserved. Furthermore, the MOC technique requires much longer run-times than finite-difference or finite-element techniques.
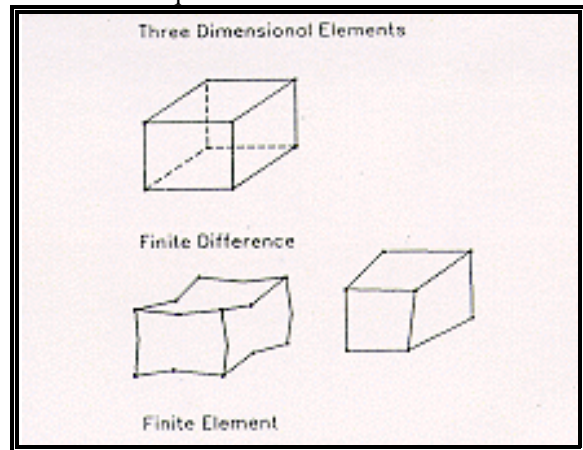

Figure C-2.   Three-Dimensional Elements

Time Stepping

As mentioned previously, while finite-element and finite-difference methods are used to approximate the spatial terms of the transient flow and transport equations, techniques are used to approximate the temporal term. While there are several commonly used variations of the finite-difference method, it is beyond the scope of this discussion to elaborate on the specifics for each of the techniques; what is important, however, is an introduction to the technical terms and a general understanding as to how the various methods influence the model run-times as well as the results. Four of the most common time-stepping schemes include Explicit, Implicit, Mixed Explicit-Implicit, and Alternating Direction Implicit Procedure. Characteristics of each method are listed below.

Explicit:

! Numerical solution is conditionally stable.

! Often requires an excessive number of time steps to simulate a practical problem.

! Due to numerical inefficiencies, method is unsuitable for simulation of field problems with a high degree of heterogeneity and/or nonlinear flow conditions.

Implicit:

! Usually produces unconditionally stable numerical solution for flow and transport.

! Much more flexible and robust than the explicit time-stepping scheme.

! Matrix formulation and solution require substantial computational effort (i.e., relatively long computer times are necessary to model practical field problems).

Mixed Explicit-Implicit:

! Based on combined use of explicit and implicit temporal approximations.

! Usually produces unconditionally stable numerical solution for flow and transport.

! More robust than the explicit time-stepping scheme, and generally more efficient than the implicit scheme for ground-water flow and transport solutions.

! Time-stepping scheme can be weighted in favor of either method (i.e., explicit or implicit) using a factor that ranges from 0 to 1. Weighting factors of 0, .5, and 1 result in explicit, Crank-Nicholson, and fully implicit formulations, respectively.

Alternating Direction Implicit Procedure:

! Usually produces unconditionally stable numerical solution for flow and transport.

! Much more flexible and robust than the explicit time-stepping scheme.

! May be prone to mass balance problems when applied to field problems with high degree of heterogeneity and/or nonlinear flow conditions.

! Unsuitable for variably saturated flow simulations.

! Limited to rectangular finite-difference grids.

The end result of applying the time-stepping schemes described above is that the flow and transport problem is broken into multiple equations with multiple unknowns for each pre-specified point in the model domain (i.e., nodes). These multiple equa-tions will, in turn, be solved through matrix algebra methods which are discussed in a later section.

Linearization of Flow and Transport Equations

In earlier sections, several situations were presented in which the equations describing ground-water flow and contaminant transport are nonlinear. For transport problems, the equations are nonlinear when changes in concentration, pressure, and temperature cause changes in viscosity, effective porosity, or density (e.g., multiphase fluid conditions). Nonlinear flow problems involve those where the transmissivity is a function of saturated thickness (i.e., water-table aquifers) or hydraulic conductivity is a function of moisture content (i.e., unsaturated zone).

Under nonlinear flow and transport conditions each node in the model domain has associated multiple nonlinear equations. Prior to solving for the unknowns of these equations through matrix algebra, an intermediate step is required in which the equations are linearized. Two of the most common procedures used to perform this linearization are the Picard and Newton-Raphson methods.

The Picard method:

- ! Is relatively simple to formulate as compared to the Newton-Raphson procedure.

- ! Generally produces a symmetric matrix for the flow problem and thus requires considerably less computer effort for the matrix solution than the Newton-Raphson method.

- ! May be prone to convergence difficulties for highly nonlinear cases.

Qualities of the Newton-Raphson method include:

- ! Suitable for handling highly nonlinear cases.

- ! Generally requires substantially greater computational effort for matrix formulation and solution.

- ! Convergence of the procedure may depend on continuity or smoothness of the nonlinear functions.

As far as model selection is concerned, if it is expected that the problem will be highly nonlinear, the code selected should be able to apply the Newton-Raphson method. It should also be recognized that in this situation the calculations will take a relatively long time for the computer to solve. Flow and transport through the unsaturated zone become more nonlinear as the contrast between ambient moisture content and volume of recharge (e.g., rainfall) becomes more pronounced. Therefore, the regional climate can provide an indication as to whether unsaturated zone flow and transport are likely to be nonlinear or highly nonlinear. For example, high-intensity rainfall events in the arid southwest would create very sharp contrasts between the ambient moisture content and the infiltrating pulse. Under these conditions, the code would most likely need the Newton-Raphson

formulation. However, in areas of the humid northeast, the ambient moisture contents are generally high enough that the wetting front saturations are not significantly different from the ambient moisture content and therefore the nonlinear equations could be adequately solved with the Picard method.

Matrix Solvers

As stated previously, following the spatial and temporal discretization of the flow and transport equations and in the case of nonlinear problems, the linearization of the equations, it then becomes necessary to solve the systems of multiple equations with multiple unknowns. The most efficient means of accomplishing this task is through matrix algebra. Matrix equations can be solved by several means. Some of the more common ones include:

- ! Direct Matrix Solution Techniques

- ! Iterative Alternating Direction Implicit Procedure (IADIP)

- ! Successive Over-Relaxation Techniques

- ! Strong Implicit Procedure (SIP)

- ! Preconditioned Conjugate Gradient (PCG)/Orthomin Techniques

It is important to recognize that matrix solving techniques will rarely be the deciding factor in the code selection process. However, some familiarity with the capabilities of the matrix solvers will not only provide a general recognition of the technical terms but will also give some indication as to potential hardware requirements. Therefore, the following provides a superficial description of the various matrix solvers listed above.

The following qualities are inherent in the Direct Matrix Solution techniques:

- ! Produces highly accurate solution of the matrix equation with minimal round-off errors.

- ! Generally applicable to both finite-difference and finite-element schemes.

! Performs well for 2-D problems with up to 2,000 nodal unknowns; unsuitable for large problems with many thousands of nodes.

Qualities of the Iterative Alternating Direction Implicit Procedure (IADIP) include:

! Accommodates large 2-D and 3-D problems with many thousands of nodal unknowns.

! Applicability limited to rectangular grids.

! Convergence rate is usually sensitive to grid spacings and material heterogeneity and anisotropy.

! Prone to asymptotic convergence behavior and may require several hundreds or thousands of iterations to reach satisfactory convergence for a steady-state analysis.

Qualities inherent in Successive Over-Relaxation Techniques (i.e., Point Successive Over-Relaxation (PSOR), Line Successive Over-Relaxation (LSOR), and Slice Successive Over-Relaxation (SSOR)) include:

! Accommodates large 2-D and 3-D problems with many thousand nodal unknowns.

! Applicable to finite-difference and finite-element approximation schemes.

! Convergence rate is dependent on the choice of relaxation factors and is usually sensitive to grid spacings and material heterogeneities and anisotropies.

! Prone to asymptotic convergence behavior and may require several hundreds or thousands of iterations to reach satisfactory convergence for a steady-state analysis.

Qualities inherent in the Strong Implicit Procedure (SIP) include:

! Accommodates large 2-D and 3-D problems with many thousand nodal unknowns.

! Much more robust than IADIP and PSOR/LSOR/SSOR techniques.

! Convergence rate is sensitive to iteration parameter and grid spacings.

! Applicable to finite-difference approximation and flow problems only.

Qualities inherent in the Preconditioned Conjugate Gradient (PCG)/Orthomin Techniques include:

! Accommodates large 2-D and 3-D problems with many thousands of nodal unknowns.

! No relaxation factor or iteration parameters are required and convergence rate is usually insensitive to grid spacings and material anisotropy and/or heterogeneity.

! Much more robust than other alternative iteration techniques.

! Applicable to both finite-difference and finite-element approximation schemes but requires substantially less storage and computer (CPU) time with finite-difference approximation, particularly for 3-D problems.

APPENDIX D

CODE ATTRIBUTE TABLES

Site-Related Features of Ground Water Flow and Transport Codes

COMPUTER CODE	BOUNDARY/SOURCE CHARACTERISTICS							AQUIFER SYSTEM CHARACTERISTICS					SOIL/ROCK CHARACTERISTICS							REFERENCE CITATION
	POINT SOURCE	LINE SOURCE	AREALLY DISTRIBUTED	SPECIFIED	SPECIFIED SOURCE RATE	TIME-DEPENDENT	MULTIPLE SOURCES	CONFINED AQUIFERS	AQUITARDS	WATER-TABLE	CONVERTIBLE AQUIFERS	MULTIPLE AQUIFERS	HOMOGENEOUS	HETEROGENEOUS	ISOTROPIC	ANISOTROPIC	FRACTURED	MACROPORES	LAYERED SOILS	

COMPUTER CODE	TRANSPORT & FATE PROCESSES									MULTIPHASE FLUID CONDITIONS			FLOW CONDITIONS			TIME DEPENDENCE	
	DISPERSION	ADVECTION	MATRIX DIFFUSION	DENSITY-DEPENDENT	RETARDATION	NON-LIN. SORPTION	CHEMICAL REACTIONS/	SINGLE SPECIES	MULTI-SPECIES TRANSPORT WITH CHAINED	TWO-PHASE	TWO-PHASE WATER/AIR	THREE-PHASE WATER/ NAPL/AIR	FULLY SATURATED	VARIABLY SATURATED/ NON-HYSTERETIC	VARIABLY SATURATED/	STEADY-STATE	TRANSIENT

Code-Related Features of Ground Water Flow and Transport Codes

COMPUTER CODE	SOLUTION METHODOLOGY																GEOMETRY				
	Analytical			Numerical																	
				Spatial Discretization				Temporal Discretization			Matrix Solvers										
	APPROX. ANALYTICAL	EXACT ANALYTICAL	SEMI-ANALYTICAL	FINITE DIFFERENCE	INTEGRATED FINITE-	FINITE ELEMENT	METHOD OF CHARAC.	EXPLICIT	IMPLICIT	MIXED IMPLICIT-	ADIP	DIRECT SOLUTION	ITERATIVE ADIP	SOR/LSOR/SSOR	SIP	PCG/ORTHOMIN	1-D	2-D CROSS SECTIONAL	2-D AREAL	QUASI 3-D (LAYERED)	FULLY 3-D

COMPUTER CODE	OTHER RELEVANT FACTORS											
	Source Code Availability		Code Testing and Process				Output					
	PROPRIETARY	NON-PROPRIETARY	VERIFIED	FIELD-VALIDATED	PC-VERSION 386-SR486	PRE AND POST	CONTAMINANT MASS/ RATE OF RELEASE TO GROUNDWATER FROM	CONTAMINANT PLUME EXTENT	CONTAMINANT CONCENTRATION AS A FUNCTION OF DISTANCE	AS A FUNCTION OF	CONTINUOUSLY DISTRIBUTED IN SPACE	CONTAMINATION AVERAGE AT SELECTED POINTS / PROFILES AT SELECTED POINTS OVER TIME

APPENDIX E

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