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Fact Sheet: A Technical Guide to Ground-Water Model Selection at Sites Contaminated with Radioactive Substances

Quick Reference Fact Sheet

BACKGROUND

Mathematical models that characterize the source, transport, fate, and effects of hazardous and radioactive materials are used to help determine cleanup priorities and select remedial options at sites contaminated with radioactive materials.

A joint Interagency Environmental Pathway Modeling Working Group has been established by 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 Nuclear Regulatory Commission (NRC) Office of Nuclear Material Safety and Safeguards (NMSS). The purpose of the Working Group is to promote the more appropriate and consistent use of mathematical environmental models in the remediation and restoration of sites contaminated by radioactive substances.

The Working Group has published reports intended to be used by technical staff responsible for identifying and implementing flow and transport models to support cleanup decisions at hazardous and radioactive waste sites. This fact sheet is one of a series of fact sheets that summarize the Working Group's reports.

REPORT

Purpose

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

Contents of the Report

The report is divided into five sections. Following the introduction, Section 2 presents an overview of the types of ground-water modeling decisions facing the site remediation manager. Section 3 describes the construction of a site conceptual model and how it is used in 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 conditions that require specific model capabilities. Section 5 describes the review and evaluation process for screening and selecting computer models that are best suited to meet site-specific modeling needs.

The report also contains five appendices, including a glossary (Appendix A). Appendix B provides a list of electronic ground-water modeling resources. Appendix C describes the mathematical techniques used in ground-water model codes. Appendix D presents site- and code-related features of ground-water flow and transport codes that should be considered when selecting a model.

Deciding Whether to Model

Ground-water flow and transport modeling can be useful in making informed and defensible remedial decisions. Site remediation managers must determine whether ground-water modeling is needed and how modeling will support the remedial decision-making process.

The ground-water pathway may be considered a potentially significant exposure pathway if radionuclide concentrations in the ground water exceed, or could eventually exceed, acceptable levels. It is likely that ground-water modeling will be useful if the concentrations of radionuclides in ground water downgradient from the site or in leachate at the site exceed acceptable levels 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. The drinking-water standards set forth in 40 CFR 141 currently guide 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. In combination with field measurements, fate and effects models are used to screen sites that may need remedial action, support the design of environmental measurement/sampling programs, help understand the processes that affect radionuclide behavior at a site, and predict the effectiveness of alternative strategies for mitigating impacts.

However, models are not substitutes for data acquisition and expert judgement. Models should not be used until the specific objectives of the modeling exercise are defined and the limitations of the models are fully appreciated.

Developing a Site Conceptual Model

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, and how they are being transported off site. The conceptual model helps visualize the source and movement of contaminants, potential receptors, and the ways in which receptors may be exposed.

The components that make up the initial conceptual model of the site include contaminant characteristics, site characteristics (hydrogeology, land use, demography), and exposure scenarios and pathways. As information about a site accumulates, the site conceptual model is continually revised and refined. The figure on the following page is an example of a conceptual model (from EPA, *Guidance for Conducting Remedial Investigations and Feasibility Studies Under CERCLA*, EPA/540/G-89/004, OSWER Directive 9355.3-01, October, 1988).

Contaminant Characteristics. The site conceptual model should address the characteristics of the waste and contaminants, including the types and chemical composition of the radionuclides, waste form and containment, and source geometry (volume, area, depth, homogeneity). These characteristics are used to model the source term, which is the rate at which radionuclides are mobilized from the source and enter the unsaturated and saturated zones of a site.

Site Characteristics. The site conceptual model should begin to address the complexity of the environmental and hydrogeological setting. Complex settings, such as complex lithology, a thick unsaturated zone, or streams on site, generally indicate that ground-water flow and radionuclide transport at the site can be reliably simulated only by the use of complex models.

The site conceptual model also should identify where ground water currently is 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 to predict the likelihood that the contaminated plume will affect active wells.

Exposure Scenarios and Pathways. The site conceptual model also should define exposure scenarios and pathways at the site. Depending on the regulatory requirements and the phase in the remedial process, exposure scenarios to be modeled can include any one or a combination of: the no action alternative, trespassers, inadvertent intruders, routine emissions, accidents, and alternative remedies. For each scenario, an individual or group of individuals may be exposed by direct (dermal) contact, inhalation, or ingestion.

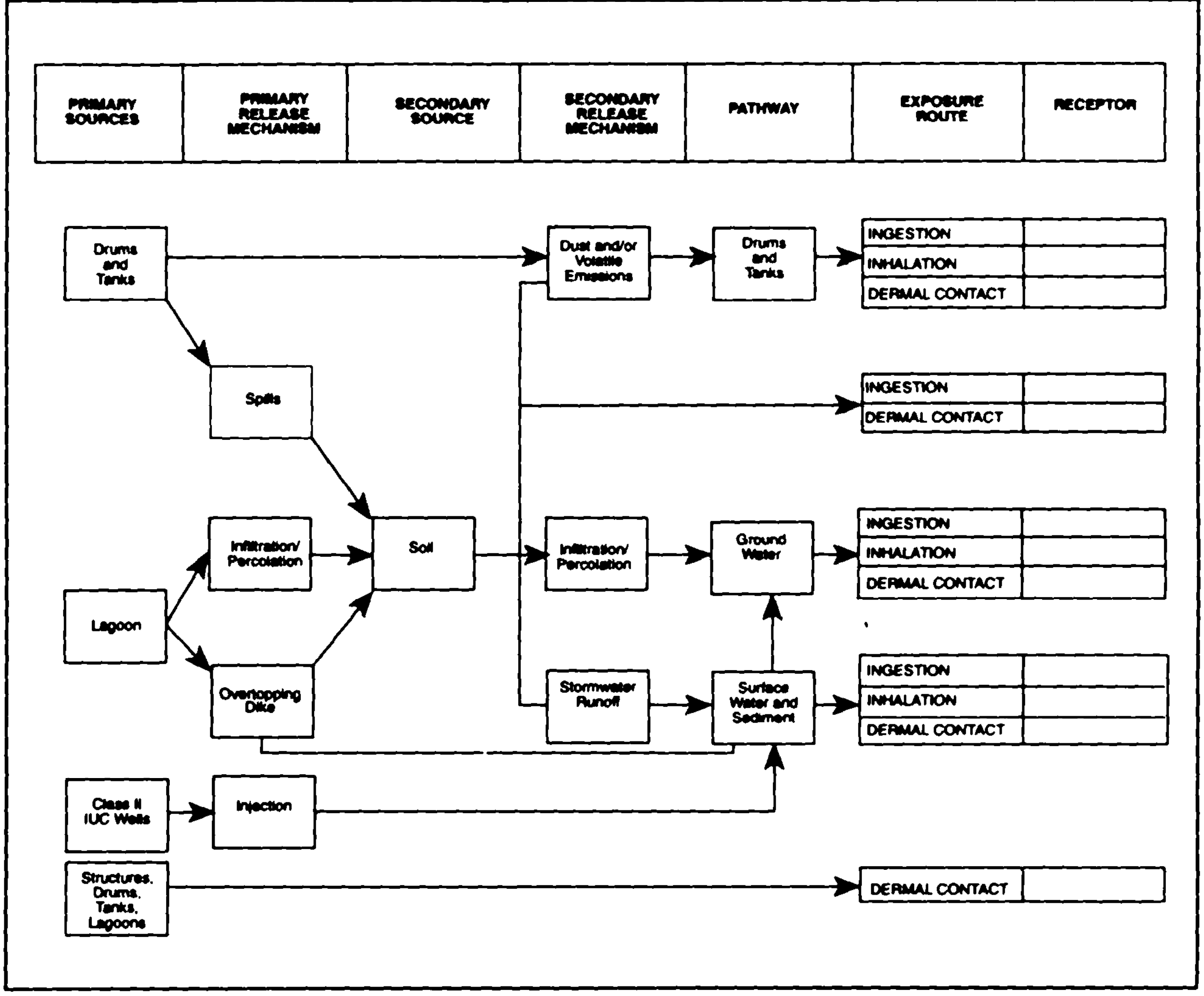
The number of possible scenarios is virtually unlimited. Scenarios that reasonably bound what may occur at the site must be determined. The scenarios selected for consideration define the receptor locations and exposure pathways that need to be modeled.

Establishing Modeling Objectives

Modeling objectives are determined by site managers based largely on existing regulatory requirements and potential exposure scenarios at the site. Exposure pathways that initially need to be modeled are determined during the planning phase based on judgement regarding the likelihood that a given pathway may be an important contributor to risk.

Modeling endpoints must be clearly defined because the type of endpoint will help to determine the ground-water model selected. In general, endpoints are expressed as a concentration, such as pCi/L, in

Example of a Site Conceptual Model



ground water at a specific location. Radionuclide concentrations also can be expressed as a function of time or as a time-averaged value. Some computer codes convert ground-water radionuclide concentrations to individual risk expressed in mrem/yr or lifetime risk of cancer. Other codes present results in terms of cumulative population impacts expressed in person-rems/yr or total number of cancers induced per year.

A baseline risk assessment at a site contaminated with radioactive material is used to determine the annual radiation dose to an individual drinking water from a potentially contaminated well. The endpoint in this case is the dose to an individual expressed in mrem/yr. To estimate this dose, it is necessary to estimate the average concentration of radionuclides in the well water over a year. Modeling objectives at each stage of the remedial investigation must be well defined early in the project. 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 available. If the modeling objectives demand more sophisticated models and input data, the necessary data should be obtained.

A mathematical model translates the conceptual model into a series of equations that simulate the fate and effects of the contaminants and displays the results in a manner convenient to support remedial decision making. The next step in the model selection process requires detailed analysis of the conceptual model to determine the degree to which specific contaminant and site characteristics need to be modeled. Once these are determined, the model selection process becomes a matter of identifying the models that meet the defined modeling objectives.

Remedial Phase

The greatest difficulty faced during model selection is determining which capabilities are required to support remedial decision making during each remedial phase at a specific site. Successful groundwater modeling requires the selection of a computer code that is consistent with the site characteristics and modeling objectives, which are strongly dependent on the phase of the remedial process. The following figure presents an overview of how the approach to modeling a site differs as a function of the phase of the remedial process.

The most common model selection mistakes are selecting codes that are more sophisticated than appropriate for the available data or result desired, and the application of a simpler code that does not account for the dominant flow and transport processes. The simplest code appropriate to the problem should be used first and more sophisticated models should be applied later until the modeling objectives are achieved.

The remedial process generally parallels this progression. The data available in the early phases of the remedial process may limit the modeling to one or two dimensions, which may be sufficient to support remedial decision making. Generally, it is during the later phases of the investigation that sufficient data have been obtained to meet more ambitious objectives through complex three-dimensional modeling.

Source Characteristics

Computer codes can accommodate the spatial distribution of contaminant source in a number of ways. The most common are point sources (drums or tanks), line sources (trenches), and area sources (ponds, lagoons, landfills). How the spatial distribution of the source term should be modeled 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 compared to the contaminant source area, even sizable lagoons or landfills could be considered point sources.

Modeling objectives also are important in determining how the source term should be modeled. For

General Modeling Approach as a Function of Remedial Phase

Model Trait	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

example, if simple scoping calculations are being performed, modeling the source as a point will yield conservative approximations of contaminant concentrations because of limited dispersion. However, if more realistic estimates of concentrations and plume geometry are required, generally it will be necessary to simulate the source term more accurately, especially if the receptor is close to a relatively large source.

Another consideration in code selection is whether the source is to be modeled as an instantaneous, continuous, or time-varying release. The need to model the source as a continuous or time-varying release primarily depends on the half-life of the radionuclide relative to the time period of interest and whether average or time-varying impacts of a release are of interest. In general, the simplest calculations, which assume a continuous release,

Model Selection Criteria

Administrative Data

Author	Documentation
Objective (research, general use, education)	Hardware requirements
Organizations distributing the code	Accessibility of source code
Organizations supporting the code	History of use
Date of first release	Cost
Current version number	Programming language

Phase of Remedial Process

Scoping	Remediation
Characterization	

Site-Related Criteria

Multiple sources	Heterogeneity
Source geometry (line, point, area)	Anisotropy
Release type (constant, variable)	Fractures
Confined aquifers	Macropores
Unconfined aquifers (water-table)	Layered soils
Aquitards	Dispersion
Multiple aquifers	Advection
Convertible (aquifer systems)	Diffusion
Two-phase: water/NAPL	Density dependent
Two-phase: water/air	Partitioning: solid-gas
Three-phase: water/NAPL/air	Partitioning: solid-liquid
Flow: fully saturated	Equilibrium isotherm
Flow: variably saturated	Radioactive decay and chain decay
Temporal discretization (steady-state or transient)	Speciation

Code-Related Criteria

Code usability	Code output
Quality assurance: code documentation	Code dimensionality
Quality assurance: code testing	Solution methodology
Code support	

are sufficient when determining the average annual doses to ground-water users.

Aquifer Characteristics

The most common aquifer characteristics that influence code selection include confined aquifers, water-table (unconfined) aquifers, convertible aquifers, multiple aquifers/aquitards, heterogeneous aquifers, anisotropic aquifers, fractures/macropores, and layered soils/rocks. Recognizing when and if these processes need to be modeled is critical to code selection.

Fate and Transport Processes

The transport of radionuclides is affected by various physical and chemical processes, including advection, dispersion, matrix diffusion, retardation, and radioactive decay. Geochemical processes are important primarily because they reduce the velocity of the radionuclides relative to the ground water, which increases transit time and results in additional radioactive decay.

Evaluating Models

This section presents the basic procedure that should be followed in evaluating ground-water flow and transport codes. Given that an investigator understands the various contaminant and site characteristics that need to be modeled, there often will be several suitable models in the scientific literature. Ideally, each candidate should be evaluated in detail to identify the one most appropriate for the particular site and modeling objectives.

The first aspect of the review concentrates on the appropriateness of the particular code to meet modeling objectives. The data requirements of the code also should be consistent with the quantity and quality of data available from the site. Next, the reviewer 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 be available to the public.

The model evaluation process involves the following steps:

1. Contact the author of the code and obtain documentation, other model-related publications, list of users, and information on code validation.

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 a written evaluation using the criteria shown in the list of Model Selection Criteria (see table on page 5).

Much of the information needed for a thorough evaluation can be obtained from the author or distributor of the code. Inability to obtain the necessary publications can be an indication that the code is not well documented or is proprietary. Inaccessibility of the documentation and related publications should be grounds for considering the code unacceptable.

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

The evaluation process must rely on user opinions and published information. User opinions are especially valuable in determining whether the code functions as documented or has significant problems. In some instances, users have performed extensive testing or are familiar with published papers documenting the use of the code. In essence, the evaluation process substitutes user experience for hands-on testing to shorten the time to perform a review.

CONTACTS

If you have any questions or want a copy of this or other reports, contact:

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REPORTS

Computer Models Used to Support Cleanup Decision-Making at Hazardous and Radioactive Waste Sites, EPA 402-R-93-005, March 1993. Also available from the National Technical Information Center (NTIS), (703) 487-4650, PB93-183333/XAB.

Environmental Characteristics of EPA, NRC, and DOE Sites Contaminated with Radioactive Substances, EPA 402-R-93-011, March 1993. NTIS, PB93-185551/XAB.

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Technical Guide to Ground-Water Model Selection at Sites Contaminated with Radioactive Substances, EPA 402-R-94-012, September 1994. NTIS, PB94-205804/XAB.