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Fact Sheet: Documenting Ground-Water Modeling at Sites Contaminated with Radioactive Substances

Quick Reference Fact Sheet

At many sites currently regulated by EPA or NRC or managed by DOE, the principal concern is the existence of—or potential for—contamination of underlying aquifers. Compared to air, surface water, and terrestrial pathways, ground-water contamination is more difficult to sample and monitor, which results in a greater reliance upon mathematical models to predict the locations and levels of environmental contamination. The types of models used to simulate the behavior of radionuclides in ground water are more complex than models for surface water or atmospheric transport, primarily due to the diversity of physical settings possible at different sites. Also, the methods used to model ground water are not as standardized as those for other pathways, and there is much less written on appropriate methods.

In 1991, a joint Interagency Environmental Pathway Modeling Working Group was initiated among EPA's Offices of Radiation and Indoor Air and Solid Waste and Emergency Response, the Department of Energy's Office of Environmental Management, and the Nuclear Regulatory Commission's Office of Nuclear Material Safety and Safeguards. The purpose of the Working Group is to promote the appropriate and consistent use of mathematical models in the remediation and restoration process at sites containing—or contaminated with—radioactive materials or mixed waste substances.

This fact sheet is one in a series that summarize reports published by the Working Group. These reports, which are identified in the References section, are intended to assist those responsible for identifying and implementing flow and transport models in support of cleanup decisions at hazardous and radioactive waste sites.

PURPOSE

The Working Group directed that a report be written to describe a recommended method of documenting ground-water modeling results for hazardous-waste remediation sites. This fact sheet summarizes the report, which is entitled *Documenting Ground-Water Modeling at Sites with Radioactive Contamination*. The method described in the report is consistent with the seven standards published by the American Society for Testing and Materials Subcommittee on Ground-Water and Vadose Zone Investigations.

Adoption of the tenets in the report will enhance the understanding between modelers and their managers of what may be expected in model documentation; facilitate the peer-review process by ensuring that modeling documentation is complete; ensure that institutional memory is preserved; and institute greater consistency among modeling reports.

INTRODUCTION

The report provides a guide to determining whether proper modeling protocol has been followed, and that common modeling pitfalls have been avoided. As a guide to modelers, the report demonstrates a thorough approach to documenting model applications in a consistent manner. A review of 20 site-specific modeling studies at hazardous-waste remediation sites[1] described mistakes in all aspects of the modeling process, including a misunderstanding of the model, misapplication of boundary or initial conditions, misconceptualization, inappropriate data, improper calibration or verification, insufficient uncertainty analysis, and misinterpretation of simulation results. Any of these errors could lead to faulty remediation decisions. A proper documentation of modeling results answers the following questions:

- Do the objectives of the simulation correspond to the decision-making needs?
- Are there sufficient data to characterize the site?
- Is the modeler's conceptual approach consistent with the site's physical and chemical processes?
- Can the model satisfy all the components in the conceptual model, and will it provide the results necessary to satisfy the study's objectives?
- Are the model's data, initial conditions, and boundary conditions identified and consistent with geology and hydrology?
- Are the conclusions consistent with the degree of uncertainty or sensitivity ascribed to the model study, and do these conclusions satisfy the modeler's original objectives?

The recommended approach to evaluating models consists of three steps: (1) determining one's objectives and data requirements for the project; (2) properly developing a conceptual model for the site, which describes the physical and chemical system that must be simulated; and (3) selecting and applying the model in a manner consistent with the objectives and the site's known physical characteristics and input variables.

MODELING OBJECTIVES AND DATA REQUIREMENTS

Ground-water modeling objectives usually depend upon the stage of the remedial process. Early (scoping) stages often need fast, efficient, order-of-magnitude estimates of the extent of contamination and the probable maximum radionuclide concentrations at specified locations. Preliminary characterization data are often sparse, and subsurface flow and transport processes can be limited to general considerations such as whether flow is controlled by porous media or fractures, or whether the wastes are undergoing phase transformations. One of the most useful analyses at this phase is to evaluate the interdependencies of controlling parameters: How do changes in one parameter affect the others and the outcome of the modeling exercise? This understanding assists in properly focusing the site characterization activities. At this early stage in the process, it is important to use a modeling approach where parameter values can be selected systematically from the probable range to evaluate what effects one or multiple parameters have on rate of flow or concentration of contaminants. Either a sensitivity analysis or—in the absence of reasonable data—a conservative bounding approach (high and low probable estimates) can be used, as long as the modeler properly documents the uncertainty such assumptions create. For example, distribution coefficients are often published at neutral pH values. However, if acid wastes are involved, even conservative values could be too high. Because site-specific information is often limited in the scoping phase, early modeling objectives are usually designed to support the design of more ambitious site characterization studies. Such relatively simple objectives can often be satisfied by one- or two-dimensional models.

The site characterization phase typically provides the first opportunity to gain a detailed understanding of the overall behavior of the system. This leads in turn to a refinement of the conceptual model, and follows the iterative process of data collection, analysis, and decision making.

The primary reasons for ground-water modeling in the site characterization phase of the remedial process are to refine the conceptual model; optimize the site characterization program; support the baseline risk assessment; and provide preliminary input into the remedy selection.

In many instances, several different approaches to modeling will be taken to accomplish the objectives. For example, the output of analytical modeling of the vadose zone, in the form of radionuclide concentrations at the saturated/unsaturated interface, may be used as input to numerical models of the saturated zone. Similarly, governing geochemical processes may have a

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[1] "Evaluation of Subsurface Modeling Application at CERCLA/RCRA Sites," U.S. EPA Center for Subsurface Modeling Support, Ada, OK, 1995.

significant impact on the transport of radionuclides, and can be simulated indirectly in the analysis.

Table 1, on page 4, summarizes a checklist of key questions a model documentation report should answer in order to provide evaluators with a reasonable opportunity to judge the model's suitability for the application. For convenience, the checklist is grouped into three categories: Objectives and Data Requirements, which considers whether the modeler has adequately considered the purpose and scope of the model; Conceptual Model Development, which ensures that the modeler has documented the physical relationships between the conceptual model and the actual system; and Modeling Application, which focuses on the model code selection, source term, parameterization, uncertainties, and results. A more detailed list of criteria is included in the full report.

CONCEPTUAL MODEL DEVELOPMENT

The conceptual model of a site is a diagrammatic or narrative description of the condition of a site and its setting. It describes the subsurface physical system, the variability of the aquifer, and the types of contaminants found and their transport mechanisms. As information about a site accumulates, the conceptual model is revised and refined into a set of hydrogeologic assumptions and concepts that can be evaluated quantitatively. The conceptual model must be consistent with the physical system and consistent internally. At a minimum, the conceptual model must include the geologic and hydrologic framework, hydraulic properties, sources and sinks, boundary and initial conditions, transport processes, and spatial and temporal dimensionality.

The formulation of a conceptual model is an integral component of the modeling process. Since the conceptual model is iteratively redesigned as more data become available and as the remediation process progresses, some components of the conceptual model may be simplified to meet limited objectives or data limitations. Such simplification is valid because early modeling focuses on the significance of specific parameters and their effects on transport rather than on modeling specific hydrogeologic transport processes. One-dimensional models (point/receptor) or two-dimensional models (plume transport from source to receptor horizontally and vertically) are commonly used in the scoping phase of a remediation. Since trends (rather than precision) are more important during the early phase, ground-water modelers make a number of simplifying assumptions early in the investigation: steady state conditions; one- or two-dimensions; simplified boundary and initial conditions; homogeneous media; and simplified flow and transport processes.

The conceptual model, which is based on the modeler's experience and judgment, will become more complex as more processes are identified and interrelationships are incorporated. The transformation of the conceptual model into a mathematical model will result in intrinsic simplifications of the system. For example, mathematical models assume that input data may be scaled up or down according to the needs of the simulation—the same algorithms are applied whether the simulation covers centimeters or kilometers. Besides inherent simplifications, the modeler may deliberately simplify the physical processes through such typical assumptions as:

Scoping Phase Simplifying Assumptions

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

Site Characterization Phase Assumptions

- Steady-state flow/transient transport
- Three-dimensional flow and transport
- Steady-state boundary and nonuniform initial conditions
- Complex flow and transport processes
- System heterogeneity

As the site investigation proceeds into the remedial phase, data are acquired that will be used to evaluate feasible remedial alternatives. Optimizing a remedial design involves evaluating alternative screen depths, pumping rates, and well locations to identify the most effective configuration. Modeling objectives associated

Table 1. Key Issues in Model Documentation

Objectives and Data Requirements

Are the purpose and scope outlined and consistent with decision making needs?
Are the data requirements outlined for the proposed modeling?
Are the sources of data and data uncertainties adequately discussed?

Conceptual Model Development

Are the physical and hydrological frameworks adequately described?
Is the nature of the contaminant source term described?
Is the conceptual model consistent with the field data?
Are the uncertainties and simplifying assumptions of the conceptual model justified?

Model Application

Code Selection

Is the rationale for code selection clearly presented for proposed code(s), and are the general features, assumptions, and limitations, of the code(s) presented?
Is the code well documented and adequately tested?
Are the hardware requirements compatible with those available?

Model Construction

—Layering and Gridding
Do the nodes fall near pumping centers on wells and along the natural boundaries?
Is the grid oriented along the principal axes of hydraulic conductivity?
Is the grid at the appropriate scale for the problem?
Are strong vertical gradients within a single aquifer accommodated by multiple planes or layers of nodal planes?

—Boundary and Initial Conditions
Are model boundaries consistent with natural hydrologic features?
Are the uncertainties associated with the boundaries and initial conditions addressed?
Are transient boundaries discussed?

—Model Parameterization
Are data input requirements fully described?
Are the model parameters within the range of reported or measured values?

Model Calibration

Are the calibration criteria presented and are the calibration procedures described in detail?
Does the calibration satisfactorily meet specified criteria?
Has the calibration been tested against actual field data and are discrepancies explained?
Is the calibrated model consistent with the conceptual model?

Sensitivity Analyses

Was a sensitivity analysis performed and is the approach to the sensitivity analysis detailed?
Was the relevance of the sensitivity analysis results to the overall project objectives discussed?
Are the results presented so that they are easy to interpret?

with remedial alternative design generally are more ambitious than those associated with the site characterization phase. The remedial design is the most challenging phase of the investigation. A number of processes that may not be important to assessing baseline risk or to site characterization may be essential to remedial design:

- Three-dimensional flow and transport
- Matrix diffusion (pump-and-treat)
- Desaturation and resaturation of the aquifer
- Heat-energy transfer
- Sharp hydraulic conductivity gradients or thresholds
- Multiple aquifers
- Movement from confined to unconfined conditions
- Simulation of complex flow conditions.

MODEL APPLICATION

The proper application of a model is perhaps more important than its selection. No matter how well a model is suited to a particular application, it will give misleading results if used improperly or with incomplete or incorrect data. Conversely, even a model with limited capabilities, or one used at a site with limited data, can give useful results if applied properly and with a full appreciation of the model's limitations. A conceptual model is a description of the present conditions of a site. To predict future behavior, it is necessary to develop a physical scale, analog, or mathematical model. Mathematical models are more widely used simply because they are easier to develop and manipulate.

Model application is the process of choosing and applying the appropriate algorithms capable of simulating the hydrogeologic system as defined by the conceptual model. Mathematical groundwater models are classified as either *deterministic* or *stochastic*. Deterministic methods assume that a process leads to a uniquely definable outcome, while stochastic models presume that all outcomes are inherently uncertain and must be characterized in terms of probabilities. Put another way, deterministic models result in a specific value for specified points, stochastic models provide the probability of a specific value occurring at any point. Stochastic models are relatively recent, and are still used primarily for research. Deterministic models—both numerical and analytical—are more widely used.

Analytical deterministic models are based on the solution of applicable differential equations that describe an idealized system. The solution of these equations give quantitative estimates of the extent of contaminant transport. These models are relatively easy to use, can be solved with a calculator, and generally require only limited site-specific data. Most available analytical models assume a uniform and steady flow, which requires the system to be homogeneous and isotropic with respect to hydraulic conductivity. Unfortunately, these models do not lend themselves to solutions when boundary conditions are complex. Therefore, if a realistic expression for hydraulic head or concentration over the site cannot be written from the governing equations and boundary or initial conditions, more sophisticated *numerical* methods must be used. Numerical methods can account for complex geometry and heterogenous media, as well as for dispersion, diffusion, and chemical processes (sorption, precipitation, radioactive decay, ion exchange, degradation). Numerical methods require a digital computer, greater quantities of data than analytical methods, and an experienced modeler.

Scoping Calculations

In practice, it is usually not necessary to develop mathematical expressions for all elements of the conceptual model, particularly in early phases of the project. There are four primary sources by which radioactivity can contaminate groundwater: leaching from surface impoundments; wastes injected below the water table; leaching from contaminated surface soils; and recharge from contaminated surface waters such as rivers or lakes. Detailed methods to calculate release rates and analyze fates are presented in Appendix B of the report, and may be used either to develop initial conditions or verify the methods used by modelers for their scoping phase.

When analyzing a radionuclide release to ground water, potential release mechanisms should be evaluated first, including the source mechanism or mechanisms, their physical and chemical properties, and their age. Estimation of release involves quantifying radionuclide concentrations present in the waste or leachate and the volume of the leachate or direct release rate. There are usually two processes that control the fate of radionuclides during transport from the source area: geochemical transport processes (such as sorption, ion exchange, and precipitation) and radioactive decay. The former processes can either facilitate or retard contaminant flow, but decay always results in a loss of activity of the original radionuclide. However, the modeler must consider the potential ingrowth of toxic daughter products, depending upon the time scale of the model.

Mathematical screening methods do not explicitly simulate processes that influence the transport of radionuclides; these processes are generally combined into a single term designated the *distribution coefficient* (K_d). Distribution coefficients are discussed qualitatively in Appendix A of the report, along with a number of limitations inherent to the assumptions surrounding the use of K_d. Analytical models are generally able to simulate steady-state flow conditions. However, because the data available during the scoping phase rarely support transient simulations, common analytical methods may be more effective than numerical methods that depend on more sophisticated (but inadequate) data. It is much easier to conduct sensitivity analyses with analytical rather than numerical models.

Uncertainty in the analyses should be emphasized in the scoping phase model. Data collection itself can introduce uncertainty, and, when combined with the system's natural randomness, may lead to wide variations in results. In practice, much of the effort in early modeling studies should focus on the significance of uncertainty associated with specific parameters rather than on modeling specific hydrogeologic properties. Since uncertainty is expressed as a probability distribution around each of the parameters, it is important to select a model where individual values can be selected systematically from the range of results and substituted into the governing flow equations. If this is done properly, the effects of a single parameter may be evaluated. Where the possible range is impracticably large, the analyst may have no other recourse than to evaluate the high and low values and await the collection of better data. Sensitivity analyses are therefore very useful in guiding the design of monitoring or site characterization studies. It is relatively easy to develop conservative estimates of the extent of contamination or the down-field concentration of contamination based on high- or low-end values of probable data values.

Site Characterization Modeling

One of the primary objectives in site characterization modeling is to obtain sufficient data for a defensible (and more realistic) site-specific approach. Reliance on conservatively high values may lead to problems during site characterization or baseline risk assessment phases. For example, reliance on conservatively high hydraulic conductivities could interfere with calibration to known values, or predictions of higher ground-water flow and concomitantly lower down-field contaminant concentrations. For these reasons, application of the model during the site characterization phase is more sophisticated and should be managed by experienced personnel.

The four steps in model application are (1) code selection; (2) model construction; (3) model calibration; and (4) sensitivity / uncertainty analysis. The greatest difficulty in selecting appropriate computer code is not in determining capabilities but rather in determining which capabilities are necessary to support remedial decision making at a particular site. However, the model's "pedigree" is also important to consider, and must be described. Availability of source code, history of use, documentation, testing, and necessary hardware each should be considered when deciding whether the model will produce acceptable—and accepted—results.

Model construction is the process of transforming the conceptual model into mathematical terms that comply with physical boundaries and accepted laws. For example, the continuum of possible values inherent in natural systems is replaced by a series of discrete blocks or elements, and three-dimensional space is divided into grids. The issue is to divide up the domain in as realistic a manner as possible. The finer the size of each "block" in the grid, the more accurate the numerical solution. However the more blocks there are, the more difficult and time-consuming it will be to run the model. Similarly, any model that simulates transient concentrations requires the use of time steps. There is a direct relationship between numerical accuracy, grid density, and time-step size. Fortunately, there is a satisfactory numerical criterion for selecting the time step for a model. Boundary conditions must be described in terms of where water is flowing into and out of the system. Since physical boundaries can be permeable, impermeable, or semipermeable, the model boundaries can be treated either as a constant or variable specified flux, or as a constant head, depending upon which best describes the physical conditions.

Model calibration refers to the trial-and-error adjustment of parameters of the ground-water system by comparing the model's output and measured values. A model is calibrated by determining a set of parameters, boundary conditions, and hydraulic stresses that generate simulated potentiometric surfaces and fluxes that match field-measured values within an acceptable range of error. Ground-water flow models may be calibrated automatically against preset criteria. A contaminant transport model is usually calibrated more subjectively, since data on concentrations are usually inadequate to permit accurate calibration. Also, contaminant transport equations contain more parameters than flow transport equations, so it is more difficult to develop an automated method. No established protocol currently exists for determining whether a model has been satisfactorily calibrated. However, there are several common ways of reporting calibration results, the most common of which is to list the measured and simulated heads together with their differences and some average of the differences.

After the model has been calibrated, sensitivity analyses should be conducted and reported to determine the sensitivity of the model's output to variations (or uncertainties) in the input parameters. The most common practice for carrying out sensitivity analyses is to repeat simulations using a series of simulated values, and to compare results with those obtained using the calibrated values. Sensitivity analyses will identify the main contributors to the observed variation in results, and are performed iteratively. However, sensitivity analyses alone will not identify a flawed conceptual model. Uncertainties arising from the numerical solution of a mathematical model are resolved when verifying the computer programs. Uncertainty resulting from the scenarios selected for modeling is best addressed by a systematic examination of a scenario's possible components and by assigning probability through such techniques as a Monte Carlo analysis.

Baseline Risk Assessment

A baseline risk assessment typically addresses three objectives: (1) assessing the magnitude and sources of current and potential health risks; (2) refining site characterization studies; and (3) identifying contaminants of potential concern and exposure assumptions. In most cases, estimating flow and transport through the unsaturated zone is an integral component of the risk assessment, particularly if the compliance point is near the source. The release rates, concentrations, and retention times within the unsaturated zone will influence receptor concentrations far more than flow and transport in the aquifer. Risk-based model subcomponents consist of infiltration, source release rates, source and leaching strength, fate and transport in the unsaturated zone, and fate and transport in the saturated zone. Risk-based codes typically are not calibrated, however, because the required data from the unsaturated zone are rarely available. Evaluation of the parameters during sensitivity analysis is therefore especially important.

Predictive Simulations

The final stage of model application is to perform predictive simulations with the optimal parameters obtained from model calibration. These simulations test specific issues of the contamination problem and provide guidance for risk-management decisions. Typical objectives of predictive simulation studies include: (1) the future behavior of ground water and contaminant plumes; (2) comparing alternative remediation schemes such as barriers or pumping wells; and (3) the responses of the ground-water system to various design configurations, such as different pumping or recharge operations.

CONCLUSIONS

Modeling reports must be evaluated in the context of the model's purpose. The most common mistakes are in using a model that is more sophisticated than appropriate for the available data, or in using a model that does not accurately account for the flow and transport processes that dominate the physical system. The reviewer should determine whether the modeler's analysis is consistent with the requirements for the decision at the specified stage of the regulatory or remediation project. The data required should be relevant to the flow, fate, and transport processes being simulated, and the sources for each data element should be described. A common problem with modeling studies lies with their discussion (or lack of one) of uncertainties, including uncertainties in data, assumptions, and sensitivities. The conceptual model should be consistent with the field data, and should be well within recommended boundary and initial conditions. The calibration process should be described in detail. While calibration may not be required in all cases, the report should explain why calibration was not done. Source terms, release rates, leachate concentrations, and decay and daughter-ingrowth (of radioactive decay products) must be documented carefully.

Evaluations of models often receive more attention from decision makers than the simulations themselves. For this reason, it is the reviewer's responsibility to judge whether he or she has the necessary expertise to interpret the data and assess the model's concept, as well as to evaluate the results.

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REPORTS IN THIS SERIES

- *Documenting Ground-Water Modeling Results At Sites Contaminated with Radioactive Substances,* EPA 540-R-96-003, March 1996.
- *Three Multimedia Models Used at Hazardous and Radioactive Waste Sites,* EPA 540-R-96-004, March 1996.
- *Technical Guide to Ground-Water Model Selection at Sites Contaminated with Radioactive Substances,* EPA 402-R-94-012, September 1994.
- *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-93-011, March 1993.
- *Computer Models Used to Support Cleanup Decision-Making at Hazardous and Radioactive Waste Sites,* EPA 402-R-93-005, March 1993.