PHASE 1 DEMONSTRATION OF THE NUCLEAR REGULATORY COMMISSION'S CAPABILITY TO CONDUCT A PERFORMANCE ASSESSMENT FOR A HLW REPOSITORY

Final Draft

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Preface

The work described in this report was a team effort that included input from the authors as well as from additional staff members.

The contributors to this report are:

J. Bradbury, NMSS
K. Chang, NMSS
R. Codell, NMSS
N. Coleman, NMSS
N. Eisenberg, NMSS
D. Fehringer, NMSS
W. Ford, NMSS
T. Margulies, RES
T. McCartin, RES
T. Mo, NMSS
J. Park, NMSS
C. Peterson, NMSS
J. Pohle, NMSS
J. Randall, RES
J. Trapp, NMSS

The authors of this report, who are responsible for the text, are:

R. Codell, NMSS
N. Eisenberg, NMSS
D. Fehringer, NMSS
W. Ford, NMSS
T. Margulies, REs
T. McCartin, REs
J. Park, NMSS
J. Randall, RES

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EXECUTIVE SUMMARY

The objective of this effort was to expand and improve the NRC staff capability to conduct performance assessments independently. By expanding and developing the NRC staff capability to conduct such analyses, the NRC would be better able to conduct an independent technical review of the DOE licensing submittals for a HLW repository.

These activities were divided into Phase 1 and Phase 2 activities. The Phase 1 activities were conducted primarily in CY 1989 by the NRC staff with minimal input from NRC contractors. The Phase 2 activities were to involve NRC contractors actively and to provide for the transfer of technology. Phase 2 activities are scheduled to start in CY 1990 to allow Sandia National Laboratories to complete development and tranfer of computer codes and the CNWRA to be in a position to assist in the acquisition of the codes.

The results presented here have had limited peer review, have numerous simplifying assumptions, consider only a limited number of scenarios, and are based on limited data; thus, the numerical results should not be taken as representative of the performance of the proposed repository at Yucca Mountain, NV. The analysis is also replete with uncertainties regarding conceptual models, data, physicochemical models, and models and data for predicting scenarios. The authors did not encounter any problems which indicated the EPA standard could not be implemented. However, due to the incomplete scenario analysis in this demonstration, not all aspects of the standard were tested (e.g. the difficulties in estimating scenario probabilities). Therefore, taking these tentative results of a preliminary analysis out of context or separating these tentative results from these caveats, may lead to the inappropriate interpretation and use of the results.

This report is intended to demonstrate the capability to conduct a performance assessment. The report is not intended to provide guidance on performance assessment methods or on the conduct of NRC staff reviews of performance assessments. Furthermore, it should not be considered as NRC staff guidance on the interpretation and implementation of NRC rules and regulations.

Purpose

Given this background, the primary focus of the Phase 1 activities was to demonstrate the capability of the staff to conduct a total system performance assessment in an independent fashion. By demonstrating such an independent capability, the NRC staff has provided evidence of a degree of readiness for the forthcoming review of licensing material to be provided by the DOE. In addition, by exercising this capability for independent review, the NRC staff has accomplished several secondary objectives, including:

1. Performing an evaluation of the adequacy of existing analytical tools, both methodologies and computational methods.

2. Obtaining valuable insights into the need for further development of methodologies and computational tools.

3. Obtaining valuable insights into the data needed from the DOE Site Characterization Program to conduct performance assessments, including the priority of these data needs. (Because of the uncertainties in the analysis, these insights are limited, especially for this Phase 1 effort.)

Scope

The performance assessment is considered to be comprised of two parts:

(1) quantitative estimation of total system performance through the use of predictive models, and

(2) documentation, including detailed auxiliary analyses where appropriate, to support the assumptions, data, and modeling approaches used to obtain quantitative estimates of performance.

Both of these aspects of performance assessment were addressed in the Phase 1 effort.

The focus of this Phase I demonstration was the EPA containment standard that requires the total system performance measure for a high level waste repository to be expressed by a complementary cumulative distribution function (CCDF) of radionuclide releases to the accessible environment, weighted by a factor approximately proportional to radiotoxicity, integrated over an appropriate period of time (10,000 years is the current regulatory requirement). This performance measure was estimated by following the steps outlined in the information flow diagram (Figure 0.1). For the Phase 1 effort, these steps were all executed, but some (for example steps 2 and 3) were only executed to a limited degree. These steps are described briefly below:

1. System Description - In this step the various important components of the waste disposal system - the waste form, the engineered barrier (the canister, the repository, backfill, if any), and the site - are described in terms useful to modeling radionuclide migration to the environment. This step usually requires the synthesis of inputs from many different disciplines in the natural sciences and engineering.

2. Scenario Analysis - Scenarios representing alternative futures for the system and possible future states of the environment are screened and chosen. Probabilities are estimated for the scenarios chosen. This step usually requires the synthesis of inputs from many different disciplines in the natural sciences and engineering.

3. Consequence Analysis - The consequence in terms of cumulative release of radionuclides to the accessible environment over a specified time period (usually 10,000 or more years) is calculated for each scenario and usually numerous realizations of possible parameter values.

4. Performance Measure Calculation (CCDF) - The consequences for each scenario, in terms of normalized cumulative releases of radionuclides to the environment over a specified period of time, are calculated and the results are displayed in a curve of consequences versus the probability that such consequences will be exceeded. Compliance with the performance criteria is determined by comparing the CCDF to a compliance curve, which the CCDF must not exceed.

5. Sensitivity and Uncertainty Analysis - Sensitivity analysis investigates the change in performance measures caused by incremental changes in the values of input parameters and data. Uncertainty analysis attempts to quantify the uncertainty in performance estimates in terms of the major sources of uncertainty, including uncertainty in input parameters, uncertainty in modeling (both the conceptual model of the geometry and characterization of the system and the process model of what physicochemical processes occur and how they are manifested), and uncertainty about future states-of-nature. Modeling uncertainty was not quantified in Phase 1.

6. Documentation - The most effective documentation must make clear the assumptions used in the analysis, their basis, and the implications of their use explicit.

Two types of uncertainty are usually treated explicitly in the generation of the CCDF: (1) uncertainty due to future states of nature and (2) uncertainty in the values of parameters determining system performance. Modeling uncertainty is usually not treated explicitly in the generation of the CCDF. The complementary cumulative distribution function is a curve of the likelihood that the consequence is a certain magnitude or less. For the repository system considerable uncertainty exists concerning the values of parameters used to estimate the consequences of the repository. The uncertainty from this source is displayed on the CCDF, by combining the probability of a given scenario with the probability of a given set of input parameters for that scenario.

Because of the complexity of the calculation of the CCDF, the staff deemed it appropriate, but not absolutely necessary that the generation of the CCDF be performed by a computer code.

As explained above, only a rudimentary performance assessment is intended for Phase 1 of the MOU, because of limited data, resources, and time and because input from NRC contractors, which could contribute to the goals of the MOU, is not currently available. Because of the constraints on this activity the scope of the effort was limited. Some of these limitations were:

- Only a preliminary analysis was intended in Phase 1.

- Use of currently available modeling tools was to be maximized; additional computer code development was to be minimized.

- The analysts were to take advantage of the limited data available for the Yucca Mountain Site.

- The scopes of the analyses were constrained by the time and resources made available to do it; the effort was scaled down from the original plan for this work.

- As many components of the methodology as possible were to be executed, given the limited time and resources available; this required reducing the depth to which certain aspects were demonstrated.

- For the Phase 1 effort the EPA containment standard was to be the major focus; other regulatory standards were considered only incidentally.

- Phase 1 was executed by NRC staff only ; other than existing reports, papers, and computer software packages already delivered, no contractor input was available for Phase 1, except infrequent and short personal communication.

- CNWRA involvement in Phase 1 was primarily as an observer, but would become more active as the CNWRA PA capability expands.

Accomplishments

The NRC staff demonstrated its capability to conduct independently performance assessments for a HLW repository. Figure 0.2 shows how a CCDF for the total system can be constructed from curves for separate scenario classes (N.B. The caveats stated on the next page indicate why this CCDF is not considered to be representative of total system performance of a proposed Yucca Mountain repository). In doing so the staff gained insight into the capabilities and limitations of the currently available performance assessment methodology. In achieving this primary objective the NRC staff also achieved the following major accomplishments during Phase I:

1. Modeled a potential liquid pathway of the undisturbed scenario class for the Yucca Mountain repository using:

    (1) the NEFTRAN computer code to simulate transport in the unsaturated zone,

    (2) four vertical transport legs under the repository to account for spatial variability,

(3) a modified treatment of waste form dissolution, and

(4) a nonmechanistic model of waste package failure.

This liquid pathway modeling was extended to treat pluvial conditions.

2. Developed and used a total system code to represent total system performance as a CCDF for a limited set of scenario classes using preliminary data and numerous assumptions.

3. Developed a model and the corresponding computer code to treat human-intrusion by drilling.

4. Performed a preliminary statistical analysis of results (sensitivity and uncertainty) using several techniques including Latin Hypercube Sampling (LHS) and regression analysis methods.

5. Executed several auxiliary analyses:

   - potential for non-vertical flow
   - sampling requirements for CCDF generation
   - consequences of C-14 gaseous releases
   - statistical analysis of available hydrologic data for input to flow and transport models

<u>Tentative Results</u>

In considering these tentative results, some important caveats should be recognized. Taking these tentative results of a preliminary analysis out of context or separating these tentative results from these caveats, may lead to the inappropriate interpretation and use of the results.

1. The results presented here have had limited peer review, have numerous simplifying assumptions, and are based on limited data; therefore, the numerical results should not be taken as representative of the performance of a repository at Yucca Mountain, NV.

2. The analysis is replete with uncertainties regarding:

   o conceptual models
   o data
   o physicochemical models
   o models and data for predicting scenarios

3. Only a limited set of scenario classes were incorporated in the modeling, so the total CCDF presented in this report cannot truly represent total system performance.

4. The modeling of waste package failure is nonmechanistic and rudimentary; therefore, this aspect of repository performance is probably not adequately represented.

5. The liquid flow and transport models used attempt to simulate key aspects of the performance of a repository at Yucca Mountain, but do so indirectly through modifications of transport analysis for saturated rock. A more direct representation of flow and transport in partially saturated, fractured rock is needed to assure an adequate level of confidence in the results.

Given the caveats stated above, the reader is reminded that the tentative conclusions stated below should be used only with these substantial limitations kept in mind. Based on a preliminary analysis, the staff has reached some tentative conclusions:

1. The fact that the Yucca Mountain repository like others is designed so that the waste is emplaced over a substantial area appears to be an important aspect determining performance and should be included in models of performance; important aspects appear to be areal variability of:

   - o waste package failure
   - o depth of rock to water table
   - o potential of rock units to sustain fracture flow

2. The gaseous release of C-14 could be an important factor in repository performance, but more analyses and data are needed to determine how important.

3. Two dimensional modeling of the HYDROCOIN Yucca Mountain description resulted in significant lateral movement of water for unsaturated groundwater infiltration rates greater than 0.2 mm/yr. Nonvertical flow could be an important factor in repository performance, which warrants additional analysis and data.

4. For the "liquid pathway" scenario class, the most significant contributors to the consequences represented by the CCDF are isotopes of plutonium. Because plutonium behavior is poorly understood, large uncertainties exist regarding:

   - o colloids
   - o retrograde solubility
   - o sensitivity of chemistry to oxidation state

5. For the "liquid pathway" scenario class, the important input parameters appear to be:

- o infiltration flux
- o fraction of infiltrating groundwater contacting the waste
- o uranium matrix solubility
- o saturated hydraulic conductivity for the Calico Hills Vitric unit

6. Consequence codes used in this study may not be sufficiently efficient to allow analyzing many scenarios each with many input parameter vectors, so that total system performance is adequately characterized.

Preliminary Suggestions for Further Work

Based on this preliminary analysis and the limitations noted, the authors have some preliminary suggestions regarding the directions for further technical work to take. These do not represent an official NRC position, but are the views of the individual staff members who wrote this report. Several of these suggestions relate to aspects of the methodology that are missing or need improvement or that have not yet been incorporated into the NRC performance assessment capability. Other suggestions relate to the general lack of data for Yucca Mountain. Some of this suggested work is clearly the responsibility of DOE; other items could be performed by NRC, DOE, or a third party. These suggestions are based on the work described in this report; they have not been correlated with other NRC staff views or with the DOE site characterization program. Therefore, these suggestions are not intended to and should not be taken as indications of deficiencies in the DOE Site Characterization Plan. These recommendations for technical improvements include the following:

Recommended improvements to modeling of performance:

General

1. Add the capability for modeling additional scenario classes.

2. Test the system code using the consequence codes as subroutines, instead of generating data sets external to the system code.

3. Acquire, test, and evaluate codes developed by SNL for a repository in the unsaturated zone.

4. Explore, with the CNWRA, the adaptation of the FPPA (Fast Probabilistic Performance Assessment) methodology to generate the total system CCDF.

5. Evaluate additional codes, which could not be acquired and evaluated during this short-time effort, to determine whether existing codes can meet the NRC modeling needs or whether additional code development is needed.

Flow and Transport

1. Refine groundwater modeling (e.g., by considering higher dimensions).

2. Incorporate a model of gas-pathway transport in the calculation of the CCDF.

3. Include flow and transport through the saturated zone.

4. Directly model transport through a partially saturated, fractured rock, instead of the indirect, approximate representation used in Phase 1.

5. Explicitly model fracture/matrix coupling.

Source Term

1. Attempt to develop or use a previously developed mechanistic model of waste package failure

2. Develop a mechanistic model of contact between groundwater and the waste

3. Treat the repository as a source of radionuclides distributed in time and space, instead of as a point source

Recommended improvements to and extensions of auxiliary analyses:

1. Perform detailed geochemical analyses to investigate:

   - use of K_D's (distribution coefficients)
   - effects of spatially varying saturation on radionuclide migration
   - waste form, groundwater, tuff reactions
   - waste package degradation
   - oxidation of the spent fuel matrix
   - plutonium behavior

2. Evaluate heat effects at early time periods; estimate the thermal, hydrologic, and geochemical environment of the repository at early times.

3. Evaluate importance of thermally and barometrically driven air flow on repository performance at Yucca Mountain.

4. Perform detailed hydrologic analysis for Yucca Mountain, to provide a better input to the transport analysis and to examine, in more detail, various alternative hypotheses regarding hydrology at Yucca Mountain.

Recommendations for additional scientific input (N.B.: some of these items could be performed by either the DOE or NRC, while others are clearly the responsibility of DOE):

1. Develop and demonstrate a mathematically rigorous, scientifically robust method for scenario analysis.

2. Obtain geoscience input for modeling volcanism.

3. Obtain geoscience and hydrologic input to modeling faulting, uplift, and subsidence at Yucca Mountain.

4. Obtain laboratory chemical analysis to determine the partitioning of radionuclides in various compartments of the spent fuel waste form.

5. Obtain field and laboratory data on phenomena important to the near-field behavior of the repository, especially the effects of heat.

6. Obtain more data on plutonium geochemistry.

7. Obtain a better understanding of waste package corrosion in the unsaturated zone.

8. Obtain field and laboratory data and perform analyses to investigate the issue of non-vertical flow at Yucca Mountain.

9. Obtain field data on the transport of gaseous radionuclides (C-14) at Yucca Mountain.

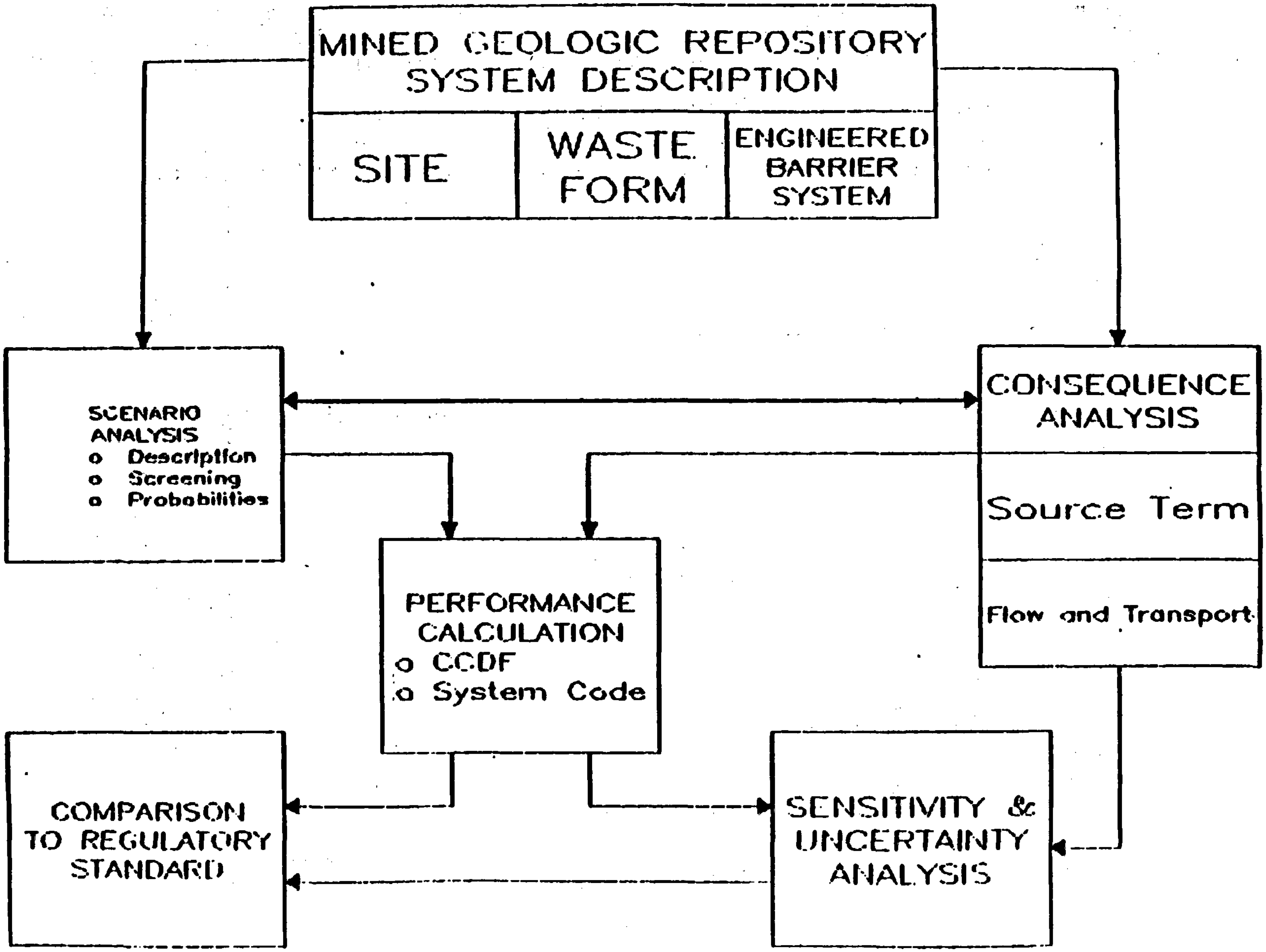

Figure 0.1 Components of a total system performance assessment.

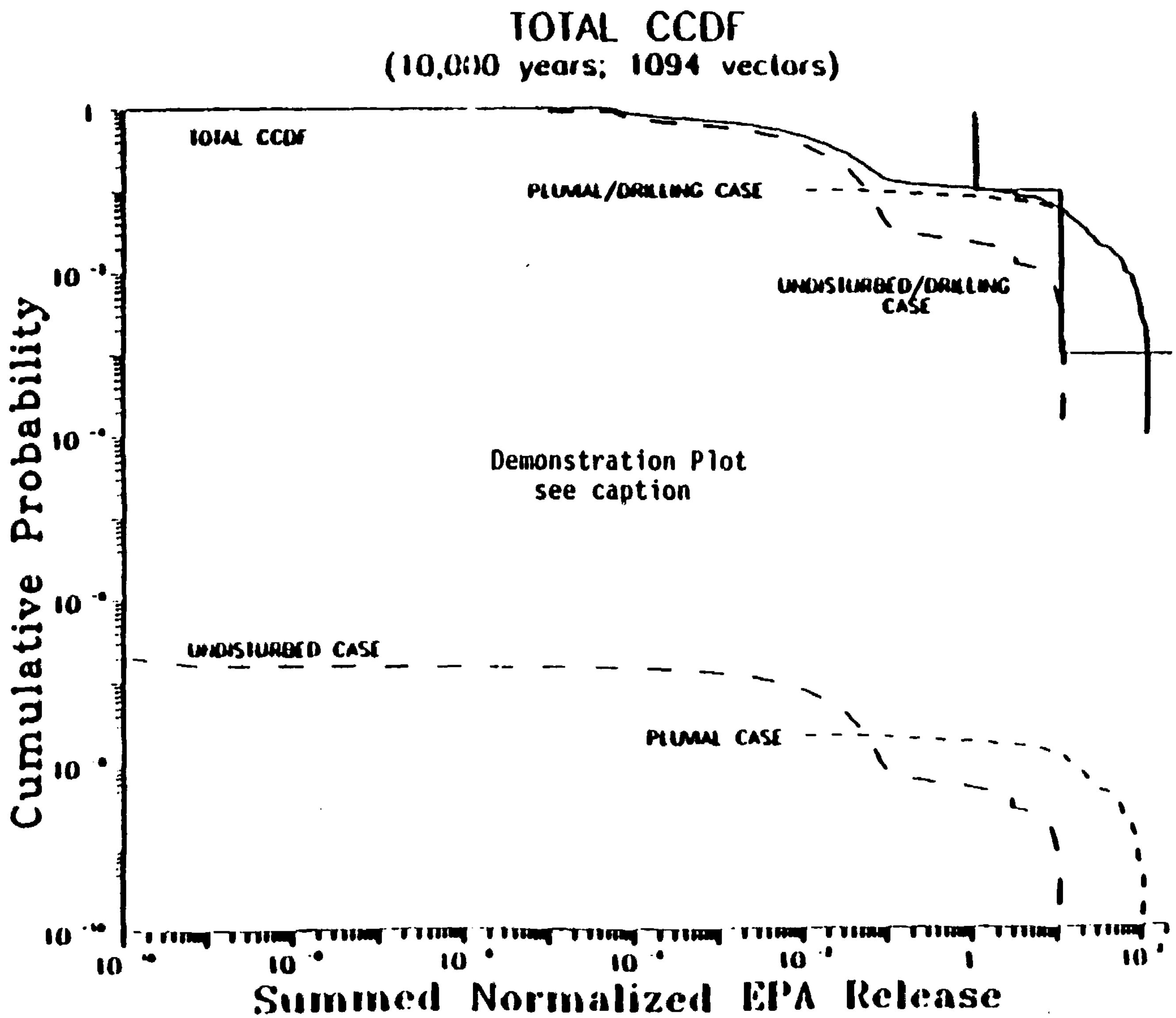

Figure 0.2 Composite CCDF curve for the scenario classes considered in Phase I of the Iterative Performance Assessment. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse d

1.0 INTRODUCTION

This report describes the results of the Phase 1 demonstration of the NRC capability to conduct a performance assessment (PA) of a high level waste repository.

This demonstration was undertaken as the initial step in a sequence of planned iterative performance assessments to be undertaken by the NRC staff and NRC contractors. Performance assessment of a high level waste repository, like other systematic safety assessment methodologies, benefits substantially by being conducted in an iterative manner, primarily because the lessons learned regarding modeling improvements, data needs, and methodology can be addressed in subsequent iterations. This activity was undertaken to maintain and to enhance the independent NRC staff capability to evaluate performance assessments submitted as part of a license application. This capability consists of at least two aspects: (1) the capability to provide an independent check on key aspects of the licensee's assessment and (2) the capability to probe the licensees assessment for potential weaknesses, based on a familiarity with the methods, data and assumptions used in the assessment.

In addition, these iterative performance assessments are expected to provide insights helpful in developing regulatory products, including: (1) technical positions, rulemakings, and other regulatory guidance; (2) evaluation of site characterization activities; and (3) evaluation of NRC research program.

These iterative performance assessment activities, are currently planned to proceed in two phases: Phase 1, a demonstration, was intended to: (1) result in a framework for PA modeling; (2) with the limited resource allocated to perform this activity, provide only a rudimentary demonstration of a PA modeling capability; (3) be accomplished with a minimum of technical input and interaction with NRC contractors, except for work already documented and products delivered to the NRC. Phase 2, is intended to: (1) be accomplished in FY 90 and beyond; (2) incorporate significant products to be delivered by NRC contractors, most notably the Tuff Performance Assessment Methodology currently under development by Sandia National Laboratories under FIN-A1266; and (3) provide a more complete, accurate, sophisticated, and realistic PA modeling capability. Additional phases (iterations) may be added as this work proceeds.

An interdisciplinary, integrated approach was envisioned when the initial plans for this activity were developed from late 1988 to early 1989. Although some work was continued by some staff for a time, sustained effort by several staff on this Phase 1 demonstration did not resume until August/September 1989. At that time, the effort was restructured. The major features of this restructuring included:

- o Conclusion of the Phase 1 work in three months, no later than November 30, 1989.

- o Attempting to execute as many steps in the performance assessment methodology, while at the same time tailoring the activities to fit into the time and resources allowed.

- o Establishing a smaller core group of participants to be responsible for the work. The involvement of other staff and continual peer review as originally envisioned in late 1988, would be deferred until after November 30, 1989, to expedite the effort.

- o The work would be divided into five parts:

  1. Scenario Analysis
  2. Flow and Transport
  3. Source Term
  4. System Code
  5. Auxiliary Analyses

The first four topical areas corresponded to four working groups or Teams. These Teams roughly correspond to the methodological steps of performance assessment shown in Figure 1.1. The members and leaders of these teams and other details of the project organization are discussed in Section 3.

This report is largely structured along the same lines used to organize the work. Thus, the central part of this report describes the work performed by the various teams:

Section 4 - System Code
Section 5 - Source Term
Section 6 - Flow and Transport Models
Section 7 - Methodology for Scenario Development
Section 8 - Auxiliary Analysis Summaries

Because Phase 1 was a demonstration of capability, these Sections may be taken as a status report on progress made to date. They should in no way be taken as the description of a definitive approach to these components of performance assessment. Sections 0 through 3:

Section 0 - Executive Summary
Section 1 - Introduction
Section 2 - Purpose and Scope
Section 3 - Organization and Staffing of Phase 1

are largely self-explanatory, front material. Section 9, Analysis and Results, presents the limited results of this Phase 1 demonstration. Section 10, Preliminary Suggestions for Further Work, presents some preliminary thoughts on the direction for Phase 2 efforts. Because of the limited nature of the analysis, no conclusions or recommendations about the proposed repository at Yucca Mountain are given or intended to be given. The authors did not encounter any problems which indicated the EPA standard could not be implemented. However, due to the incomplete scenario analysis in this demonstration, not all aspects of the standard were tested (e.g. the difficulties in estimating scenario probabilities).

Finally, the appendices present material too detailed to be included in the main text.

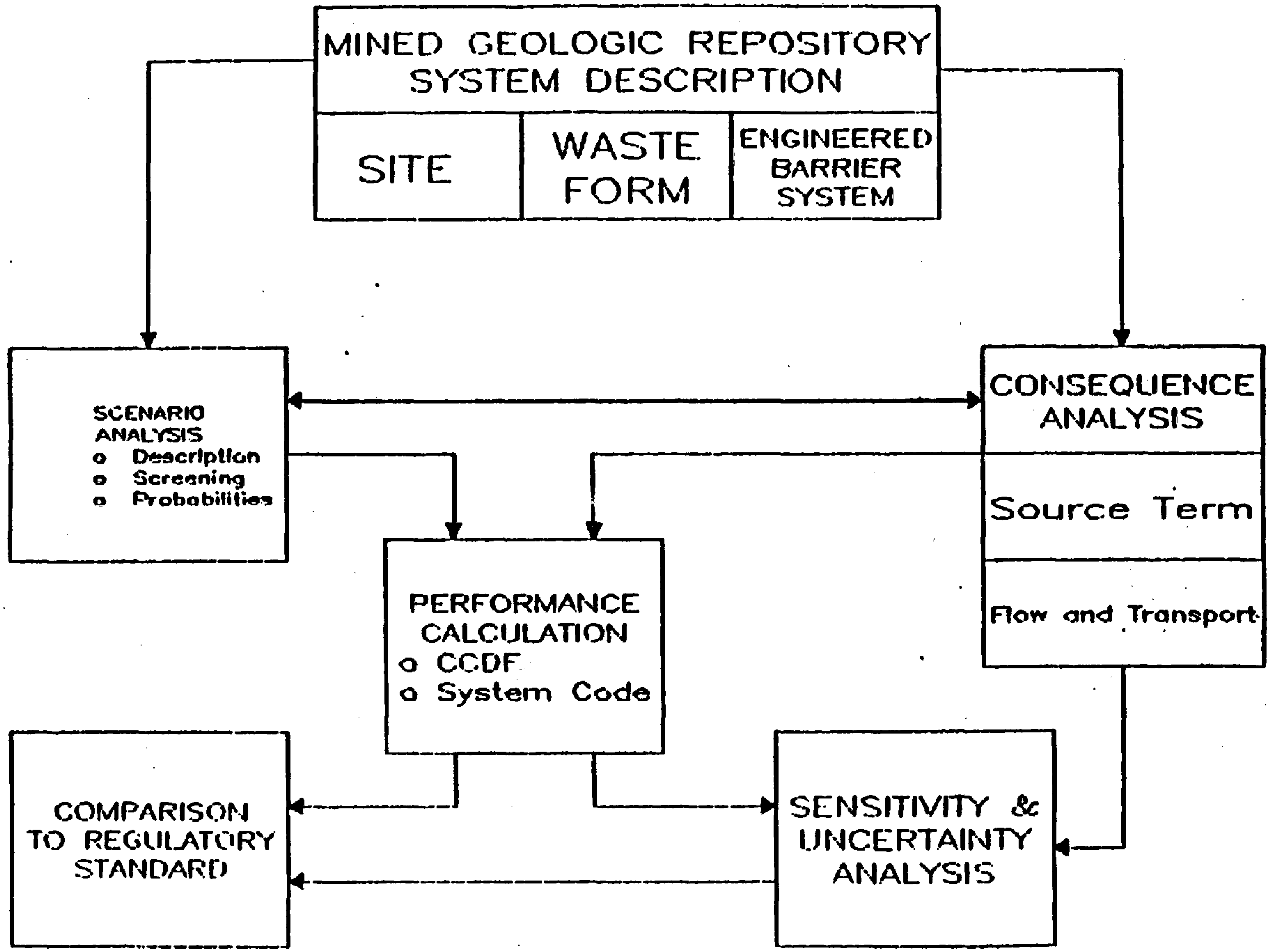

Figure 1.1 Components of a total system performance assessment.

2.0 PURPOSE AND SCOPE

The primary purpose of Phase 1 of the iterative performance assessment activity was to demonstrate the capability of the NRC staff to conduct, independently, a performance assessment of a proposed repository. An independent assessment capability is considered to be an important aspect of the licensing review to be conducted by the NRC staff. In order to achieve these goals a limited, preliminary total system performance was conducted.

The performance assessment is considered to be comprised of two parts:

(1) quantitative estimation of total system performance through the use of predictive models and

(2) documentation, including detailed auxiliary analyses where appropriate, to support the assumptions, data, and modeling approaches used to obtain quantitative estimates of performance.

Both of these aspects of the performance assessment were addressed in the Phase 1 effort.

By accomplishing this primary goal, some worthwhile secondary goals were achieved:

- The existing analytical tools to conduct a performance assessment (both methodologies and computer codes) were evaluated

- Insight was obtained into the needs for the development or improvement of methodologies

- Insight into the needs for site characterization was obtained.

The total system performance measure for a high level waste repository can be expressed by a complementary cumulative distribution function (CCDF) of radionuclide releases to the accessible environment, weighted by a factor approximately proportional to radiotoxicity, integrated over an appropriate period of time (10,000 years is the current regulatory requirement). This performance measure is mandated by the EPA standard (40 CFR 191) for the containment of waste by a HLW repository. This performance measure is incorporated into the NRC's regulation (10 CFR 60), along with additional performance measure relating to (1) waste package lifetime, (2) fractional release of radionuclides from the engineered barrier system, and (3) ground water travel time. The representation of repository performance by a CCDF of weighted cumulative releases incorporates (a) consideration of the various components impeding the movement of radionuclides to the environment and (b) consideration of a range of conditions and events that could affect future performance. This performance measure is estimated by following the steps in the outlined flow diagram, Figure 1.1, located in the prior section. For the Phase 1 effort, these steps were all executed, but some (for example steps 2 and 3) were only executed to a limited degree and only parts of others (for example step 5) were done. These steps are described briefly below for the Phase 1 effort:

1. System Description - The repository is broken into its component parts for the purposes of modeling. These include the source term model and the flow and transport model. Computer codes are adapted or written to simulate models of these components. Ranges of parameter values are chosen to bound the expected behavior of the system models.

2. Scenario Analysis - Scenarios representing alternative futures for the system and possible future states of the environment are screened and chosen. Probabilities are estimated for chosen scenarios.

3. Consequence Analysis - Consistent with the requirements of the EPA standard, the consequence in terms of cumulative release of radionuclides to the accessible environment over a specified time period (usually 10,000 or more years) is calculated for each scenario and usually numerous realizations of possible parameter values. In addition to being incorporated by way of cumulative releases into the CCDF (step 4), certain types of consequences might also be considered separately to compare to standards for maximum doses to individuals and for maximum concentration in groundwater (but are beyong the scope of Phase 1). For purposes of dividing up the work, the consequence analysis was conducted by the Source Term Team and the Flow and Transport Team.

4. Performance Measure Calculation (CCDF) - The consequences for each scenario, in terms of normalized cumulative releases of radionuclides to the environment over a specified period of time, are calculated and the results are displayed in a curve of consequences versus the probability that such consequences might be exceeded. Compliance with the performance criteria is determined by comparing the curve to a compliance curve, that provides limits that the calculated the curve must not exceed.

5. Sensitivity and Uncertainty Analysis - Sensitivity analysis investigates the change in performance measures caused by incremental changes in the values of input parameters and data. Uncertainty analysis attempts to quantify the uncertainty in performance estimates in terms of the major sources of uncertainty, including uncertainty in input parameters, uncertainty in modeling (both the conceptual model of the geometry and characterization of the system and the process model of what physiochemical processes occur and how they are manifested), and uncertainty about future states-of-nature. Uncertainty in modeling was not quantified in Phase 1.

6. Documentation - A largely self explanatory effort, documentation must make the assumptions used in the analysis, their basis, and the implications of their use explicit and clear.

Two types of uncertainty are usually treated explicitly in the generation of the CCDF: (1) uncertainty due to future states of nature and (2) uncertainty in the values of parameters determining system performance. In a safety analysis for a more conventional type of system, the response of the system to any single future state of nature to be considered would be a single-valued estimate of system performance (in the parlance of the repository system, a single value of consequence). System performance would then be described by the plot of consequences versus the likelihood of the future state of nature (scenario) producing that consequence; such a curve would be the distribution function. The integral of such a curve over probability would yield a cumulative distribution function; i.e. the likelihood that the consequence would be at least of a certain magnitude. The CCDF would be the curve of the likelihood that the consequence would be a certain magnitude or less. For the repository system considerable uncertainty exists concerning the values of parameters used to estimate the consequences of the repository. Traditionally the uncertainty from this source is also displayed on the CCDF by: (1) describing some or all of the parameters used to estimate consequences as distributions of values rather than point estimates, (2) choosing a value of each parameter required to describe system performance from these distributions representative of some portion of the various distributions, (3) estimating performance based on a given realization of parametric values, (4) noting the conditional parametric probability, i.e. the joint probability density for the given realization or region of parameter space (for uncorrelated parameters this would be the product of the individual parameter probabilities), and (5) calculating the CCDF using the parametric probability multiplied by the probability of the scenario. This process is complicated further when consideration of different scenarios makes it is necessary to vary: (1) the consequence models for different scenarios, and/or (2) the distributions of parameters (either the range of parameters, the magnitude of the parameters, or the shape of the distribution) depending on the scenarios.

Because of the complexity of the calculation of the CCDF, it was decided that the generation of the CCDF be performed with the aid of a computer code. At a minimum such a code is needed to: (1) sequence through all the scenarios to be considered, (2) choose the consequence models and parametric distributions corresponding to the scenario being analyzed, (3) sample the parameter space appropriate to the given scenario, (4) estimate consequences based on the models and parameter values for the scenario, and (5) combine the parametric and scenario probabilities and the calculated consequences to generate a CCDF.

Although the primary focus of the Phase 1 demonstration was the EPA containment standard and the associated performance measure (cumulative releases to the accessible environment), some calculation of performance measures related to the NRC subsystem requirements, such as groundwater travel time, fractional release rate, and waste package lifetime were performed. These calculations were performed to demonstrate the capabilities of the performance assessment methodology and the ability of the staff to exercise the methodology. These calculations are intended as examples and should not be considered to be methods for calculating quantities in a regulatory context that the NRC staff considers acceptable.

As explained in Section 1, only a rudimentary performance assessment is intended for this Phase 1 demonstration, because of limited resources and time and because input from NRC contractors that could contribute to the goals is not currently available. Because of the constraints on this activity the scope of the effort was limited; some of these limitations were:

- only a preliminary analysis was intended in Phase 1
- the effort was scaled down from the original 1/89 plan for this work
- only currently available modeling tools were to be used; computer code development was to be minimized
- the analysts were to take advantage of the limited data available for the Yucca Mountain Site
- the scope of the analyses were constrained by the time and resources made available to do it
- As many components of the methodology as possible were to be executed, given the limited time and resources available; this required reducing the depth to which certain aspects were demonstrated.
- For the Phase 1 effort the EPA containment standard was to be the only performance standard considered. The EPA standards for individual protection and groundwater protection will be investigated later. Also the 10 CFR Part 60.113 subsystem requirements were not to be a subject of the Phase 1 work and perhaps not included in the Phase 2 work.
- Phase 1 was executed by NRC staff only.
- Other than existing reports, papers, and computer software packages already delivered, no contractor input was available for Phase 1, except infrequent and short personal communication.
- CNWRA involvement in Phase 1 was primarily as an observer, but would become more active as the CNWRA PA capability expands.

In order to perform this preliminary performance assessment and demonstrate the staff capability to conduct such work, the following types of activities were performed: 1) Computations and support, including, data input, model setup, code development and testing, code execution, and output analysis; 2) auxiliary analyses, including, evaluation of assumptions and preprocessing raw data; and 3) documentation.

3.0 ORGANIZATION AND STAFFING OF PHASE 1

NRC staff members from both NMSS and RES worked on Phase 1. In order to coordinate the efforts of the two offices, the organizers of Phase 1 designated an administrative project manager from NMSS and two office technical coordinators: One from NMSS and one from RES. The technical staff involved in Phase 1 came from both offices. The assignment of technical staff to technical efforts in Phase 1 was done without regard to office affiliation.

3.1 Administration of Phase 1

Brian Thomas of NMSS/HLPD was Phase 1's administrative project manager. Norman Eisenberg and John Randall, respectively of NMSS/HLPD and RES/DE/WMB, were the technical coordinators for Phase 1. The project manager and technical coordinators facilitated communications among the various technical participants and managers. The technical coordinators also proposed plans for technical activities, schedules, and staffing for Phase 1 for approval by NMSS and RES management.

3.2 Technical Organization of Phase 1

The technical work of Phase 1 of Tasks 2 and 3 was organized as described as described in Section 1. Personnel associated with each effort are listed below.

<u>System Integration:</u> N. Eisenberg (technical leader), J. Park

<u>Source Term:</u> R. Codell (technical leader), K. Chang, T. Mo, J. Park, C. Peterson

<u>Geosphere Transport:</u> T. McCartin (technical leader), J. Bradbury, R. Codell, N. Coleman, N. Eisenberg, D. Fehringer, W. Ford, T. Margulies, J. Park, J. Pohle

<u>Scenario Analysis:</u> D. Fehringer (technical leader), N. Eisenberg, J. Pohle, J. Trapp

<u>Auxiliary Analyses:</u>
- J. Bradbury (geochemical data analysis),
- R. Codell (gas transport and sensitivity and uncertainty analyses),
- W. Ford (hydrogeologic data analysis),
- T. Margulies (volcanism),
- T. McCartin (two-dimensional transport)

4.0 SYSTEM CODE

4.1 Introduction

The system code processes information needed to generate a Complementary Cumulative Distribution Function (CCDF) representative of the performance of a HLW repository. In order to obtain the CCDF, the code treats sequentially a set of scenarios, which represent possible future states of nature. Consequence modules associated with the available release pathways calculate the cumulative radionuclide release for each scenario for the 10,000 year simulation time. These modules are products of work performed on the Source Term and Flow and Transport Tasks, which are documented elsewhere in this report. Each scenario may yield numerous cumulative release values, which result from the multiple input vectors of parameters used in a realization. Probabilities assigned to each consequence within each scenario are then combined with the likelihoods of the scenarios themselves to form the CCDF.

In accomplishing these tasks, the system code handles two types of uncertainty inherant in a CCDF. First, it treats the uncertainty in the future states of nature by looking at sets of scenarios which attempt to describe those future states. Secondly, the code handles the uncertainty related to the variability in model parameters by using multiple sets of parametric input vectors when executing the pathway consequence modules.

4.2 Requirements for the Development of the System Code

The development of the system code is a continuing process, consistent with the ongoing iterative performance assessment activity. Throughout its development, this code should meet certain minimum requirements:

1. The computational modules for calculating consequences, comprised of one or more codes for the source term and transport calculations, produce output in terms of cumulative radionuclide release to the environment. The system code must be capable of receiving this data.

2. The system code must be able to treat two of the types of uncertainty incorporated in a CCDF characterizing repository performance: (1) the uncertainty in future states of nature, and (2) the uncertainty in model parameters used to estimate cumulative releases.

3. In order to treat uncertainty in future states of nature properly, the system code must be able to treat different scenarios (or more properly scenario classes) which attempt to describe those future states and obtain the corresponding data on cumulative releases of radionuclides.

4. In order to treat properly the uncertainty related to the variability of parameters used in the consequence models, the system code must be able to collect and process cumulative release data generated from multiple sets of parametric input vectors.

5. Because many scenarios are expected to allow radionuclide releases by more than one pathway (e.g. in groundwater, by gas, and/or by direct release), the system code must be able to obtain cumulative releases corresponding to the specified pathways.

[Requirements 2 through 5 mandate that the system code will be handling a four-dimensional array of cumulative release estimates, where the dimensions are: scenario number, radionuclide number, pathway number, and input parameter vector number.]

6. The system code should have built-in protection to assure the consistency of the assumptions used within a single simulation. For example, the performance time period (10,000 years for the current EPA standard) should be the same for all scenarios and pathways in any given representation of the repository to which the system code is applied. One way to assure consistency would be to have the system code call the consequence modules as subroutines of the main program. A second method would be to have the consequence results generated outside the system code and stored in a file. This file would include a sufficient record of the critical assumptions and parameters to permit a consistency check. Note: It is not clear presently whether the consequence modules can be called as subroutines by the system code and still be practicable in terms of program size and run-time. The NRC system code allows both methods of operation, but only the latter has been tested.

7. Tabular and graphical presentations of the results should be obtainable from the system code.

4.3 Survey of Existing Codes

The staff evaluated several codes to determine their suitability (as a whole or in part) for use as a system program in this effort. Although all the surveyed codes are not "system codes" per se, each was reviewed in terms of how well it fit the requirements expressed in Section 4.2. The codes are described briefly in Table 4.1, while Appendix A provides a more detailed look.

Based on the results of the review, the staff decided to develop its own system code rather than to adopt an existing one. There were several reasons for this choice. First, adapting an existing program to meet the staff's needs and to be compatible with the NRC computing environment would likely be as time consuming as development of a new code. Secondly, an NRC written code could be more closely tailored to the specific requirements and needs of the project than one developed outside the NRC. Finally, the more promising system codes for potential use in this work would not be available to the staff within the timeframe set.

4.4 Description of the System Code

4.4.1 Introduction

This section presents a brief description of the system code developed by the staff for this demonstration. The manner of code execution (i.e. internal vs. external), the input data requirements, the type of output available, and a brief outline of the system program are all presented.

4.4.2 Internal vs. External Runs

The system code can be executed in either the "internal" or the "external" mode (Figure 4.1). This distinction refers to the time at which the output files from the consequence models are generated. In the internal mode, consequence modules are run and cumulative radionuclide releases calculated as the code is executed. This requires that the modules be incorporated as subroutines in the main program. For external runs however, the modules are separate from the system code, and as a result, the cumulative releases can be generated and placed in files at any time prior to iteration of the code.

Internal executions would appear to make sensitivity analyses easier, because simulation parameters are global. Thus changes to the input files for subsequent runs need only be made once. This decreases the opportunity for error, while offering increased convenience and quality assurance to the analyst.

Simulations in the external mode offer the opportunity to repeat earlier runs as long as the output files from the consequence modules are uniquely identifiable. In addition, external runs would appear to be more economical in terms of both computer time and money since they do not require the execution of either the LHS routine or the consequence models.

Note: As yet, the system code has been demonstrated only in the external mode.

4.4.3 Input to the System Code

The system program requires input data in the following five areas:

1) general run information
2) the particular scenarios to be considered,
3) probabilities of those scenarios occurring,
4) EPA limits for the initial radionuclide inventory, and
5) cumulative releases due to the effects of the scenarios.

The analyst creates a file which consists of both the general run data and the scenario-specific information. This file supplies the execution mode, the simulation time period, and the amount of output desired, as well as the scenarios (total number, names, release pathways) to consider.

A scenario's probability is estimated by combining the probabilities of the processes and events making up the scenario. For this demonstration, the staff modeled four scenario classes based upon two fundamental events: a pluvial period (or not) and drilling at the site (or not). Figure 4.2 shows the probabilities assigned to the events and scenarios.

The EPA limits are taken from 40 CFR Part 191 Appendix A Table 1. Given in curies released per 1000 Metric Tons of Heavy Metal (MTHM), these limits are converted in the system code to limits for the initial inventory of 70,000 MTHM assumed for this demonstration. EPA ratios are calculated, using these limits, for each released radionuclide.

The cumulative releases of radionuclides are calculated by the consequence modules, which model the repository release via the pathways assigned per scenario.

4.4.4 System Code Operation

In order to obtain a Complementary Cumulative Distribution Function (CCDF) estimating repository performance, the system code treats a set of scenarios describing possible future states of nature, and accesses the estimated cumulative releases corresponding to each scenario. The code next combines this data from the scenarios into the CCDF, and finally it prints the CCDF out in the form of a graph and/or a table. This section, along with Figures 4.3 and 4.4, provides a more detailed explanation of how the system code accomplishes these tasks.

The effects of each scenario are assessed in the following manner. Consequence modules for the potential release pathways specified for a scenario are executed if the simulation is run in the internal mode. Next, the cumulative releases calculated by the modules either internally or externally (using Latin Hypercube Sampling (LHS) generated input vectors) are read into the program and stored in temporary arrays. Each nuclide-release pair is compared to its EPA limit and a corresponding normalized EPA ratio calculated by the following formula:

$$\text{Normalized Release of Radionuclide } i = \frac{\text{Cumulative Release of Radionuclide } i}{\text{EPA Limit for Radionuclide } i}$$

These normalized releases are then placed into a four-dimensional array arranged by scenario, radionuclide, vector, and release pathway (Figure 4.5). Once the effects of all scenarios have been modeled, this array is used as a data base over which different summation routines take place. These routines create a second array of summed normalized EPA releases ordered by scenario and vector by adding up normalized releases for all radionuclides over all release pathways.

Then, for each scenario, probabilities are calculated for the consequences associated with a particular input vector. These likelihoods are based on the assumption that every vector within the scenario is equally probable. For example, given this assumption, the likelihood of occurrence of a single vector within a scenario containing 500 vectors is equal to 1/500 or .002. Following the assignment of probabilities, the consequences within each scenario class are sorted, duplicates eliminated, and the likelihoods adjusted accordingly.

The array for each scenario now contains unique, ordered consequences with associated likelihoods of occurrence. Then, in order to obtain a representative cumulative distribution function, scenario probabilities are factored in by multiplying the probability of each consequence by the likelihood of its scenario.

Finally, the results from all scenarios considered are combined, the summed normalized releases with their probabilities ordered and sorted, and a running sum of the probabilities created. This outcome can be graphed as a CCDF on a log-log plot of summed normalized EPA release against cumulative probability.

4.4.5 System Code Output

Results generated by the system code can be written to two output files. In addition to the data needed to graph the total CCDF, these files can contain normalized releases broken down by scenario, vector, release pathway, and radionuclide, or various combinations of these categories.

Plotting the CCDF can be accomplished using any of the variety of graphics packages currently available.

Table 4.1 System Code Survey

1.	AREST	EBS code; partially documented by PNL; code not available
2.	SPARTAN	DOE total system code; oversimplified flow and transport; does not treat radionuclide chains; documented by SNL and DOE; code not available
3.	TOSPAC	DOE total system code; documented by SNL; code not available
4.	REPRISK	EPA total system code; considers four scenario classes; developed for saturated porous media; calculates EPA ratios and health effects; code and documentation available as of 10/89
5.	SUNS	SNL sensitivity and uncertainty analysis shell; interactive; code and limited documentation available
6.	Code Coupler	Provides linkage between different scale models in a total PA; designed for set suite of models including NEFTRAN; LHS used to create common site description for all models; code and documentation available as of 11/89

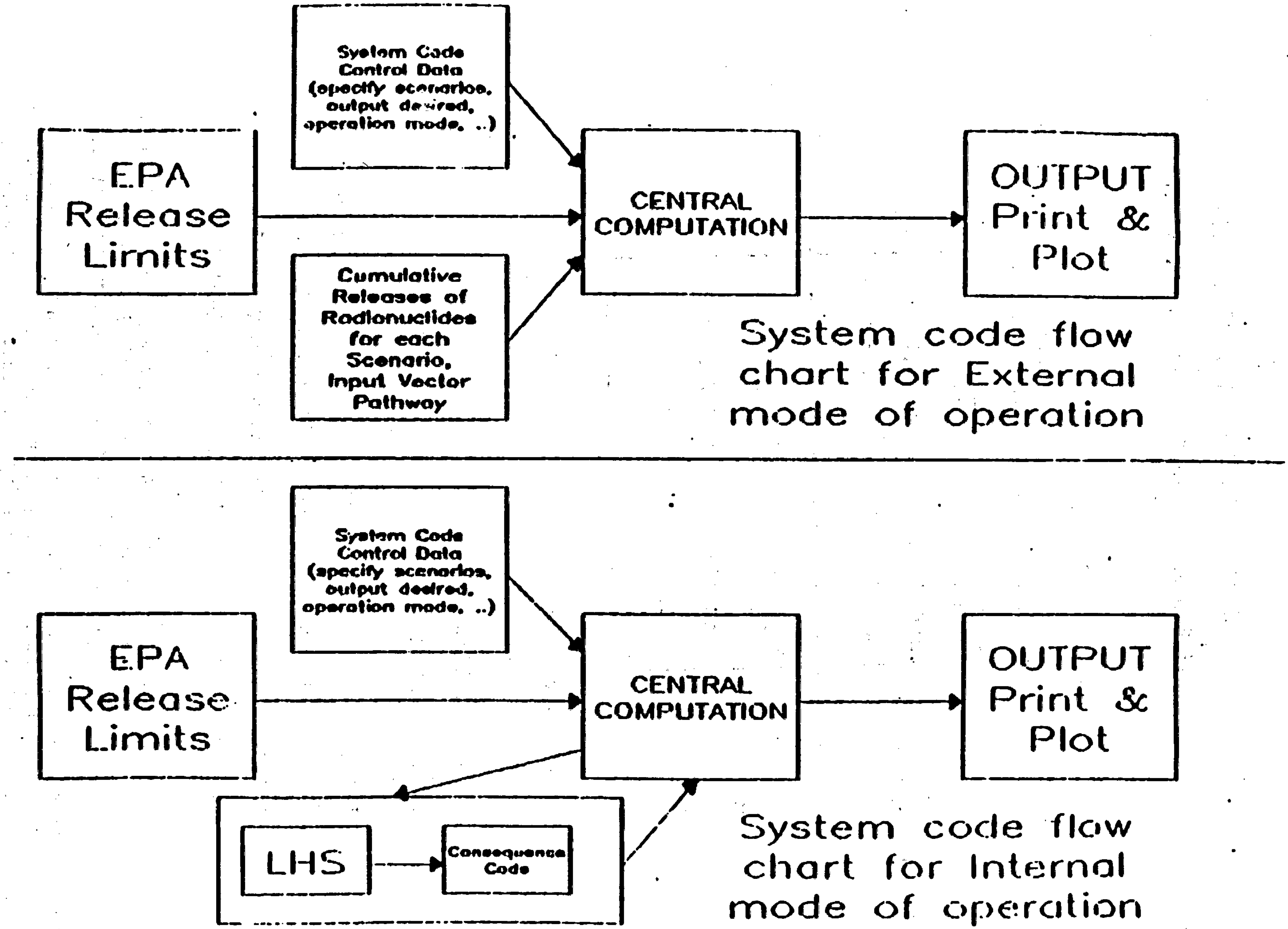

Figure 4.1 Flow diagram of external and internal modes of operation.

DETERMINATION OF SCENARIO PROBABILITIES FROM THE PROBABILITIES OF FUNDAMENTAL EVENTS

	$\bar{P}$ 0.9	P 0.1
$\bar{D}$ 2.3×10^{-7}	scenario class # 0 probability $= 2.0 \times 10^{-7}$	scenario class # 1 probability $= 2.3 \times 10^{-8}$
D ~ 1.0	scenario class # 2 probability ~ 0.9	scenario class # 3 probability ~ 0.1

$\bar{P}$ is not pluvial

P is pluvial

$\bar{D}$ is no drilling

D is drilling

scenario class # 0 is no drilling, not pluvial

scenario class # 1 is no drilling, with pluvial

scenario class # 2 is drilling, not pluvial

scenario class # 3 is drilling and pluvial

Note: Probability combinations assume that fundamental events have independent probabilities of occurence; this is not a general restriction.

Figure 4.2 Determination of scenario probabilities from probabilities of fundamental events. This figure presents results from an initial demonstration of staff capability to conduct a performance assessment. The figure, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

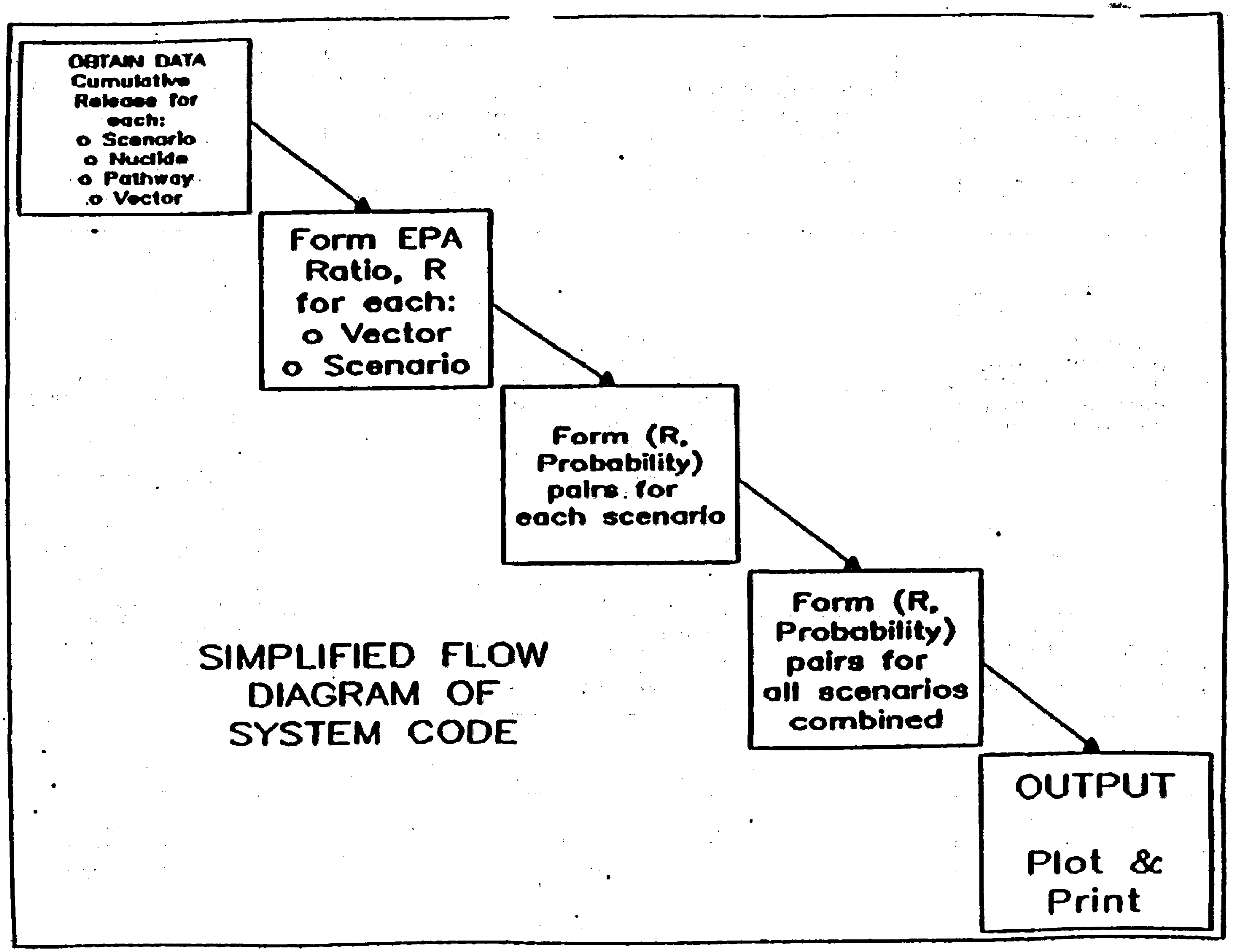

Figure 4.3 Simplified flow diagram of system code steps.

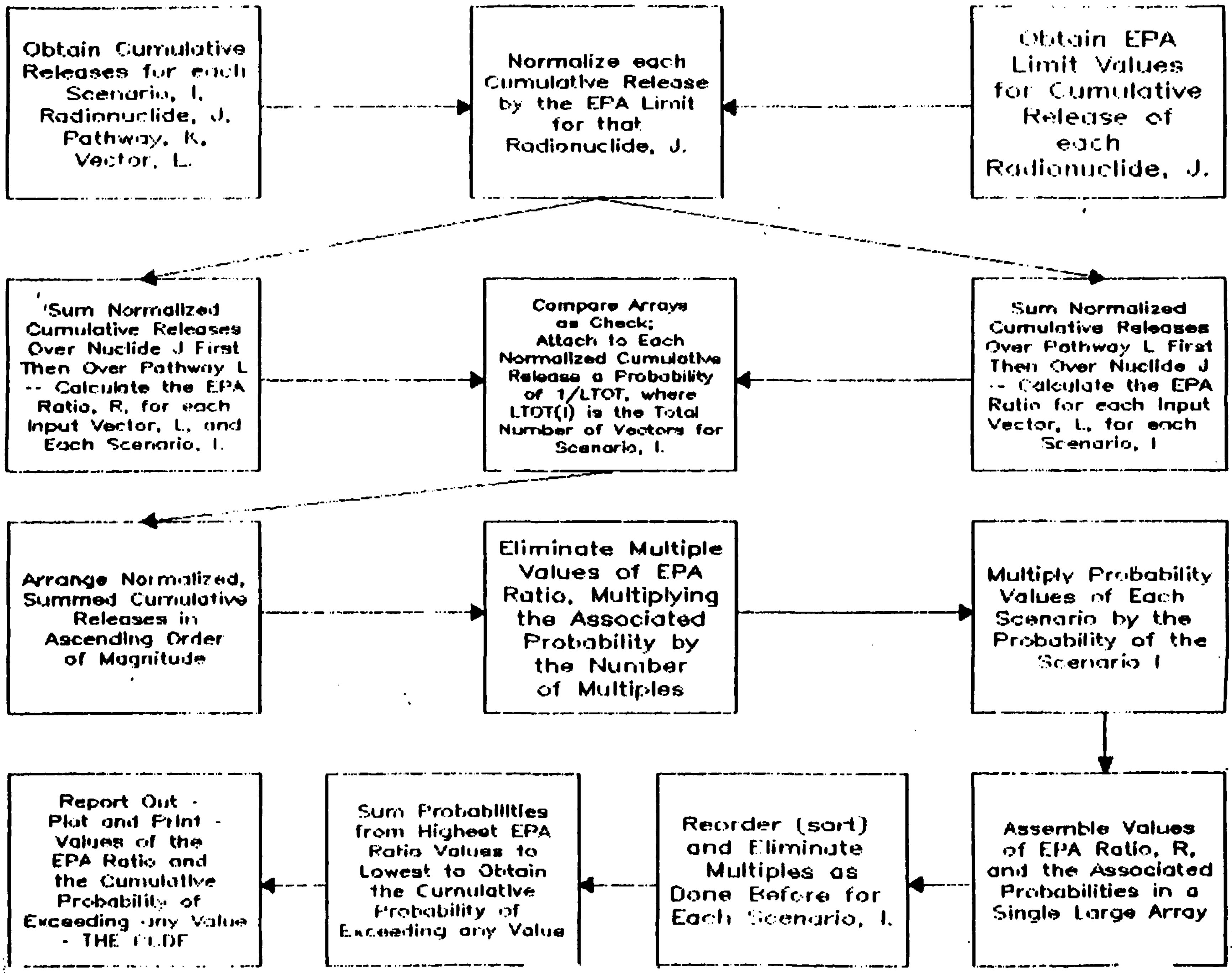

Figure 4.4 Detailed flow diagram of system code steps.

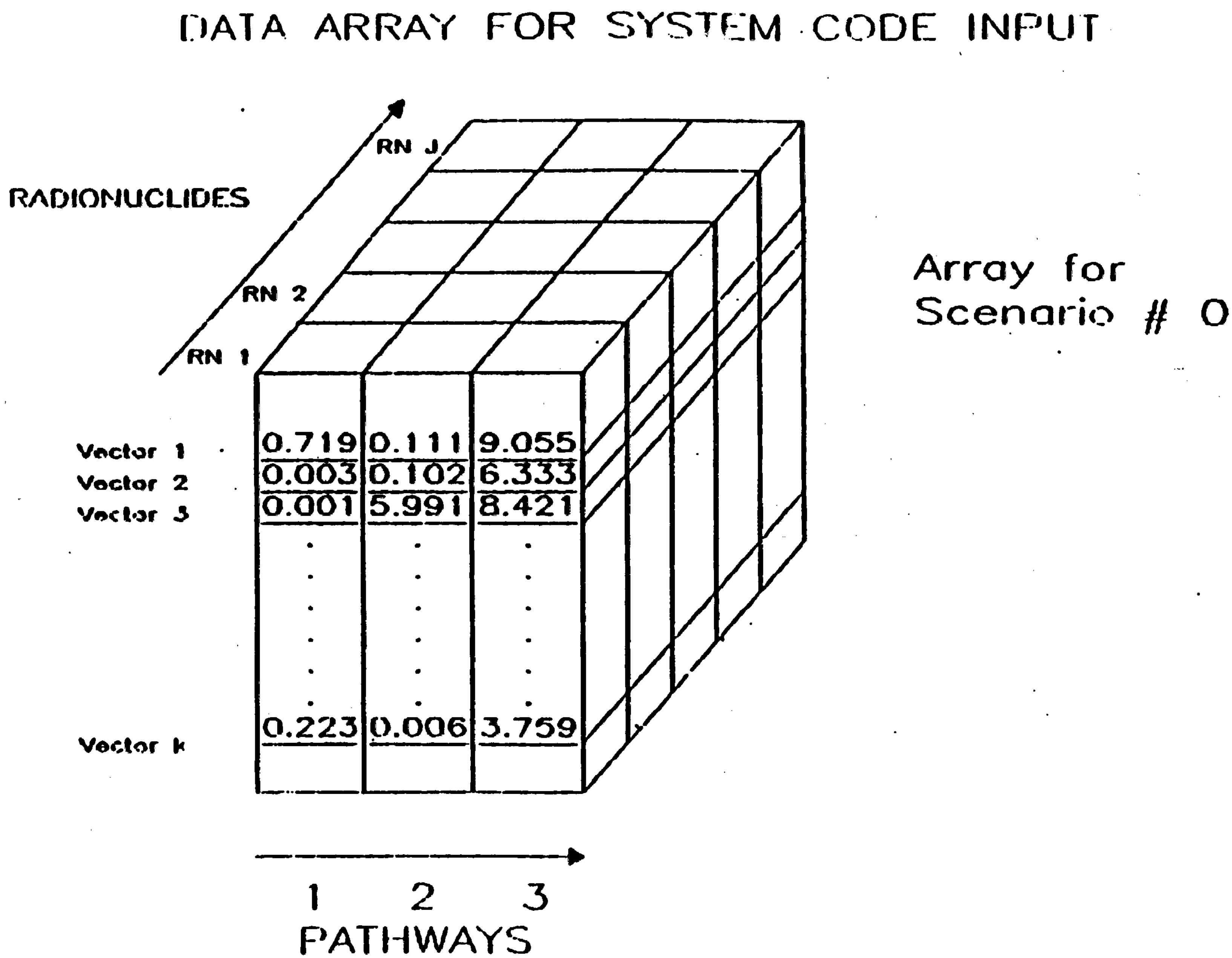

Figure 4.5 System code data array for normalized radionuclide releases.

- Corrosion by hot steam or water dripping through fractures.
- Corrosion by direct contact of canister with rock; e.g. loss of air gap because of spallation of rock or infilling by water-borne sediment.
- Corrosion by immersion because of rise in regional water table or perched water table.
- Heat pipe effect.

5.2.2 Cladding Failure

Most of the spent fuel will be protected by thin cladding, usually zirconium alloy, but in some cases stainless steel. In a small fraction of the cases, the cladding will be flawed by pinhole leaks or damaged (Van Konynenberg, 1987). The cladding is an additional layer of corrosion resistance for the fuel. It would protect the fuel from oxidation or water contact for a time. Since it is very thin (typically 0.6 mm) relative to the canister thickness, cladding has usually been ignored in performance assessment studies.

Aside from the potential corrosion protection offered by the cladding, the cladding itself is likely to contain C-14 produced by activation of impurities in the zirconium metal or picked up from the circulating water in the reactor. Cladding corrosion thus might prove to be a source for the release of C-14 from the waste. Releases of gaseous C-14 are discussed in Appendix D.

5.2.3 Oxidation of uranium dioxide matrix

Uranium dioxide is unstable in an oxidizing environment (Grambow, 1989). Because the repository will be located in unsaturated rock, there will be oxygen available to oxidize the uranium dioxide following failure of the waste package and cladding. Prior to failure, the canisters will most likely be filled with an inert gas to prevent oxidation, although it is possible to have oxidation directly from water that might be contained in the fuel rods, particularly those fuel rods that have already failed. The rate of oxidation depends among other things on temperature, so the time that the waste package fails might be important. Oxidation of the uranium dioxide is potentially important to the performance model, because uranium in higher valence states is much more soluble than in low valence states. If the fuel is immersed in water, the rate of oxidation may be the limiting rate for congruent dissolution of the fuel matrix (Doctor, 1988). In addition, oxidation of the fuel under dry or moist steam conditions can cause an increase in its volume and porosity, with the consequence that the ease at which the gaseous radionuclides such as C-14 could be released might increase.

5.2.4 Release of dissolved radionuclides from the fuel

Initially, the canisters and the spent fuel are likely to produce sufficient heat to dry out their surroundings or create a dry steam environment.

5.0 SOURCE TERM

5.1 Introduction

The demonstration of the performance assessment methodology depends in part on developing or adopting a source term model that considers the rate of release of the radionuclides from the engineered barrier system. The Staff has reviewed several assessments of the Yucca Mountain site performed for DOE by national laboratories. The Staff has also reviewed other source term models not developed for the Yucca Mountain case. A synopsis of our reviews is given in Appendix B. None of these models is fully satisfactory because important data on actual spent fuel under expected repository conditions are not yet available.

The staff's model draws on the features found in these assessments. In many cases, the Staff has found it necessary to make simplifying assumptions. These assumptions are believed to lean on the side of conservatism.

5.2 Review of Important Issues for Selecting Source Term Models

The radioactive waste, consisting mainly of spent light water reactor fuel will be stored in metal canisters. A typical canister according to current DOE plans is about 4.8 meters long, 0.66 meters in diameter and have a wall thickness of 1 cm (SCP, section 7.3.1.3). Small amounts of nuclear wastes in other forms may also be stored in the repository such as vitrified defense wastes, but the present study will focus only on the spent fuel wastes. The source term model must account for the processes in the near field that determine the rate at which radionuclides are released, including corrosion and physical destruction of the waste package, oxidation of the cladding and the spent fuel, gaseous releases, contact between liquid water and the fuel, and transport of the released radionuclides beyond the confines of the engineered barrier.

5.2.1. Waste Package Lifetime

The canisters will be sealed and most probably filled with an inert gas. They must first be breached before there can be any release of radionuclides. Several measures will be used to reduce the likelihood of canister breaching. The canisters will be made of corrosion resistant material. There will be an air gap between the canister and the host rock to prevent any direct contact with pore water. The decay heat may create a dry zone for several hundreds of years after emplacement, further isolating the canisters from contact with liquid water.

Irrespective of these measures, canisters may still fail. Some of the mechanisms that might lead to failure are:

- o Mechanical damage by excavation failure, earthquakes, magmatic intrusions or human intrusions.

Eventually however, liquid water might come into contact with the spent fuel, allowing it to dissolve and release its inventory of radionuclides to the environment. Most of the inventory of radionuclides will be entrapped by the uranium dioxide matrix of the fuel, and will be released slowly as the matrix disintegrates. Some of the radionuclides released from the matrix might precipitate immediately because of their low solubility, thereby limiting their release (Ogard, 1983), or may form colloids (Thompson, 1989) Some of the more-volatile radionuclides such as C-14, cesium and iodine tend to migrate from the matrix and collect at intergranular boundaries and in the gap between the fuel and the cladding, particularly while still in the reactor. These volatile radionuclides will be released more quickly than those released by congruent dissolution.

5.2.4.1 Water contact fraction

DOE plans to emplace the canisters in the host rock in a manner that they expect to reduce the likelihood of water coming into contact with the waste (SCP, Section 8.3.5.9). A proposed emplacement plan would have the canisters stored vertically with an air gap between the canister and the rock walls. Furthermore, DOE believes that the heat generated by the waste may create a significant zone of dry rock around the canisters, isolating them until such time that the water can resaturate the rock. Water might still come into contact with the canisters by several mechanisms:

- o Circulating water generated by the decay heat
- o Infiltrating water flowing through fractures and dripping onto the canisters.
- o Loss of the air gap caused by failure of the emplacement holes through mechanical and thermal stresses, or mineral and sediment infilling.

There are other possible sources of water available to the fuel other than vertically infiltrating precipitation, but the Staff has not explicitly included them in its calculations. Two potentially important sources are (1) lateral inflows from areas of perched water and (2) liquid water circulation caused by heat-driven evaporation and condensation. Lateral infiltration might divert infiltrating ground water causing some of the waste packages to come into contact with liquid water, but at the same time, the water would be diverted away from other waste packages.

The significance of the issue of thermally driven water circulation is difficult to determine at this time. If all heat generated by the nuclear waste went into evaporation of water, the flux would far exceed the likely infiltration rate. It may be the case that these phenomena are short-lived, and unimportant during the period of canister integrity, during which most of the water driven off would be diverted from the canisters rather than returning. Of course, the relationships between heat production, evaporation and circulation are far from simple, and must be approached with sophisticated modeling tools. Models such as TOUGH would be required to carry these arguments further. They are beyond the scope of the Phase 1 study, but should be planned for subsequent studies.

We characterized the water contact by a factor relating the fraction of water infiltrating the site coming into contact with the waste. The staff performed simple calculations to estimate the fraction of the waste canisters exposed to purely vertical infiltration by taking the ratio of the cross-sectional area of the canisters to the total area of land surface. This ratio was about 0.00078. In its uninterrupted state infiltrating water is likely to flow around the canisters because of the matrix suction of the unsaturated rock, so this simple figure does not capture the true nature of water contact. The analysis in the Environmental Assessment (DOE, 1986) assumed a contact fraction of 0.025, but the authors specified no basis for this choice. Other analyses have specified that all water infiltrating the site contacts the waste (Doctor, 1988). DOE design goals specify that 95% of the canisters should be essentially dry and the remaining 5% have less than 5 liters per year contact with water for the first 300 years. For years 300 to 1000, up to 10% of the cansisters can have 5 liters per year contact (SCP, Section 8.3.5.9). Section 8.3.5.10 of the SCP allows contact of less than 20 liters per year per canister for up to 10% of the canisters, however. This figure was estimated as 80 times the expected maximium flux for canisters emplaced vertically.

5.2.5 Release of Gaseous Radionuclides

There are several gaseous radionuclides in spent fuel, although many of these are short-lived and of no long-term concern. The most significant radionuclides are C-14 and possibly I-129 (only at elevated temperatures). Carbon-14 would be released from the cladding, the cladding-fuel gap, and the matrix. The gaseous releases would be partitioned between the groundwater and air, depending on environmental factors such as saturation, temperature and concentration of bicarbonate ions.

None of the models reviewed in Appendix B handle the releases of C-14 in a very sophisticated way. The models either treat the C-14 as a component of the fuel released to the groundwater by congruent dissolution of the fuel matrix, or all is released instantaneously upon failure of the waste canister.

The release of C-14 from the repository is of interest to disposal in unsaturated rock because there is at least the possibility of a fast pathway to the accessible environment through fractures, excavations and tunnels. Two models of transport of C-14 in the geosphere of Yucca Mountain indicate that the time for C-14 released at the repository level to reach the atmosphere would be on the order of hundreds to a few thousand years, too short a time to depend on decay to diminish the importance of C-14 cumulative releases to the accessible environment (Knapp, 1987, Amter, 1988). An assumption of instantaneous release from failed canister may be too pessimistic. On the oth hand, the assumption that all C-14 is contained in the matrix and released on as the matrix dissolves may be too optimistic, because a substantial fraction of the C-14 may be contained in places other than the matrix, e.g, the cladding. Laboratory data on the location of various radionuclides in spent fuel under different conditions will reduce this modeling uncertainty.

5.3 Model Selection and Justification

5.3.1. Model for Dissolved Radionuclides

The source term model provides calculations of radionuclide releases to the flow and transport calculations. For this study, the Staff decided to adopt the source term model currently incorporated in NEFTRAN. Radionuclide releases would occur only after failure of the engineered barrier characterized as a single failure time t_f (the Staff recognized that waste canister failure would probably be distributed in time and space, but the NEFTRAN model was incapable of dealing explicitly with the source term in this manner).

Upon failure of the engineered barrier at time t_f, radionuclide release will be governed by either the leaching rate determined by the rate of dissolution of the waste form, or limited by the solubility of the individual radionuclides, S_i. For the former, the rate of release would be:

$$R_i(t) = \lambda_L M_i(t) \qquad (5.1)$$

The leach rate λ_L was determined by the combination of the infiltration rate I, the fraction of water contacting the waste f, the surface area of the repository A, the solubility of the waste form S_u and the initial inventory of the waste form M_o:

$$\lambda_L = I \times f \times A \times S_u/M_o \qquad (5.2)$$

where M_i = the inventory at time t of the radionuclide in the waste and S_i = solubility of radionuclide i.

If the solubility limit would be exceeded by the release calculated by Eq. 5.1, i.e., if $R_i(t) > S_iIAf$, then the release rate is cut off at the solubility limit:

$$R_i(t) = S_iIAf \qquad (5.3)$$

The release rate $R_i(t)$ becomes a flux boundary condition to the transport equation.

5.3.2 Limitations of Model for Dissolved Radionuclides

The most significant limitations of the dissolved radionuclide source term model are believed to be:

- The model ignores the diffusion-limited case where there might be the buildup of a boundary layer limiting the release of solubility limited radionuclides (this mechanism would apply only if there were a continuous liquid water path between the fuel and the rock).

- For larger infiltration rates, the model cannot represent phenomena that would tend to limit the rate of release such as the forward rate of reaction for oxidation of the spent fuel, and the possibility that oxidants might not be available in unlimited quantities because they would be consumed within the canisters.

- The model assumes intimate contact between the groundwater and the waste, ignoring features such as the air gap designed to prevent such contact. It in effect assumes there is no protection for the fuel from the water, even though the fuel has multiple layers of protection including the air gap, waste package and cladding.

- The model incorporates a single time to failure, even though it is more likely that waste packages would fail in a distributed manner in time and space.

- Releases from the matrix of low-solubility radionuclides might result in colloid formation rather than a precipitation.

- The model does not take into account radionuclides which might not fit neatly into the three compartments (unleached, undissolved and dissolved), such as those collecting in the grain boundaries and in the cladding gap.

- The model ignores the potentially significant amount of liquid water circulation through evaporation and condensation of groundwater that might be caused by the repository heat, i.e., a "heat-pipe".

The use of this model was based on expediency because the fundamental framework was already in place in the NEFTRAN code and required a minimum of reprogramming to adjust the coefficients to represent the Yucca Mountain case. Adjustment of the coefficients of the model allows a wide latitude of potential source term conditions to characterize either congruent dissolution of the uranium matrix or solubility limited releases.

5.3.3 C-14 Release Model

Very little is known about the long-term release of gaseous radionuclides from spent fuel under conditions anticipated at Yucca Mountain. The only data on releases from spent fuel indicate a rapid, small release of C-14 upon failure of the fuel rod, and very slow release thereafter (Van Konynenberg, 1984).

Because of the speculative nature of the C-14 release model, gaseous release pathways were not included into the overall systems analysis, but are treated separately as an auxiliary analysis in Appendix D.

5.4 Source Term Inventory

The inventory of radionuclides assumed for the source term in the Phase 1 study is typical of previous analyses of the performance of a high-level repository at Yucca Mountain and is given in Table 5.1 (Doctor, 1988). The list was restricted to 29 isotopes, chosen from a more-extensive list of fission and activation products found in spent fuel, on the basis of half lives, potential inventories and radiotoxicity (in terms of their EPA cumulative release limits).

Table 5.1 - Radionuclide Initial Inventory (Doctor, 1988)

Radionuclide	Halflife, yrs	Inventory, Ci
Cm-246	5.50E03	2.45E03
Pu-242	3.79E05	1.12E05
U-238	4.51E09	2.24E04
Cm-245	9.30E03	1.26E04
Pu-241	1.32E01	4.83E09
Am-241	4.58E02	1.12E08
Np-237	2.14E06	2.17E04
U-233	1.62E05	2.66E00
Th-229	7.34E03	1.96E-03
Am-243	7.95E03	9.80E05
Pu-239	2.44E04	2.03E07
U-235	7.10E08	1.12E03
Pu-240	6.58E03	3.15E07
U-236	2.39E07	1.54E04
Pu-238	8.60E01	1.40E08
U-234	2.47E05	5.18E03
Th-230	8.00E04	2.87E-01
Ra-226	1.60E03	5.18E-04
Pb-210	2.23E01	4.90E-05
Cs-137	3.00E01	5.25E09
Cs-135	3.00E06	1.89E04
I-129	1.59E07	2.31E03
Sn-126	1.00E05	3.36E04
Tc-99	2.15E05	9.10E05
Zr-93	9.50E05	1.19E05
Sr-90	2.90E01	3.64E09
Ni-59	8.00E04	2.10E03
C-14	5.73E03	9.80E04

5.5 References

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6.0 FLOW AND TRANSPORT MODELS

6.1 Introduction

The quantification of the consequences of high-level waste (HLW) disposal is anticipated to require the analysis of ground-water flow and transport of radionuclides in liquid, gas, and direct release pathways. These analyses typically will be based on site conceptual models which are then implemented in computer programs for calculational use in a performance assessment. For this study, a review of information on unsaturated fractured tuff and transport pathway phenomena, and flow and transport computer programs was conducted to select computer programs to provide calculational tools with which to demonstrate the performance assessment capability. The purpose of this section is to describe the information that was collected and used to select the programs for quantifying consequences.

It should be pointed out that the definition of the site conceptual model(s) will typically be based on detailed laboratory and field investigations for the site under consideration. This site conceptual model(s) will undoubtedly be the most important factor in selecting a computer program for site analyses. However, a well characterized HLW site does not currently exist. As described above, the model selection, for this study, is based on a review of published information. The authors do not consider the review comprehensive and do not intend the model selection to represent an endorsement of any particular conceptual model(s) for the Yucca Mountain site or a recommended approach to modeling flow and transport in unsaturated fractured tuff.

6.2 Definition of Issues for Selecting Performance Assessment Transport Models

The definition of the technical issues for defining and selecting flow and transport models was based on the characteristics of an unsaturated fractured tuff medium and the pathways anticipated to be analysed. This information was obtained from published reports concerning performance assessment in geologic media and ground-water flow and transport in the geosphere with an emphasis on unsaturated fractured media.

6.2.1 Site Concepts

The Yucca Mountain site is located on and immediately adjacent to the southwestern portion of the Nevada Test Site. Yucca Mountain is a prominent group of north-trending, fault-block ridges. The terrain at the site is largely controlled by high-angle normal faults and eastward-tilted volcanic rocks. Slopes are locally steep (15 to 30 degrees) on the west-facing side of Yucca Mountain and along some of the valleys that cut into the more gently sloping (5 to 10 degrees) east side of the mountain.

For this study, the hydrostratigraphic units of interest at Yucca Mountain are primarily comprised of ash-flow and ash-fall tuffs which originated from eruptions during the development of calderas. The amount of welding, fracturing, unit thickness, and chemical alteration varies greatly from one layer to the next. The major hydrostratigraphic units beneath Yucca Mountain starting at the surface are: alluvium, Tiva Canyon welded unit, Paintbrush nonwelded unit, Topopah Springs welded unit, Calico Hills (vitric and zeolitic) nonwelded unit, Crater Flat welded and nonwelded unit (Prow Pass member and Bullfrog member) (see Figure 6.1).

Three broad categories which describe these tuffs are: densely welded tuffs, nonwelded vitric tuffs, and nonwelded zeolitized tuffs. The densely welded tuffs are highly fractured. These tuffs have a very low saturated matrix conductivity (less than 1 mm/year) and a saturated conductivity for the fractures which is probably several orders of magnitude or more higher than the matrix value. The nonwelded vitric tuffs have fewer fractures and a higher matrix saturated conductivity (100 - 10,000 mm/year). The fractures for this unit would have a relatively low saturated conductivity. The nonwelded zeolitized tuffs have few fractures and low matrix-saturated conductivity (less than 1 mm/year) and low fracture saturated conductivity. The contacts between these units generally tend to occur over short distances and involve large differences in hydrologic properties (Prindle, 1987).

Based on current information on hydrogeologic units and theories of flow at Yucca Mountain, the DOE (from page 3-195 of the Yucca Mountain Site Characterization Plan, SCP) described the conceptualization of flow from the Topopah Springs unit to the water table as follows (DOE, 1988):

1. "Flow in the TSw unit is expected to be essentially vertical and under steady-state conditions to occur as flow within the matrix for fluxes less than some critical value of flux related to the saturated matrix hydraulic conductivity, and predominantly as fracture flow at fluxes higher than the critical value.

2. Lateral flow may be induced in the TSw unit at its contact with the underlying Calico Hills nonwelded unit (CHn). The circumstances under which this may occur depend on the magnitude of the flux in the TSw unit and whether this unit is underlain by the low-conductivity zeolitic facies (CHnz) or the relatively higher-conductivity vitric facies (CHnv) of the CHn unit. At low fluxes within the TSw unit, lateral flow may be produced by capillary-barrier effects within the matrix of the TSw unit where it overlies the CHnv unit. At high fluxes, efficient fracture flow in the TSw unit may produce lateral flow as well as vertical flow where the low-conductivity CHn unit underlies the TSw unit.

3. Flow in both the CHnv and CHnz units is predominantly vertical through the matrix (although a lateral component may occur parallel to the bedding within the vitric CHnv unit) and continues directly to the water table wherever the latter transects the CHn unit. Where the CHn unit lies above the water table, flow is presumed to proceed vertically downward to the water table through the Crater Flat undifferentiated unit (CFu).

4. The nearly vertically oriented fault zones and their associated fracturing may be highly effective pathways for vertical moisture flow, especially in the competent TCw and TSw units. But faults may impede lateral flow and may thus produce perched-water bodies where the faults transect zones or horizons of significant lateral flow."

Additionally, very little data are available on estimated infiltration rates and deep percolation rates past the repository. Estimates of deep percolation rates past the repository horizon are described on page 3-205 of the SCP (DOE, 1988) as:

"Wilson (1985) reviewed available site and regional hydrogeologic data in order to set conservative upper limits on the present, net vertically down-ward moisture flux below the repository horizon at Yucca Mountain and on the present rate of net recharge to the saturated zone in the vicinity of Yucca Mountain. Wilson (1985) concludes (1) that the liquid-water percolation flux, directed vertically downward in the matrix of the TSw unit below the repository horizon, probably is less than 0.2 mm/yr and (2) that the area averaged rate of net recharge to the saturated zone in the vicinity of Yucca Mountain probably is less than 0.5 mm/yr. Although Wilson (1985) considered a number of processes, such as upward water-vapor flow in the fractures of the TSw unit at the repository horizon, these upper bounds on percolation and recharge fluxes must be regarded as preliminary estimates that have as-yet-unknown limits of uncertainty."

The definition of a conceptual model for flow and transport in unsaturated fractured tuff was considered by the authors to be dependent on fracture-matrix interactions and the rate of infiltration. The current review indicates that the effects of fractures on ground-water flow and of flow diversion at layer boundaries will need to be assessed and their sensitivity to infiltration rates determined. However, for the present study, it was assumed that ground-water flow would be one-dimensional and in the vertical direction.

The role of fractures and flow diversion at unit boundaries could have significant effects on flux rates through a repository. Although flow diversion was the subject of a limited auxiliary analysis (see Appendix G), future analyses will need to consider fracture-matrix interactions and further consider flow diversion where fractures can affect the flow.

6.2.2 Pathways

The assessment of a repository in the unsaturated zone could involve the following three pathways: (1) liquid, (2) gas, and (3) direct. The most obvious release path for radionuclides away from the repository is the liquid pathway. For the present study it was assumed that radionuclides would be transported vertically in the unsaturated zone towards the water table and releases were calculated at the water table.

The gas pathway is a potential concern for a repository located in the unsaturated zone due to the presence of carbon-14. It is present in the emplaced waste in quantities at least one order of magnitude greater than the release limit specified in Appendix A of the EPA standard. It can exist as one of several gasses (CO_2, methane, acetylene), and could therefore move relatively rapidly compared to its halflife (5720 years) through the unsaturated fractured rock and along pathways such as access tunnels and excavations. In addition, unlike most of the other radionuclides in the waste, transport in the geosphere is not likely to depend strongly on the influx of water to the repository, and can proceed under totally dry conditions. (However, its release from the waste may depend on the water influx.)

Finally a release pathway could occur as a result of a "direct" release. The "direct" release pathway encompasses a couple of possible scenario types such as a release due to drilling into the repository and a release due to a disruptive event like a magmatic eruption. The consideration of the consequences due to volcanic activity was too involved to be included in the current study, therefore, the direct release pathway considered only releases due to drilling. Releases resulting from volcanism will need to be addressed in future work.

6.2.3 Flow and Transport Pathway Phenomena

Performance assessment of potential releases of radioactivity from nuclear waste requires an understanding of a number of complicated transport phenomena for the pathways under consideration. The transport pathways to be analysed are the liquid pathway, the gas pathway (primarily involving the transport of carbon-14), and a direct release pathway (due to a drilling scenario). This section describes, in a preliminary way, some phenomena associated with the transport of radionuclides in ground water and the phenomena considered in this study.

6.2.3.1 Liquid Transport

A common starting point in the development of a transport model is a qualitative statement of the conservation of mass in the liquid phase for an elemental volume (Freeze, 1979):

net rate of change of mass within the element	=	flux of solute out of the element	-	flux of solute into the element	+	loss or gain of solute mass due to reactions and sinks and sources

The processes that control flux into and out of the elemental volume are advection (transport via the bulk motion of the ground water) and hydrodynamic dispersion (transport resulting from mechanical mixing and molecular diffusion). Chemical reactions and radioactive decay will affect the loss or gain of solute mass (for the present analysis phenomena such as Knudsen diffusion and coupled processes are considered of minor importance).

The transformation of the above qualitative statement into differential equation(s) typically involves a number of simplifying assumptions with respect to dimensionality, variability, and processes associated with the intended application. This section will review some of the processes associated with the pathways to be considered in this study.

Physical Processes

It is generally assumed that the bulk movement of fluid will be the primary source of transport away from a HLW repository. In a porous medium it is commonly assumed that the average rate of solute transport by advection is equal to the average linear velocity of the fluid times the concentration. The presence of a fracture system complicates the advective flow system by providing a high permeability flow path separate from but interacting with the matrix path.

In the unsaturated zone, water is held in the pore space by surface tension. Geologic media are comprised of a variety of pore space and fracture dimensions, therefore, these volumes will not empty at the same suction. During drainage the large pores (or larger fractures) will empty at low suctions, while small pores (smaller radius of curvature) will empty at higher suctions. Most models of unsaturated flow in fractured media, therefore, assume that under high suction the dominant ground-water pathway will be in the matrix (i.e. the fractures will be dry). However, it is worth pointing out that many factors (transient infiltration rates, fracture coatings, fracture dimensions, and the presence of perched water) can dramatically influence the degree of fracture flow and validity of a single continuum model for unsaturated fractured media. Many assumptions which preclude fracture flow under unsaturated conditions have not been substantiated by laboratory or field data and, therefore, cannot be ruled out as a possible transport pathway in unsaturated, fractured rocks (Olague, 1989).

Based on the lack of information to support a detailed fracture flow model, we have assumed a steady state flow model where the fractures contribute to flow only when the infiltration rate exceeds the saturated conductivity. Further work will need to determine the degree of conservatism or pessimism in this assumption.

While advection moves solute in the direction of flow, hydrodynamic dispersion and matrix diffusion affect solute concentration along its flow path. Hydrodynamic dispersion includes dilution due to mechanical mixing and molecular diffusion. Mechanical mixing (a direct result of a tortuous path, variation in pore sizes or fracture apertures, and surface roughness) is related to the heterogeneity of the geologic media and is typically characterized by the dispersivity.

For the present analysis we have assumed that dispersivity can be represented with a single dispersion length. This treatment was assumed adequate for the present study because the performance measure of interest (cumulative release at the accessible environment over 10,000 years) would generally be insensitive to longitudinal dispersion when the cumulative releases include a majority of the waste and small cumulative releases are not as important as large releases. The degree to which this is or is not a conservative assumption will need to be examined in further work.

Matrix diffusion couples the solute concentration in the fracture and matrix systems and is generally thought to provide a retardation of radionuclide transport in the fractures. As with the flow of water across the fracture-matrix interface, a large uncertainty in evaluating this phenomenon is determining the effect of fracture coatings on the diffusion rate. Quantification of the effect of fracture coatings will be needed to better determine the best approach for performance assessment. For the present study matrix diffusion is assumed not to occur. This assumption should be conservative for the situation when contaminant being transported in the fractures is diffusing into the matrix. However, this assumption may not be conservative when contaminant is diffusing from the matrix into the fractures.

Chemical Processes

There are several chemical processes that affect the movement of radionuclides in ground water. One of the most significant chemical processes that occurs is sorption (Olague, 1989). Solute species adsorb to the matrix or fracture surfaces by forming bonds with the molecules on the solid surface. The strength of these bonds and the kinetics depend on many chemical factors such as: 1) electric charge of solute and solid, 2) saturation of bonding sites, 3) pH, 4) oxidation and reduction potential, and 5) temperature and pressure of the hydrogeologic system (Freeze, 1979).

Adsorption can be physical (generally considered a reversible process) or chemical (generally considered an irreversible process). At any moment some of the solute particles are bonded to the solid surface and some are free to move with the ground water. The adsorption-desorption process has typically been represented in most ground- water transport models using a retardation equation that employs a distribution coefficient. The assumptions in this model include instantaneous and reversible adsorption and desorption (equilibrium), linear sorption isotherms, and single-valued sorption isotherms (i.e., no hysteresis effect) (Rasmussen, 1987). The distribution coefficient model was adopted for this study. Future work will need to perform supporting geochemical analyses to determine the degree of validity of the present approach.

The model ignores precipitation of radionuclides along the flow path, although solubility is taken into account in the source term. This assumption is conservative because it would overestimate the cumulative release.

Table 6.1 Identification of liquid pathway processes and estimated effect on calculating cumulative release from the liquid pathway.

Processes	Estimate of Importance
1. Advection	High
2. Sorption	High
3. Radioactive Decay and Production	High
4. Fracture-Matrix Interactions	High
5. Matrix Diffusion	Medium
6. Precipitation of Radionuclides	Low
7. Dispersion	Low

6.2.3.2 Gas Transport

The gas pathway is an alternative pathway for radionuclide transport to the accessible environment. Futhermore gas phase source terms (i.e., carbon-14, tritium, krypton-85, and iodine-129) could potentially be released from spent fuel buried at Yucca Mountain. Gas phase carbon-14 in the form of carbon dioxide appears to be the most important for considerations of performance assessment. The half-lives of tritium and krypton-85 are relatively short (12.3 years and 10.7 years, respectively) and it is possible that elemental iodine could quickly partition into the liquid phase. Because of the complexity of the issue and the relatively poor state of knowledge about gaseous release and transport, carbon-14 release to the atmosphere is not included into the total system analysis. An auxiliary analysis for carbon-14 release to the atmosphere is presented in Appendix D.

6.2.3.3 Direct Transport

Potentially significant scenarios for the assessment of repository performance involve the possibility of volcanism in the form of a disruptive event such as a magmatic eruption, or an intrusive event involving human drilling activities. Both scenario classes involve events whose estimated likelihood of occurrence and consequences are very uncertain over the regulatory period of performance for the repository (i.e., 10-100,000 years). Considerations for magmatic events and human intrusion are discussed below. However, due to the complexity in understanding and predicting magmatic events, simulation work in this area was not performed in this study.

Magmatic Events

Basaltic eruptions are noted to have occurred near the Yucca Mountain site and west and south of it during the Quaternary period. Basalt flows and cinder cones have been observed on Crater Flat, and volcanic centers in Amargosa Valley have deposited ash falls as recently as 20,000 to 30,000 years ago. The consequences assuming that a magmatic eruption occurs are very uncertain; however, it is believed that this class of scenarios would need to consider the following in estimating consequences: (1) entrainment of the waste and deposition on the surface, for example, as a result of a physical (steam) explosion, (2) dispersal of fine-grained ash and radioactivity into the atmosphere, (3) mechanical and thermal loading that can affect rock stresses and permeabilities and flow conditions for radionuclide migration from the repository to the accessible environment, even if the event does not compromise the structural integrity of the repository, (4) the relative amounts of radioactivity that would be released due solely to the occurrence of this natural event, (5) potential barriers to flow or water table level changes and (6) the source term.

The source term depends upon many factors, including:

- mix of waste forms for the repository (spent fuel and high level waste from defense activities)
- spent fuel inventory characteristics (reactor type and burn-up)
- time of emplacement
- emplacement configuration
- rock geochemical properties

- o time of eruption or intrusion
- o extent, location, and geometry of volcanism

For scenarios involving the interception of waste packages by feeder dikes, estimates of the distribution and size of these dikes (resulting from the feeding of basaltic cinder cones) are needed, in addition to estimates of their times of occurrence (to account for radioactive decay).

Human Intrusion

Human activities such as deep exploratory drilling of boreholes could potentially provide direct releases of radioactivity to the environment. It is believed that this issue is primarily a source term issue which depends on the amount of radioactivity brought to the surface by drilling. In general, the waste package material, emplacement configuration, age of waste at time of interception by a drill bit, altogether contribute to estimating the radioactive source term. Estimates of radioactivity brought to the surface in contaminated cores from those boreholes that intercept the repository are also needed for a more complete consequence analysis. In order to estimate the risk one needs to combine the consequence information with a probabilistic analysis of the drilling rate and penetration depth.

6.3 Computer Program Review and Selection

The analysis of any complex system often involves the use of computer implemented mathematical models to assist the analyst in presenting an "adequate" description of the risk or performance of the system. The analysis of hydrologic systems has, over the last twenty years, created an number of computer programs for analyzing a variety of problems (until recently little attention has been paid to an unsaturated, fractured, and uneconomic rock such as tuff). Based on the pathway phenomena and types of scenarios anticipated for the analysis of a repository in unsaturated fractured tuff, computer programs were reviewed for their applicability in a performance assessment.

6.3.1 Liquid Pathway

The evaluation of the liquid pathway could involve a suite of computer programs. The complexity of flow and transport in unsaturated fractured tuff could dictate the use of a set of models. A specific model could be used to evaluate a specific performance question, assist the assignment of model inputs, or justify the assumptions of simpler models used in a systems model. Some examples of the types of programs needed are: 1) two-phase flow program for analysing thermal effects, 2) two- or three-dimensional program for simulating regional flow, 3) geochemical programs for assessing retardation phenomena, 4) a program which includes the influence of fractures or allows for an interaction between fractures and matrix, and 4) an efficient transport program for use in the multiple simulations of a performance assessment.

The review of computer programs is divided into the following four sections: 1) regional or far-field ground-water flow programs, 2) two-phase flow programs, 3) geochemical programs, and 4) transport programs. The ability of the various programs to deal with the presence of fractures will be discussed under the individual programs. A summary of the review and the selection rationale is provided in the subsequent sections while individual program summaries are provided in Appendix C.

6.3.1.1 Regional Ground-Water Flow Programs

A number of unsaturated flow programs (e.g., FEMWATER and UNSAT2) were developed approximately 10 years ago to analyze unsaturated flow in near surface soils (Thomas 1982). NRC participation in the international project HYDROCOIN (Cole, 1987) revealed significant numerical limitations in these programs in simulating unsaturated problems involving large non-linearities (e.g., infiltration into a dry soil and large permeability contrasts). These and similar type programs were not examined further due to their numerical deficiencies which would be unacceptable in evaluating unsaturated fractured media. A new generation of unsaturated flow programs has been developed to better handle the non-linearities encountered in unsaturated flow.

Sandia National Laboratories reviewed 71 computer programs that simulated groundwater flow and transport in the unsaturated zone (Olague, 1989). Based on this review and recently published user manuals, it was decided to provide a description for the computer programs entitled SUTRA, VAM2D, and TRACER3D. The three programs employ similar Darcian approaches to simulating fluid flow in porous media. The ability to simulate fracture flow could only be accommodated through a dual porosity approach. (Currently, there are no existing programs which simulate fracture-matrix interactions with an approach different from dual-porosity. Sandia National Laboratories under RES contract FIN A-1266 is developing a flow program that will account for the fracture-matrix interactions in a more rigorous fashion than is currently available. This program is scheduled for completion in April of 1990.)

The VAM2D program (Huyakorn, 1989) was selected for use in modeling regional flow because of the efficiency of the non-linear numerical techniques employed and the availability of the program for NRC staff use.

6.3.1.2 Two-Phase Flow Programs

Assessing the thermal period of the HLW repository will require programs that can simulate the flow of air, liquid water, and water vapor. TOUGH, NORIA, and PETROS are existing programs which solve the two-phase flow and energy transport problem. A detailed Sandia review of these programs (Updegraff, 1989) discussed the difficulties of running two-phase flow models and the relative strengths and weaknesses of the individual programs. Overall, one program was not superior to the others. However, TOUGH successfully ran most of the test problems while NORIA and PETROS could at best simulate approximately half the test problems.

The TOUGH program (Pruess 1987) was selected to analyze two-phase flow problems because of its ability to handle a variety of problems (Updegraff, 1989) and the current availability of TOUGH to NRC staff. (Due to the complexity of two-phase flow problems, simulation work was not performed in this study.)

6.3.1.3 Geochemical Programs

The geochemical behavior of the HLW repository could have a very strong effect on the movement of radionuclides. Unfortunately, current geochemical programs are not amenable to most performance assessment systems programs due to their complexity. The primary use of the geochemical programs will be to aid the understanding of the geochemistry of the site and the assignment of lumped parameters in the simpler transport models.

The current study did not consider complex modeling associated with geochemical analyses. Summaries of various programs are included in Appendix C. Selection of a particular program was considered inappropriate until more specific performance issues or questions with respect to geochemistry could be made.

6.3.1.4 Transport Programs

The utilization of a transport program in a systems code for the performance assessment will require a number of simplifications of the real system to accomodate the large number of simulations necessary for sensitivity and uncertainty analyses (see Appendix E, Testing Statistical Convergence). Some of the simplifications being considered are: utilization of a one- or two-dimensional analysis; limited (if any) interaction between fractures and matrix; steady-state flow; and limited geochemistry (typically a lumped retardation factor which is intended to account for all the geochemical interactions).

A number of existing programs, which employ many of the above simplifications, have been reviewed (see code summaries in Appendix C). The review included numerical solutions such as SPARTAN, NEFTRAN, and TOSPAC as well as closed form solutions such as the UCB programs. The NEFTRAN (Longsine, 1987) program, developed at Sandia National Laboratories under NRC funding, was selected because: 1) it was available on NRC computer systems, 2) ready access to the Sandia developers, and 3) efficiency of the program and compatibility with the LHS computer program for analysing model sensitivity.

Although all of the reviewed programs did not fully describe fracture-matrix interactions, Sandia is currently modifying NEFTRAN (to be completed by March, 1990 to include fracture-matrix interactions). Staff use with the current version of NEFTRAN will assist technology transfer of the new version of NEFTRAN in 1990.

6.3.2 Gas Pathway

The gas pathway has been treated as an auxiliary analysis and is presented in Appendix D.

6.3.3 Direct Pathway

The staff was unable to acquire computer programs for evaluating the consequences of drilling into a repository in a timely fashion. The staff developed a model that accounts for the anticipated important aspects of a drilling scenario. The model accounts for a drilling rate, radioactive decay, the areal extent of the repository, waste package emplacement orientation (horizontal versus vertical), and boreholes intercepting both the waste package and contaminated rock. A detailed discussion of the drilling model is provided in Appendix H.

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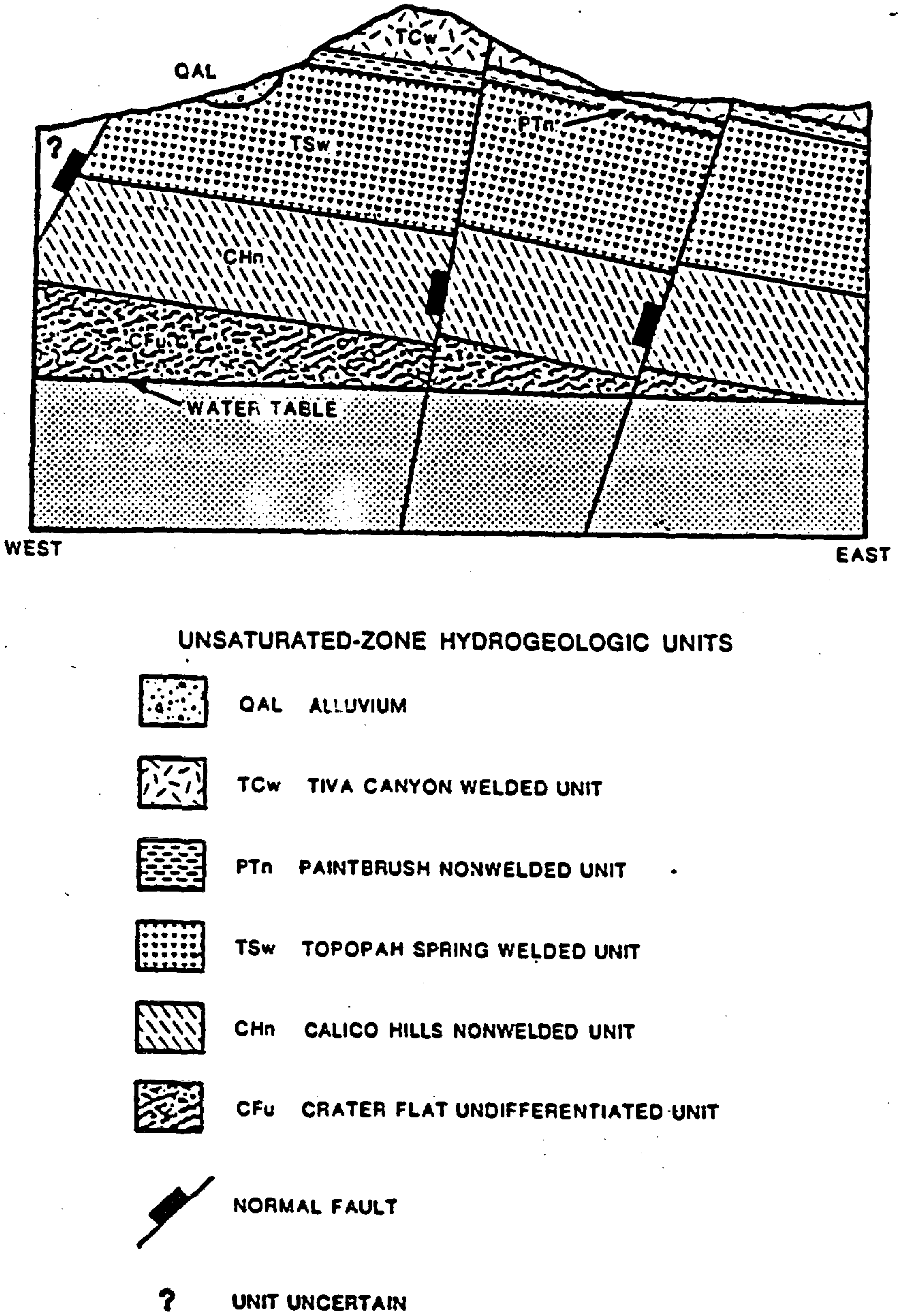

Figure 6.1 Conceptualization of a hydrogeologic cross-section through the unsaturated zone at Yucca Mountain. Modified from DOE (1988).

7.0 METHODOLOGY FOR SCENARIO DEVELOPMENT

7.1 Introduction

When this study was initiated, the staff intended to accomplish two objectives: (1) identify a methodology that could be used for scenario development, and (2) demonstrate the utility of the methodology by application to the Yucca Mountain site. Due to limitations on availability of staff resources, only limited progress was made on application of the methodology. This section is, therefore, primarily a status report of on-going work, and consists primarily of a description of the methodology selected by the staff. Because application of this methodology to the Yucca Mountain site was not completed, there is no correlation between this section of the report and the scenario classes hypothesized for analysis in other sections of the report.

An important part of a performance assessment for an HLW repository is an evaluation of the uncertainties in projected performance. Two general approaches are available for analyses of uncertainties in repository performance. Such analyses can be carried out by incorporating the uncertainties directly into the model(s) and data base(s) describing the repository system, or uncertainties can be approximated as "scenarios" -- i.e., descriptions of alternative ways in which the repository system might perform in the future. Most analyses use a combination of the two approaches, although there are generally no explicit criteria for which way to treat a specific source of uncertainty. Thus, lists of processes and events to be included in scenarios often include phenomena such as waste canister corrosion, even though such phenomena are likely to be evaluated directly within the repository model(s) and data base(s) rather than as scenarios.

This study distinguished two aspects of an uncertainty analysis: (1) uncertainty about the characteristics of the repository system and its environment as they exist at the time of analysis, and (2) uncertainty about the future evolution of the environment within which the repository will exist far into the future. For the purposes of this study, scenario analysis is limited to the second type of uncertainty. All uncertainties of the first type are assumed to be incorporated directly into the model(s) and data base(s) which describe the repository system.

The term "scenario" is defined here as a description of one of the many alternative ways in which the environment of a repository might evolve in the future. The goal of a scenario analysis is then to identify a set of such scenarios, to be used in uncertainty analyses, which is sufficiently complete to support a regulatory decision regarding the acceptability of the repository.

In this study, phenomena were considered to be either "internal" or "external" depending on the location where they are initiated. Those phenomena initiated in the accessible environment are classified as external perturbations of the repository system, even if the effects of the phenomena occur within the repository. Thus, fault movement within the controlled area of the repository is classified as an external event because the tectonic forces responsible for the movement are external. Similarly, drilling into a repository is classified as an external event because the drilling is initiated outside the controlled area. Phenomena internal to the repository system, such as corrosion of waste canisters, were assumed to be addressed in the development of model(s) and data base(s) describing the repository system, and therefore were excluded from consideration for scenario development.

The boundary of the repository system was chosen to be coincident with the boundary of the accessible environment for two reasons. First, many of the uncertainties within this boundary involve processes rather than discrete disruptive events. Simulation of processes and their associated uncertainties is often fairly simple, sometimes involving no more than specification of a range of values within the data base for the repository (e.g., a range of corrosion rates). On the other hand, phenomena outside this boundary are often rare, discrete events such as fault movement or volcanic activity. Simulation of such events within the model of the repository system may be awkward, especially when Monte Carlo or related simulation techniques are used. In such cases, the number of simulations needed to obtain a good representation of repository performance may be so large that accurate approximations of repository performance are not practical.

The second, and more important, reason for selection of the repository system boundary involves the way in which the repository is perceived by regulators and by the public. Both groups tend to view the repository system as ending at the accessible environment boundary and to visualize phenomena occurring outside this boundary as external perturbations of the repository. Scrutiny of repository safety tends to take the form of "What if" questions -- e.g., What happens to the repository if a volcano erupts nearby? Evaluation of external phenomena through scenario analysis directly answers such questions, while incorporation of external phenomena into the repository system model(s) or data base(s) would tend to obscure the results of the analysis.

It is important to note differences between the approach adopted here for scenario development versus those proposed by other analysts. Hodgkinson and Sumerling (ref. 1) describe an approach for scenario development in which no distinction is made between "internal" phenomena and those which occur outside the repository. In their approach, processes such as waste canister corrosion would be treated as phenomena to be combined into scenarios for analysis. Because these authors combine internal with external phenomena, their list of "events, features and processes" to be combined into scenarios contains approximately 150 entries and, even after screening out unimportant entries, the number of scenarios that could be constructed from a list of this length would be quite large. Treatment of internal phenomena within the repository system model greatly reduces the potential number of scenarios, keeping the complexity of the repository analysis within manageable bounds.

Hodgkinson and Sumerling also describe an alternative approach, referred to as "environmental simulation," in which an attempt is made to incorporate all identifiable uncertainties into the repository system model. As discussed above, it appears that such an approach would have difficulty satisfying the information needs of regulators, and could require excessive numbers of simulations in order to provide accurate approximations of repository performance.

7.2 Methodology

The scenario development approach adopted for this study is an adaptation of the event tree approach used in probabilistic risk analyses, and consists of the following steps:

1. Identification of Processes and Events. This step involves identification of a comprehensive set of processes and events that could adversely affect repository performance. Only "external" processes and events occurring (or initiated) in the accessible environment are included. Processes and events internal to the repository system are assumed to be treated as uncertainties within the model(s) or data base(s) describing the repository system and therefore are not included here. When the time of occurrence of a process or event (e.g., volcanic activity) is expected to have a significant effect on repository performance, the time is specified as part of the description of the event, and occurrences at several different times may be listed as separate "subevents."

2. Estimation of Probabilities. Probabilities of the processes and events are estimated from historical data, models of the processes and events, or expert judgment.

3. Screening of Events and Processes. Where possible, processes and events are eliminated from the list compiled in step 1 using the following screening criteria: a) lack of physical reasonableness, b) low probability of occurrence, and c) insignificant effect on repository performance if the process or event were to occur.

4. Scenario Construction. Processes and events surviving the screening of step 3, above, are combined to form "scenario classes" using the event tree approach described in NUREG/CR-1667. (Each "scenario class" is a unique combination of processes and/or events without regard to the order in which they occur.) For this study, different permutations of events which comprise separate scenarios were not considered. Instead, judgment was used to select a permutation to be representative for the scenario class. For the illustrative purposes of this project, it was planned that the only scenarios to be formed would be those consisting of zero, one or two processes or events -- i.e., scenarios containing three or more events would not be formed.

5. Scenario Probabilities. Scenario probabilities are estimated by combining the probabilities of the processes and events which comprise the scenarios. If the processes and events comprising a scenario are independent, the scenario probability is determined by multiplying the probabilities of the constituents. If the processes and events are not independent, correlations or causal relationships must be considered when determining scenario probabilities.

6. Scenario Screening. Scenarios are screened using the same criteria as for screening processes and events in step 3 above.

7.3 Application

Application of the selected scenario development methodology for Yucca Mountain was largely limited to the first step -- identification of processes and events. The primary source of information used to compile a list of processes and events was the staff's knowledge of the Yucca Mountain site, although limited references to literature describing similar scenario development efforts for Yucca Mountain were also made. Some progress was also made on the third step involving screening processes and events. However, because probability assignments were not completed, screening was conducted only on the bases of physical reasonableness and insignificant consequences. Combination of processes and events into scenarios, development of scenario probability estimates, and scenario screening (steps 4 - 6) must await development of probability estimates for the phenomena comprising the scenarios. The following table presents a summary of the candidate list of processes and events identified, including those that were later screened from the list. (As additional knowledge about the site is acquired, it will obviously be necessary to periodically review both the completeness of the list and the specific descriptions of processes and events making up the list.) Following the table is a more detailed description of each process and event and, where appropriate, the basis for screening.

Table 7.1 - LIST OF PROCESSES AND EVENTS[1]

I. Tectonic

- A. Volcanic
    - 1. Extrusive
        - a. On-site
            - i. Years 0 - 100
            - ii. Years 101 - 1,000
            - iii. Years 1,001 - 10,000
        - b. Off-site
    - 2. Intrusive
        - a. Upgradient
        - b. Downgradient
        - c. Intersecting repository
- B. Regional Uplift & Subsidence
    - 1. Increased rate of uplift
    - 2. ~~Subsidence~~
- C. Fault Movement
    - 1. Fault within controlled area
        - a. Within underground facility
        - b. Outside underground facility
    - 2. Fault outside controlled area
        - a. Location alters groundwater flow
        - b. Effects limited to ground motion

II. Climatic

- A. ~~Current climate - extreme weather phenomena~~
- B. ~~Increase in frequency or intensity of extreme weather phenomena~~
- C. ~~Glaciation~~
    - 1. ~~Covers site with ice~~
    - 2. ~~Causes sea level change~~
- D. Change in precipitation
    - 1. Pluvial period
    - 2. Drier period

III. Human-initiated

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[1] Cross-hatching indicates processes and events screened from further analysis.

A. Greenhouse effect
   1. Increased precipitation
   2. Reduced precipitation

B. ~~Climate control~~ -

C. ~~Weapons testing at NTS~~

D. Drilling
   1. Intersects canister
   2. Misses canisters

E. Mining
   1. ~~Above underground facility~~
   2. At or below underground facility

F. Withdrawal well(s) at or beyond controlled area
   1. Small, single-family drinking water well
   2. Large drinking water well (addition to Las Vegas supply)
   3. Agricultural irrigation well

IV. Other

A. ~~Meteorite impact~~

B. ????

Table 7.2 - DESCRIPTIONS OF PROCESSES AND EVENTS[2]

Process or Event	Description
1 (I.A.1.a.)	On-site extrusive volcanic activity. A basaltic volcano erupts through the underground facility. The volcano is fed through a dike. Waste canisters within the dike mix with the magma, and their contents are erupted. The size of the dike is assumed to be ________, which is sufficient to eject from the underground facility _____ % of the originally emplaced waste. This size is the worst credible, and is taken to be representative of all less disruptive events. Three "subevents" are defined, based on the assumed time of occurrence. (a) Subevent 1a, occurring immediately after repository closure, represents all occurrences during the first century after closure, (b) Subevent 1b, occurring at year 101, represents all occurrences between year 101 and year 1,000, and (c) Subevent 1c, occurring at year 1,001, represents all occurrences between year 1,001 and year 10,000. Screening on the basis of likelihood is done only on the overall probability of occurrence of the event during 10,000 years -- not on the probabilities of the subevents. The probability of event 1 is estimated to be _______.
2 (I.A.1.b)	Off-site extrusive volcanic activity. Off-site activity is a likely candidate for screening from the list because potentially detrimental effects seem unlikely. However, the event was retained pending a more thorough consideration of potential effects such as alterations of regional or on-site hydrological or geochemical conditions.
3 (I.A.2.a)	Upgradient intrusive volcanic activity. An igneous intrusion at __________ (location) upgradient from the underground facility forms in a way that alters groundwater flow downgradient from the location of the intrusion. The intrusion is in the form of a dike with dimensions of ____________________, and reaches to a depth of _____ below the ground surface. The location and dimensions are the worst credible values, in terms of effects on repository performance, and are taken to be representative of all less disruptive intrusions. The temperature of the intrusive material is _____, causing thermal alterations of surrounding groundwater flow conditions. The probability of event 3 is estimated to be _______.

[2] Blanks indicate information to be developed later.

4 (I.A.2.b) Downgradient intrusive volcanic activity. An igneous intrusion forms at __________ (location) downgradient from the underground facility. Except for location, this intrusion is identical to that of event 3. The probability of event 4 is estimated to be ________.

5 (I.A.2.c) Volcanic intrusion intersects underground facility. An igneous intrusion identical to that of event 3 forms beneath the underground facility, intersecting emplaced waste, but not reaching the ground surface. The probability of event 5 is estimated to be _________.

6 (I.B.1) Increased regional uplift. The existing rate of uplift at the repository site increases to a rate of ______ immediately after repository closure and then remains constant for 10,000 years. This same uniform rate of uplift also occurs within a surrounding area of dimensions ______________. The probability of process 6 is estimated to be ________.

(I.B.2) Subsidence. Subsidence was screened from the list because potentially disruptive effects could not be identified.

7 (I.C.1.a) Fault movement within underground facility. A fault intersecting the underground facility moves immediately after repository closure, resulting in an offset of ______ along the fault. (Should we specify the type of fault, dimensions, etc? Is simultaneous movement on a series of faults within the underground facility possible and, if so, should that be the description here?) This event is taken to be representative of all similar events with less detrimental effects on waste isolation. The probability of event 7 is estimated to be __________.

8 (I.C.1b) Fault movement within controlled area. A fault intersecting the controlled area, but not the underground facility, moves immediately after repository closure, resulting in an offset of ______ along the fault. This event is taken to be representative of all similar events with less detrimental effects on repository performance. The probability of event 8 is estimated to be ________.

9 (I.C.2.a) Fault movement outside controlled area alters groundwater flow. A fault located outside the controlled area moves immediately after repository closure, altering groundwater flow characteristics in a way that potentially influences waste isolation. The location of the fault is ________ and the offset along the fault is ______. This event is taken to be representative of all similar events with less detrimental consequences. The probability of event 9 is estimated to be ________. (NOTE: If both upgradient and downgradient locations of fault movement capable of altering groundwater flow are credible, separate events

might need to be defined analogous to events 3 and 4 above.)

10 (I.C.2.b) Fault movement outside controlled area causes ground motion. A fault located outside the controlled area moves causing ground motion at the underground facility and shaft and borehole seals. The maximum acceleration and the frequency of motion are ________. This event is taken to be representative of all similar events with lower acceleration or less detrimental frequencies. The probability of event 10 is estimated to be ________. (NOTE: It might be possible to combine events 9 and 10 although, in general, these events will be different since event 9 depends strongly on the location of the fault movement, while event 10 is concerned with the ground motion produced by an event at any location.)

(II.A) Current climate -- extreme weather phenomena. Extreme weather phenomena, such as tornados, hurricanes, etc. were screened from the list because potentially detrimental effects on waste isolation could not be identified.

(II.B) Increased frequency or intensity of extreme weather phenomena. These phenomena were also screened from the list because potentially detrimental effects on waste isolation could not be identified.

(II.C) Glaciation covering site with ice or causing sea level change. Glaciation causing the site to be covered with ice was screened from the list because of lack of evidence of occurrence during previous glacial episodes. Sea level changes caused by glaciation were screened from the list because potentially detrimental effects on waste isolation could not be identified.

11 (II.D.1) Pluvial period. A period of increased precipitation begins immediately after repository closure and continues for 10,000 years. Precipitation at the site and throughout the surrounding region is increased by 50% compared to current levels. This event is taken to be representative of all similar events of later onset, shorter duration, or smaller changes in precipitation. The probability of event 11 is estimated to be ________.

12 (II.D.2) Drier period. A period of reduced precipitation begins immediately after repository closure and continues for 10,000 years. Precipitation at the site and throughout the surrounding region is reduced by 50% compared to current levels. This event is taken to be representative of all similar events of later onset, shorter duration, or smaller changes in precipitation. The probability of event 12 is estimated to be ________.

13 (III.A.1) Greenhouse effect -- increased precipitation. The greenhouse effect causes precipitation to increase by 30% above levels that would have otherwise prevailed. The increase begins immediately after repository closure and continues for 10,000 years. This event is taken to be representative of all similar events of later onset, shorter duration, or smaller changes in precipitation. The probability of event 13 is estimated to be ________.

14 (III.A.2) Greenhouse effect -- reduced precipitation. The greenhouse effect reduces precipitation by 30% compared to levels that would have otherwise prevailed. The decrease begins immediately after repository closure and continues for 10,000 years. This event is taken to be representative of all similar events of later onset, shorter duration, or smaller changes in precipitation. The probability of event 14 is estimated to be ________.

(III.B) Climate control. This event was screened from the list because of low likelihood. It is presumed that the institutional controls required by Part 60 will be sufficiently effective to prevent any events of this type that could detrimentally affect waste isolation.

(III.C) Weapons testing at NTS. This event was also screened from the list by presuming that the institutional controls required by Part 60 will be sufficiently effective to prevent any events of this type that could detrimentally affect waste isolation.

15 (III.D.1) Drilling intersects a canister. Wildcat drilling for petroleum breaches a canister allowing part of the canister contents to be brought to the surface in drilling fluids. Wildcat drilling for petroleum is taken to be representative of all potential drilling at the depth of the underground facility. The frequency of drilling at the repository site is estimated to be ________, and the probability that any one drilling event will breach a canister is estimated by the geometric relationship between the area of the waste canisters and the total area of the underground facility.

16 (III.D.2) Drilling misses canisters. Wildcat drilling for petroleum penetrates the underground facility, but misses all canisters. This type of drilling is taken to be representative of all potential drilling at the depth of the underground facility. The frequency of drilling at the repository site is estimated to be ________, and the probability that any one drilling event will miss all canisters is estimated by the geometric relationship between the area of the waste canisters and the total area of the underground facility.

(III.E.1) Mining above the underground facility. This event was screened from the list because effects potentially detrimental to waste isolation could not be identified.

17 (III.E.2) Mining at or below the underground facility. Construction of shafts and other mining activities are assumed to be carried out only if direct contact with wastes does not occur. If wastes are directly contacted, it is assumed that their character will be recognized, mined openings will be sealed, and mining activities will be abandoned. The frequency of mine construction is estimated to be __________, and the probability that mining activities will contact waste canisters is estimated by the geometric relationship between the area of the waste canisters and the total area of the underground facility.

18 (III.F.1) Small water well. A small, single-family drinking water well is assumed to be located at the downgradient boundary of the controlled area and is used as a year-round domestic water supply. The well is assumed to be drilled 100 years after repository closure, and is used continually for the next 9900 years. The probability of event 18 is estimated to be __________.

19 (III.F.2) Municipal drinking water well. A municipal drinking water well is assumed to be drilled at the boundary of the controlled area at year 100 after repository closure, and the well is assumed to be used until year 10,000 after closure (or until depletion of available groundwater supplies). The effect of this well on repository performance is limited to potential alterations of regional groundwater flow characteristics. It is assumed that current requirements for monitoring the quality of municipal water supplies will continue, so that remedial actions will be taken if radioactive contamination of water supplied by the well occurs. The probability of this event is estimated to be __________.

20 (III.F.3) Agricultural irrigation well. The assumptions regarding this well are identical to those for event 19 except that monitoring for potential radioactive contamination of the water is not assumed to occur. Therefore, remedial actions will not be taken to stop potential releases of waste via this well. The probability of this event is estimated to be __________.

(IV.A) Meteorite impact. This event was screened from the list because of low probability. Several references in the technical literature demonstrate that the probability of impact by a meteorite large enough to disrupt a repository is extremely small.

7.4 Conclusions

Although only limited progress has been made in applying the selected methodology for scenario development, several tentative conclusions have already been reached.

1. The methodology appears to be workable. The distinction between "internal" and "external" processes and events appears to have merit for determining which uncertainties are to be incorporated directly into the model(s) and data base(s) describing the repository system and which are to be addressed in scenario descriptions. This distinction also appears to be capable of limiting the number of processes and events in the scenario analysis to a manageable level.

2. Scenario descriptions are necessarily only approximate descriptions of future repository performance, and must incorporate significant conservatisms in order to limit the number of scenarios to be evaluated. In particular, the time at which a processes or event is assumed to disrupt a repository may be highly conservative. If such conservatism is excessive, definition of "subevents," as was done for volcanism in this analysis, provides a way to remove conservatism and to generate a more realistic approximation of expected repository performance.

3. As for other risk analyses, no way has been found to ensure completeness of the initial list of processes and events from which scenarios are formed. An approach similar to fault tree analysis, in which the repository system is examined to identify potential failure modes, seems a useful way to check on the completeness of process and event identification.

4. Alternative approaches to scenario analysis, such as those described by Hodgkinson and Sumerling, appear to differ primarily in the degree to which they address uncertainties in the model(s) and data base(s) describing the repository system or in scenario descriptions. The approach selected for this study is intermediate between the extremes proposed by others, and appears to be a reasonable trade-off between the desire for a highly detailed simulation of repository performance and the need to limit resources expended on the simulation. The selected approach also appears to have advantages over alternatives for producing information in a form that corresponds to the needs of the NRC's regulatory process.

7.5 References

1. Hodgkinson, D. P., and T. J. Sumerling, "A Review of Approaches to Scenario Analysis for Repository Safety Assessment," paper presented at NEA Symposium on Safety Assessments for Repositories, Paris, 1989.

2. Cranwell, R.M., R.V. Guzowski, J.E. Campbell and N.R. Ortiz, "Risk Methodology for Geologic Disposal of Radioactive Waste: Scenario Selection Procedure," NUREG/CR-1667, 1982.

8.0 AUXILIARY ANALYSES SUMMARIES

8.1 Introduction

Generally the auxiliary analyses are directed towards the evaluation of the appropriateness and limitations of various computational approaches and the analysis and interpretation of data being used in this study. These analyses include: the two-dimensional cross sectional flow simulation of a layered porous site, the analysis of hydrologic data, and the analysis of statistical convergence for a CCDF. Addtionally, a separate analysis of carbon-14 releases was performed to supplement the liquid and direct pathway analysis. The above auxiliary analyses are discussed in detail in the Appendices. A brief description of the analysis will be given below.

8.2 Carbon-14 Analysis (Appendix D)

The release of carbon-14 from waste packages is a potential concern for a repository located in the unsaturated zone due to the presence of a fast pathway (gas through the fractures) to the accessible environment. Due to the complexity of the source term considerations of this problem, the analysis was not considered appropriate to be included in the total CCDF. However, it was considered important to perform some simple calculations to obtain a better appreciation and understanding of the magnitude of the problem and some of the concerns.

The analysis identified release mechanisms and the geochemistry of calcite precipitation as areas where data collection and further investigation would be most fruitful.

8.3 Statistical Convergence (Appendix E)

There are rules of thumb for determining the number of Monte Carlo simulations to perform to provide statistically representative results. Due to the highly non-linear problems currently being tackled, it was deemed appropriate to investigate the number of simulations required to obtain statistical convergence.

Approximately an order of magnitude more simulations than the rule of thumb would indicate were required for the current problem. The most likely reason for this result, was the very few simulations which provided a non-zero result in the high consequence part of the CCDF.

8.4 Analysis of Hydrologic Data (Appendix F)

An auxiliary analysis of hydrologic data was conducted to determine if spatial correlations could be identified for porosity and hydraulic conductivity parameters. A large scale trend of decreasing porosity with increasing depth was identified in data from three holes drilled into the Topopah Springs unit and a small scale correlation length of less than 40 meters was identified in data from two holes drilled into the Topopah Springs unit. However, this analysis did not identify any spatial correlation with depth for Calico Hills porosity data or for saturated hydraulic conductivity in either the Calico Hills or the Topopah Springs units. This was relevant to the flow and transport modeling, because long correlation lengths lead to a broad travel time distribution for each column (Section 9.3.1.4). Very short correlation lengths lead to the conclusion there is a single ground-water travel time per column and little likelihood of long, fast ground-water flow paths. In the flow and transport modeling, it was assumed that there was no apparent spatial correlation for saturated hydraulic conductivity beyond 10 meters separation (Section (.3.1.5).

8.5 Two-Dimensional Flow Simulation (Appendix G)

A two-dimensional flow simulation was conducted to examine the potential for flow diversion at unit interfaces or the propensity for non-vertical flow. The analysis, which considered only matrix flow, showed that considerable non-vertical flow would occur at interfaces where the saturated conductivity of the lower unit was 75 percent or less of the infiltration rate. Future work will need to consider the effect of fractures on non-vertical flow.

9.0 ANALYSIS AND RESULTS

Previous sections have described the methods and approaches for estimating performance and the evaluations used to select the various methods and approaches. This section describes the implementation of the methods and the results obtained. The following correspondence exists between the previous sections and the current section:

Previous (Methods)	Current (Implementation)
Section 4 - System Code	9.6 Total CCDF
Section 5 - Source Term	9.2 NEFTRAN Source Term Model
Section 6 - Flow and Transport Models	9.3 Flow and Transport Models
Section 7 - Methodology for Scenario Development	9.1 Treatment of Scenarios

Three additional subsections are added to this section to complete the exposition of implementing the methodology:

- 9.4 Parameters, describes values used in the analysis
- 9.5 Sensitivities and Uncertainties for Liquid Pathway Analysis, describes a demonstration of analytic methods
- 9.7 References

9.1 Treatment of Scenarios

A general approach for analysis of scenarios is discussed in Section 7. Because work on this part of the performance assessment was delayed, a less systematic approach to the treatment of scenarios was taken in the interest of expediency. In particular, the steps of: (1)identification of processes and events, (2)assignment of probabilities, (3)screening of events and processes, (4)scenario class construction, (5)scenario class probability estimation, and (6)scenario class screening were collapsed into a more direct approach. Because of the limited time available to perform the Phase 1 analysis, significant new modeling initiatives were not possible. With this in mind the staff decided to choose a small number of interesting scenario classes to incorporate in the CCDF to demonstrate how this is done and how results from various scenario classes are combined.

Two classes of fundamental events were selected. These events were: (1)Changes in climate at Yucca Mountain and (2)Human intrusion by drilling exploratory boreholes. These types of events were selected, in part, because they would demonstrate interesting aspects of repository performance and because the modeling variations needed to accomodate them were not excessive. Thus treatment of the class of climate changes, called pluvial conditions in this study, that could be represented by increased infiltration and a rise in the water table at Yucca Mountain were relatively easily accomodated by a small number of modifications to the data used as input to the model representing groundwater transport. Excavation of radioactivity contained either in the repository or in contaminated host rock could be relatively easily modeled to what is believed to be an acceptable degree of accuracy. In addition, excavation of radioactivity is an archetypical direct release event, representative of the type of modeling anticipated for similar direct release mechanisms like volcanism.

The two classes of fundamental events combine to form four classes of scenarios:

0. base case, no drilling
1. pluvial conditions, no drilling
2. base case, with drilling
3. pluvial case, with drilling.

Consequences for the base case were estimated by the output of the NEFTRAN code as described in Sections 6 and 9.2. The pluvial case was estimated by the NEFTRAN code, but with input modified to simulate a higher water table and greater infiltration rate. Because the drilling removed so little radioactivity from either the repository or the host rock, the consequences of drilling, to a first approximation, could be calculated independent of the details of the migration of radionuclides. However, some of the same factors, such as the removal of waste from the repository, influenced both pathways, so parameters important to these factors were used in calculating releases from both pathways. For scenario classes 2 and 3, consequences from both pathways were calculated and subsequently added together by the system code.

The probability of occurence of drilling was considered to be independent of the occurence of pluvial conditions (see Figure 9.6.1). Although drilling boreholes for purposes of acquifer detection or water exploration and extraction probably would depend on the climatic conditions at the site, drilling for purposes of mineral exploration would probably not depend on climate. Following the guidance provided by EPA in Appendix B of 40 CFR 191, a constant drilling rate of .0003 boreholes per square kilometer per year, a repository area of 5.1 square kilometers gives 15.3 as the expected number of boreholes over 10,000 years. This means that the probability of no boreholes at the site over the same time period is very small. Using a Poisson distribution to describe drilling, the probabiltiy of no boreholes is estimated to be 2.3×10^{-7}. Thus the probability of drilling is very close to 1. This may be an overestimate because exploratory drilling may be done preferentially in more level terrain (which is not accounted for in the average drilling rates) and because the repository's markers may be more effective than was assumed.

Had the scenario analysis procedure discussed in Section 7 been followed for this Phase 1 demonstration, the event of no drilling and all the scenarios involving no drilling would probably have been screened out, because of low probability of occurence. Alternatively the two scenarios involving no drilling probably would have been sceened out, again because of their low probability of occurence. These non-drilling scenarios were retained in this analysis for demonstration purposes and because the scenario analysis effort had not progressed sufficiently far to use the scenario screening procedure. An interesting result shown in Section 9.6 is that these scenarios, which would in all likelihood been screened out, have a negligible effect on the total CCDF, which is dominated by the scenarios with drilling. Because there were no readily available data, the probability of occurence of pluvial conditions was assumed to be 0.1 and the non-occurence of pluvial conditions was assume to be 0.9.

The two fundamental events selected for treatment here illustrate the striking differences in the importance of various scenarios to the CCDF that are to be expected when the probabilities of occurence or non-occurence of a particular event (such as drilling or pluvial conditions) are nearly equal or are orders of magnitude different. Also note that the treatment of drilling consequences, in combination with consequences from liquid pathway releases, as a separate pathway depended on the viability of the assumptions that: (1)the amount of radioactivity released by drilling is small compared to the total inventory in the repository and host rock and (2)that drilling boreholes had no substantial effect on the mechanisms important to liquid pathway releases. Had these assumptions not been good approximations, a far more complex treatment of the combination of fundamental events would have been necessary.

9.2 NEFTRAN Source Term Model

NEFTRAN (Longsine, 1987) has several built-in source term models; solubility limited, leach limited, and mixing cell. We have adopted the solubility limited and leach limited models for the present analysis.

Engineered barrier lifetime T_{eb}, a randomly sampled variable in the calculation, is the time before which there would be no radionuclides released. Beyond that time, the waste is assumed to be fully accessible to the environment and can be leached and dissolved. Once exposed to the environment, the radionuclides in the waste are assumed to be contained in the uranium dioxide matrix, and to be released at a rate determined by the "Leach time", T_L, which is the time for the matrix to be totally dissolved at a constant rate. The leach time is simply the reciprocal of the leach rate λ_L. We estimate the leach rate on the basis of the total inventory of the matrix M_0 [grams], the infiltration rate I [m/yr], the total surface area of the site, A [m^2], the fraction of infiltrating water contacting the waste f[unitless], and the solubility of the matrix S_0 [grams per cubic meter water]:

$$\lambda_L = I \ A \ f \ S \ /M_0 \qquad (9.2.1)$$

The rate of release of nuclides will be governed by either the dissolution rate of the matrix or the radionuclide itself. Most of the radionuclides must first be released from the matrix before their solubilities become limiting. Since more-oxidized fuel is likely to be more soluble, this solubility may be a function of time. The rate of fuel dissolution might be controlled either by the amount of water entering the canister, or if there is ample water, by the solubility of the fuel determined by its oxidation state.

Once released from the waste matrix, the NEFTRAN program determines if the concentration of the radionuclide exceed the solubility limit. If so, then the "undissolved inventory" for that radionuclide increases and the flux leaving the source is limited by the solubility. The undissolved inventory can be released later if the concentration of radionuclides leaving the source term drops below the solubility limit. All variables for the source term model except the initial inventories are random, generated externally to the program by the Latin Hypercube Sampling routine.

Several of the radionuclides, notably C-14, I-129 and cesium, are known to collect outside of the uranium oxide matrix (SCP, Section 8.3.5.9), and could be treated as being solubility limited rather than leach limited. We assumed that the fraction of the inventories available for immediate release of these radionuclides are not sufficiently great to affect cumulative releases over 10,000 years, so it was not necessary to make changes to the NEFTRAN code to facilitate them. All of their inventories are assumed to be contained in the matrix. However, we do consider the different inventories for C-14 for the gaseous pathway analysis. (In the present phase of this study, the staff has decided to treat C-14 releases separately from the liquid releases of radionuclides (including C-14). Release and transport of C-14 as a gas are covered in Appendix D.)

9.3 FLOW AND TRANSPORT MODELS

The movement of radionuclides could occur in the liquid, gas and direct pathways. As discussed in Section 6, the liquid pathway was simulated with the NEFTRAN computer program (Longsine, 1987), and a computer code was developed by the staff to simulate the direct pathway (for this phase of the MOU the direct pathway was a drilling scenario). The gas pathway was analyzed as an auxiliary analysis in Appendix D.

9.3.1 Liquid Pathway

Yucca Mountain is a complicated, multilayered system in three dimensions. NEFTRAN can represent the site only as an interconnected series of flow tubes. Although capable of representing a two-dimensional flow situation, NEFTRAN is further restricted to having only a single flow path for radionuclide migration. The staff considered that much important detail would be lost from the analysis of the complicated site with a one-dimensional analysis. Therefore, the NEFTRAN code was modified and run in a manner to partially overcome the limitations of the one-dimensional structure (i.e., simulate the spatially varying and uncertain conditions at Yucca Mountain). This specialized implementation can be divided into the following areas: 1) geometry or network set-up, 2) phenomena, and 3) data input.

9.3.1.1 NEFTRAN Network Implementation

The design of the one-dimensional network for NEFTRAN is based on current information on hydrogeologic units and theories of flow at Yucca Mountain. The SCP conceptualizes the flow at Yucca Mountain as essentially vertical and under steady-state conditions within the matrix for fluxes less than the matrix saturated conductivity, k_s, and as fracture flow at higher fluxes. (The potential for lateral flow at the contact between hydrologic units when a higher-conductivity unit is underlaid by a lower-conductivity unit was examined as an auxiliary analysis in Appendix G.)

Based on the assumption of vertical flow and the fact that the repository is envisioned to have a slope similar to the surrounding geologic unit (see Figure 9.3.1), the analysis was comprised of four separate networks. The network, designed to represent the hydrologic units existing below a portion of the repository and extending to the water table, is depicted in Figure 9.3.2. This representation takes into account the assumption that one end of the repository is 299 meters above the water table while the other end is 155 meters above the water table and different units exist below these two extremes. Additionally, the areal extent of the repository is rather complex (see Figure 9.3.3). The percentage of waste inventory was partitioned among the four columns based on the areal percentage of the repository determined to be above each column (see Figure 9.3.4). Table 9.3.1 presents the hydrogeologic units within the columns (labeled A through D), the thicknesses of the units and thus the distance from the repository to the water table for each column, and the fraction of waste present in the delineated by the columns.

Table 9.3.1 - Columns representing Yucca Mountain Repository Thicknesses in Meters

Column	A	B	C	D	Average Matrix Saturated Conductivity
Topopah Springs Weld	45 m	60 m	55 m	55 m	0.72mm/yr
Calico Hills Vitric	100	50	10	0	107
Calico Hills Zeolitic	20	70	120	100	0.54
Prow Pass Welded	34	45	10	0	88
Prow Pass Nonwelded	90	20	0	0	22
Bullfrog Welded	10	0	0	0	118
Fraction of waste	0.4	0.33	0.17	0.10	-

There are 6 hydrologic units in column A, 5 in B, 4 in C and 2 in D. Note that in Column D, the only layers present have very small average k_s, and that for high infiltration rates, the transport might be dominated by fracture flow, and therefore contribute to potentially high rates of transport to the water table. Column C is only slightly better, with two thin layers of the Calico Hills Vitric and Prow Pass Welded units present.

Some limitations of the one-dimensional network modeling approach (i.e., simulating the ground-water release pathway as four distinct columns of vertical flow) are:

1. Lateral flow caused by the diversion of water along interfaces between units and/or obstructions of flow near faults is not taken into account.

2. Flow and transport of radionuclides in the saturated zone from the water table beneath the repository to the accessible environment is conservatively neglected.

The source term is conservatively considered to start at the boundary of the disturbed zone, 25 meters lower than the plane of the waste emplacement, and therefore closer to the water table (NRC Draft Technical Position on the Disturbed Zone).

9.3.1.2 Implementation of Matrix and Fracture Flow in NEFTRAN

The NEFTRAN code was developed primarily for repositories located in saturated media (e.g.,in bedded salt and basalt). It represents groundwater flow and solute transport through a network of flow tubes. The groundwater flux and transport within each flow tube is considered to be fully saturated and at steady state, with each steady state velocity determined by Darcy's Law. In this form, it was not well suited for the present unsaturated flow calculations because steady state saturated conditions are not anticipated.

The guidelines for the present phase of this work limited the staff to using currently existing computer codes wherever possible. Rather than develop a new code capable of simulating the Yucca Mountain case, the NRC staff made modifications to the NEFTRAN code to facilitate the simulation of unsaturated flow and transport. First, all coding within NEFTRAN that calculated saturated flux through the flow tubes was eliminated. Instead, the flow rates through the network along the path of radionuclide migration are calculated from the infiltration flux. Second, the staff modified the NEFTRAN code to examine predominant downward bifurcated flow. Flow occurred either through the matrix or fractures, depending on the rate of infiltration relative to the saturated hydraulic conductivity of the matrix k_s. Flow through a vertical column would be driven by the infiltration rate. Since the column is one dimensional, all flux must pass through each layer. If the infiltration rate is greater than the matrix saturated hydraulic conductivity of an individual unit, then the fraction of the infiltration exceeding the saturated conductivity was assumed to flow in the fractures (in this case, all radionuclide transport occurred through the fractures, ignoring any radionuclide transport through the matrix). The possible subcases for this flow are described below:

a. Infiltration lower than saturated hydraulic conductivity

In this case, the staff assumed that because of matrix suction, water will flow entirely within the matrix, so that the velocity of a non-sorbing tracer without dispersion will be equal to the infiltration rate I divided by the water content ϕ; i.e.

$$v = I/\phi \qquad (9.3.1)$$

The water content is related to the unsaturated hydraulic conductivity through a constitutive relationship. In the present case, the Brooks-Corey formula is assumed:

$$\phi = n_e \, (q/k_s)^{1/\varepsilon} \qquad (9.3.2)$$

where ε is the Brooks-Corey factor for each hydrogeologic unit and n_e is the saturated effective porosity (Lin, 1986).

b. Infiltration Exceeding Saturated Hydraulic Conductivity

In this case the matrix will be incapable of carrying all the flow, therefore, a part of the flow will be carried by the interconnected fractures in the tuff. The matrix portion of the flow would have a transport velocity defined by:

$$v = k_s/n_e \qquad (9.3.3)$$

The fracture portion of the flow would be:

$$v' = (I - k_s)/n_f \qquad (9.3.4)$$

where n_f is the effective porosity of the fracture. This parameter should also depend on the infiltration rate. However, for the present set of calculations n_f will be taken as a constant, 0.0001, representative of a small value leading to short travel times in fractures (Lin, 1986). Since most of the potential for retardation and long travel times is in the matrix, a relatively small fraction of flow in the fracture may completely dominate the transport for bifurcated flow. Therefore, only the fraction of the infiltration carried in the fractures affected radionuclide transport for cases when both matrix and fractures should occur. The reasons for this choice are covered in the next section.

9.3.1.3 Implementation of Transport Phenomena within NEFTRAN

Radionuclides will be transported in the matrix or in the fractures if infiltration exceeds the saturated conductivity. If flow occurs in the fractures, the matrix and the fractures would be coupled by hydraulic and chemical processes. The effect of matrix diffusion on the transport through the system would depend on the transfer rate of radionuclides between the fractures and the matrix. The net effect of this transfer can be characterized in three ways, depending on the rate:

High transfer rate

At one extreme, transfer between the matrix and fractures would be high, leading to the concentration in the fractures being identical to that in the matrix. For plug flow (i.e., no longitudinal dispersion in the direction of flow) the rate of radionuclide movement would be the flux divided by the total water content ϕ_T, i.e., the total volume of the void water-filled void space:

$$v = I/\phi_T \qquad (9.3.5)$$

No transfer

At the other extreme, no coupling, the transport in the matrix and fracture pathways would be separate.

Partial transfer

For the intermediate case, the concentrations of the matrix and fracture would be coupled by a process allowing the transfer of radionuclides from the higher to lower potential; i.e., if the concentration of radionuclide in the fracture were greater than in the matrix, there would be transport of the radionuclide into the matrix by molecular diffusion. This phenomenon is generally called matrix diffusion.

By judicious choice of parameters, the NEFTRAN code can be made to approximate matrix diffusion using a simple two-zone model (Van Genuchten and Wierenga, 1976). The staff assumes that the water contained in the matrix is essentially immobile, because fracture flow is so much faster. The model accounts for the loss of the radionuclide from the mobile fluid to the immobile fluid by transfer across a boundary between the fracture and matrix. The concentration in the matrix and fracture are assumed to be uniform, and do not vary with distance from the interface. The model is only a rough approximation of true matrix diffusion because it ignores concentration gradients lateral to the direction of flow. It may capture salient features of matrix diffusion for our present purposes, however, and maintains the high efficiency of the code.

Transport due to matrix diffusion is proportional to a coefficient B. The NEFTRAN manual suggests that B can be approximated from the average fracture spacing a and effective diffusion coefficient D':

$$B = 2D'/(a/2)^2 \qquad (9.3.6)$$

The model does not account for the additional resistance that could be caused by the presence of surface coatings on the fracture. Since fracture coatings are common, the coefficient B should be reduced to take into account the reduction in transfer caused by these barriers.

For the preliminary analyses of the Phase 1 effort, the effects of matrix diffusion are ignored (the transport strategy is expressed by the "No Transfer" case). The reasons for the choice of this approach are:

1. The approach is conservative. Transfer from the fractures to the matrix would retard radionuclide transport.

2. Preliminary screening analyses show that for cases where fracture flow is important, the greatest contribution to dose is likely to come from transuranic elements such as plutonium and americium. These elements are known to have a tendency to form colloids (Thompson, 1989). The molecular diffusion coefficient of colloids is much less than that for dissolved molecules and ions, so matrix diffusion may not be effective (colloid transport is not modeled explicitly in the present exercise, however).

3. Fracture coatings would lead to a diminished effectiveness of both the diffusive transfer of radionuclides and water flow from the fractures to the matrix (Carlos, 1985).

Lacking experimental data on the actual magnitude and rates of matrix diffusion at Yucca Mountain, the staff is conservative to discount matrix diffusion in this initial demonstration.

9.3.1.4 Spatial Variability of flow and transport parameters

In order to maintain a high degree of efficiency in the Monte Carlo analyses with NEFTRAN, we represent the complicated spatially varying repository as four vertical columns, each with a small number of hydrogeologic units through which all of the radionuclides must pass. Existing data on tuff layers at the Yucca Mountain site indicate that there are considerable variations in the material properties. Available data do not support long correlation lengths for the transport parameters at the Yucca Mountain site. The data in many cases suggest small spatial correlation, or none at all on the scale for which they were collected (see Appendix F). Using constant values of transport parameters in the models therefore would be inappropriate. Assuming perfect spatial correlation within a unit could lead to a false conclusion that conditions leading to short travel time would apply over the whole unit. In actuality, short travel time might only apply to a small segment of the column and be countered by the presence of a barrier elsewhere in the column. This applies to a one dimensional analysis only in which the flow must pass through each segment in series.

Previous studies have recognized the importance of spatial correlation in the assessment of arrival time distributions. Lin and Tierney (1986) estimated the arrival time distribution for releases at the Yucca Mountain site by calculating the travel time of particles confined to a series of one-dimensional columns which represented the pathways from the repository to the water table. For each column, they varied the correlation length by changing the spatial step size, but keeping the hydraulic properties constant within a given step. They found from this analysis that longer step sizes lead to a wider arrival time distribution:

> "The implicit vertical correlation length (10 feet) of the baseline case is much less that the thickness of any of the hydrogeologic units. This results in a large number of independent random variables (travel times through each of the calculational elements) which are added together to obtain a travel time through a column. Consequently there is a low probability that fracture flow will occur through a large number of elements in any single column from the disturbed zone to water table.....
>
> ....Longer correlation lengths affect the travel time distribution, especially at the tail ends of the distribution, because of the increasing probability of fracture flow through a significant number of elements that make up each of the columns... These results indicate high sensitivity of the travel time distribution to the as yet undetermined correlation length for velocity in each hydrogeologic unit. Generally the

sensitivity of the travel times to the correlation lengths suggest how prudent it is to perform a carefully designed testing program for determining the correlation length of all key parameters influencing flow velocities."

Long correlation lengths led to an overly broad distribution for arrival time, with some very short travel times at the tail of the distribution. At the other extreme, the assumption of zero correlation length leads to the conclusion that there is only a single groundwater travel time per column. The above conclusions apply equally well to radionuclide transport, and therefore the determination of spatial correlation scales, especially for k_s, is important to the analysis.

9.3.1.5 Effective Values of Flow and Transport Coefficients

The NEFTRAN code simulates flow and transport through a network of connected tubes. For the present case, the staff represents the flow and transport model by up to 6 tubes in series, each tube representing a major hydrogeologic unit; e.g., Topopah Springs welded. Each tube is represented by coefficients expressing its physical properties for flow and transport, namely hydraulic conductivity, porosity, cross sectional area, and the retardation coefficients for each of the radionuclides considered in the present analysis.

As described in Section 9.3.1.2, groundwater transport is assumed to be either entirely in the matrix at low rates of infiltration, or entirely in the fractures at infiltration rates that exceed k_s. Since we presume that flow will be vertical and under unsaturated conditions, the primary factor for determining whether the flow in the present analysis is in the matrix or the fracture is the saturated hydraulic conductivity k_s. If infiltration exceeds k_s, then the excess will flow in the fractures.

Geostatistical analyses of the k_s data presented in Appendix F indicate that there is no apparent spatial correlation beyond about 10 meters separation distance, the smallest interval evaluated. As longer correlation lengths are more conservative, we assume that k_s is completely correlated at a distance of L meters. We represent each tube in the column by a connected series of sub-tubes, each of length L. Each sub-tube has uniform properties, but is uncorrelated to the next subtube in the series. The value of k_s for each sub-tube is picked by the Monte Carlo method from the lognormal distribution derived from the available core data presented in Table 9.4.4.

The analysis is based on the assumption that the flux of infiltrating water passes through each of the sub-tubes. The travel time across each sub-tube, depends on whether the flow is greater or less than k_s:

for $I > k_s$

$$\Delta t_i = n_f \, \Delta l/(I k_s) \qquad (9.3.6)$$

$$\Delta t_{ij} = \Delta t_i \, R_{dj,f} \qquad (9.3.7)$$

for $I < k_s$

$$\Delta t_i = \phi_i \, \Delta l/I \qquad (9.3.8)$$

$$\Delta t_{i,j} = \Delta t_i \, R_{dj} \qquad (9.3.9)$$

where Δt_i = the water travel time for subtube i

$\Delta t_{i,j}$ = the travel time for radionuclide j in subtube i

n_f = the effective porosity of the fractures (taken to be 0.0001)

ϕ_i = the water content of the matrix of subtube i

Δl = the length of the subtubes

I = the infiltration rate

R_{dj} = the matrix retardation coefficient for radionuclide j

$R_{dj,f}$ = the fracture retardation coefficient for radionuclide j

In this analysis, we consider that flow is either totally matrix or totally fracture flow for each sub-tube of length Δl. Even though there will be matrix flow in parallel with the fracture flow, in practice the fracture transport properties generally overwhelm the contributions of the matrix flow and can therefore be safely left out of the analysis.

We then sum the individual travel times and radionuclide travel times to determine effective values of porosity, ϕ_e, and retardation coefficients, R_{dej} for the main tubes representing the hydrogeologic units:

$$\phi_e = \frac{I \sum_{i=1}^{N} \Delta t_i}{N \, \Delta l} \qquad (9.3.10)$$

$$R_{dej} = \frac{\sum_{i=1}^{N} \Delta t_{ij}}{\sum_{i=1}^{N} \Delta t_i} \qquad (9.3.11)$$

where N is the number of sub-tubes.

There are two levels of sampling:

1. Within each sub-tube we sample by means of a Monte Carlo method for the values of k_s from a lognormal distribution in order to determine tube-averaged properties of effective porosity and retardation coefficients

2. From realization to realization, we sample by means of the Latin Hypercube method the mean and standard deviation of the logs of k_s and the sub-tube length L in order to represent the uncertainty in their values from borehole to borehole.

9.3.2 Gas Pathway

The discussion of this pathway is presented in Appendix D.

9.3.3 Direct (Drilling) Pathway

The analysis for the direct drilling pathway is presented in Appendix H. The drilling analysis used parameters specific to drilling (i.e., frequency of drilling) but all other parametric values were obtained by reading the NEFTRAN input files.

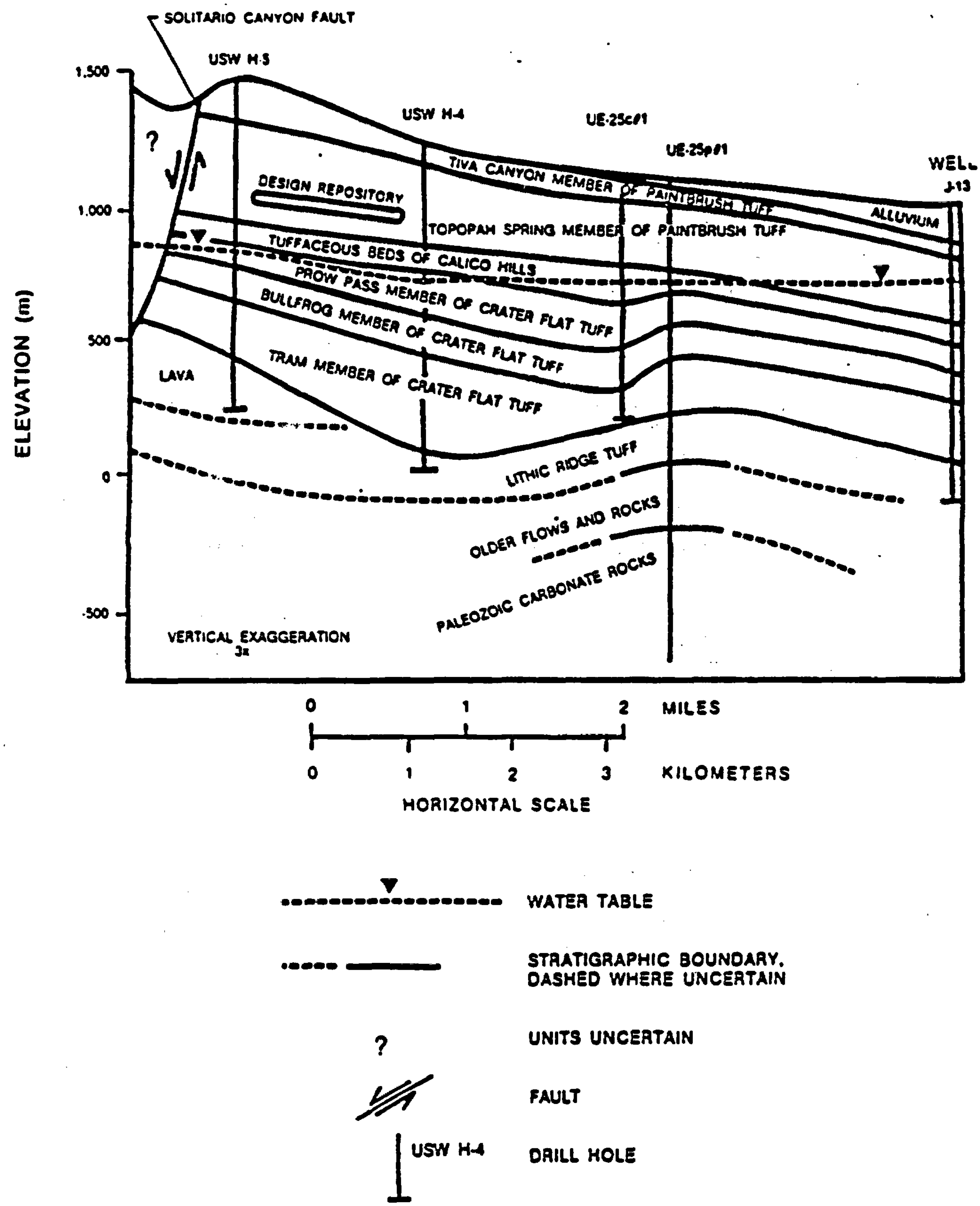
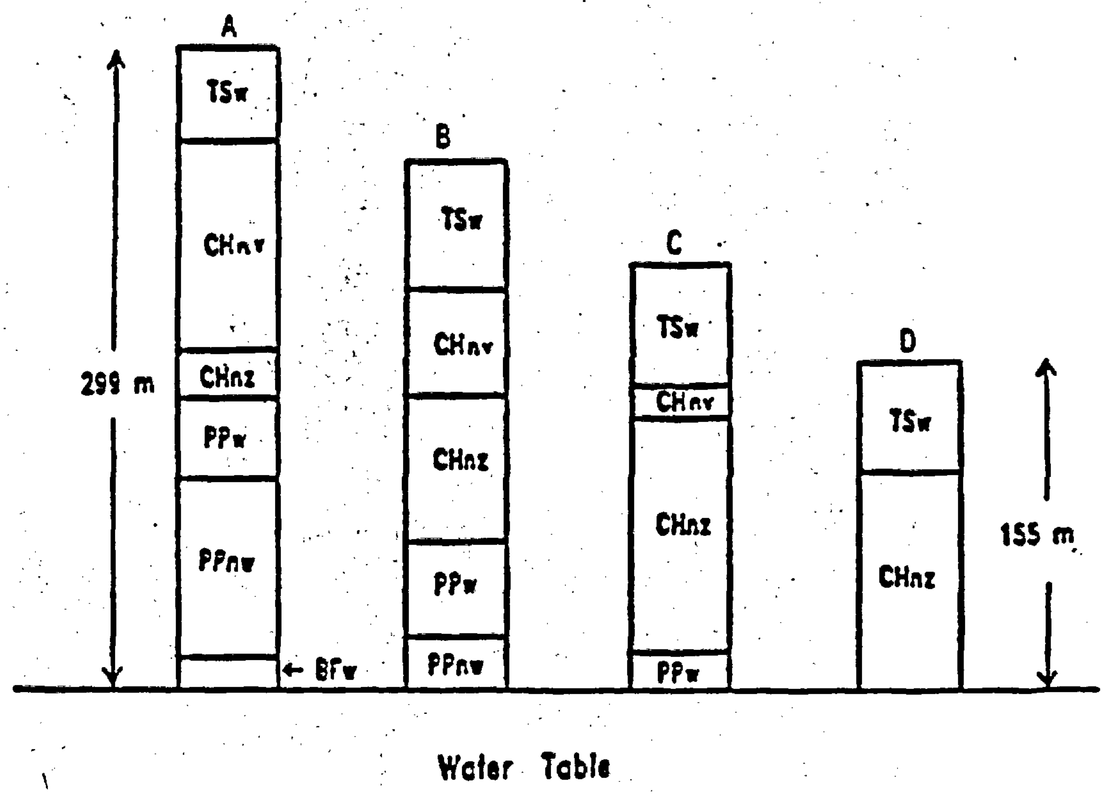


Figure 9.3.1 Conceptualization of a hydrogeologic cross-section through the unsaturated zone at Yucca Mountain (DOE, 1988).



TSw - Topopah Springs welded unit
CHnv - Calico Hills nonwelded vitric unit
CHnz - Calico Hills nonwelded zeolitized
PPw - Prow Pass welded member
PPnw - Prow Pass nonwelded member
BFw - Bullfrog welded member

Figure 9.3.2 Hydrostratagraphic units used to simulate the variation in depths and units existing below the repository. The four separate NEFTRAN representations are identified as A, B, C, or D.

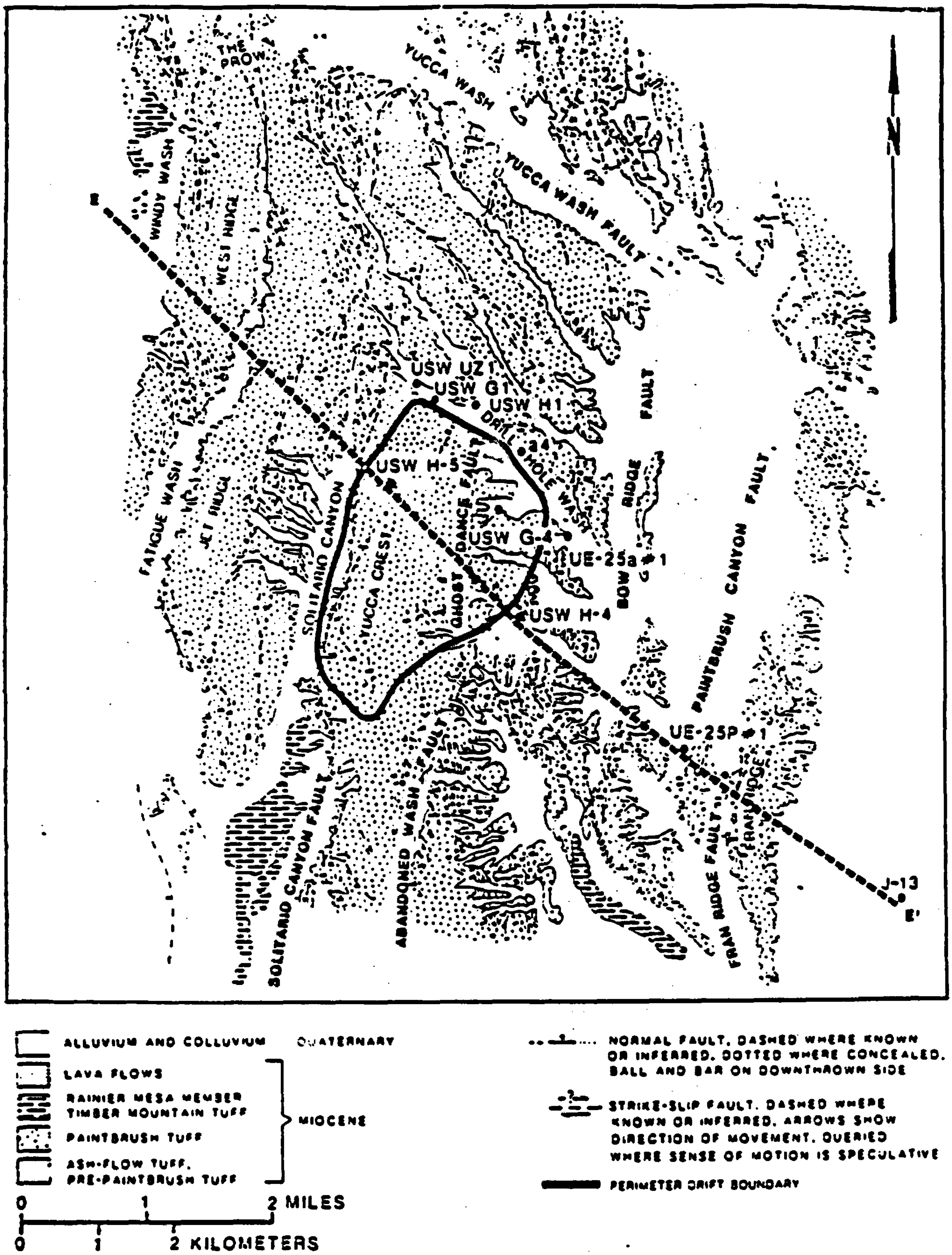


Figure 9.3.3 Geologic map of Yucca Mountain showing repository drift perimeter (DOE, 1988).

TSw - Topopah Springs welded unit
CHnv - Calico Hills nonwelded vitric unit
CHnz - Calico Hills nonwelded zeolitized
PPw - Prow Pass welded member
Pnw - Prow Pass nonwelded member
BFw - Bullfrog welded member

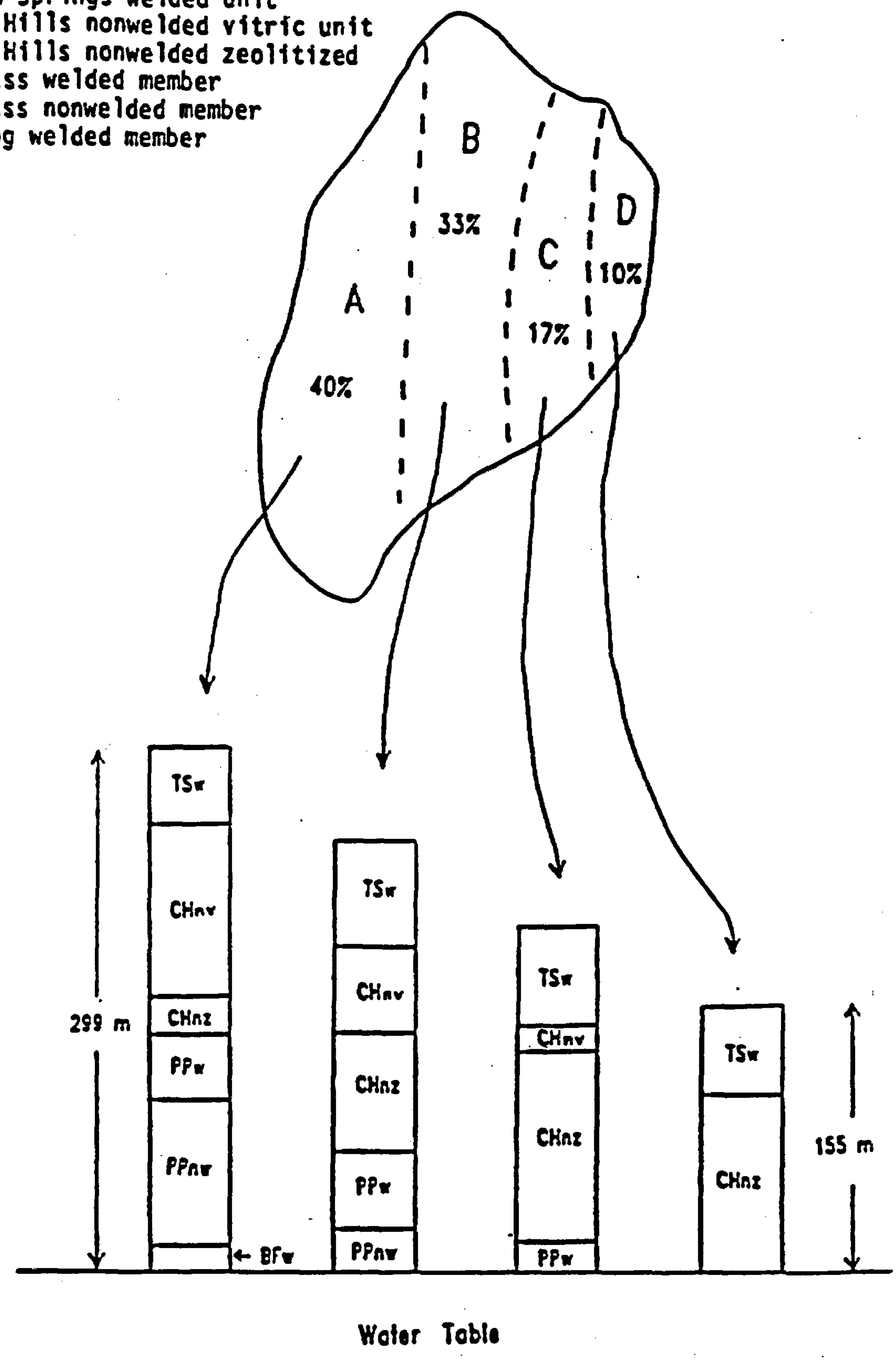


Figure 9.3.4 Representation of the allocation of repository area and radionuclide inventory of the four NEFTRAN simulations.

9.4 PARAMETERS

This section presents the ranges of parameters used in the liquid and direct pathways. Parameter values used for the gas pathway analysis are presented in Appendix D. Ranges were utilized by the Latin Hypercube Sampling (LHS) program to generate inputs for the source term and transport programs.

9.4.1 Liquid Pathway

Using NEFTRAN to simulate the liquid pathway requires the assignment of the following parameters:

saturated conductivity
porosity
volumetric flux
retardation coefficients
solubility limits
solubility of uranium matrix
waste package lifetime
water contact fraction
dispersivity
correlation length for hydraulic properties

For the liquid pathway analysis, the geologic medium is represented as a series of four vertical columns, each with up to 6 hydrologic units through which all of the radionuclides must pass. Each segment represents a single hydrogeologic unit. Subroutine GETRV in program NEFTRAN contained all of the definitions of source term and transport parameters necessary to make the code emulate the unsaturated flow and transport model.

Inputs to NEFTRAN were generated using the Latin Hypercube Sampling (LHS) program which selects random values from the input parameter ranges. Several known or suspected correlations are given in Table 9.4.1. Formal inclusion of correlations between variables should be performed in subsequent phases of this study.

Table 9.4.1 - Examples of Known and Suspected Correlations

- o Retardation coefficients for similar elements
- o Solubilities of similar elements
- o Solubilities with temperature
- o Temperature of canisters with engineered barrier failure time
- o Uranium matrix decomposition (i.e., oxidation, spallation, dissolution) with waste package failure time
- o Leach rate with infiltration rate and fraction of water contacting waste.
- o Infiltration rate with fraction of water contacting waste form

9.4.2 Sampling Parameters for NEFTRAN Analysis

The parameters necessary for this preliminary analysis of the Yucca Mountain repository came from a variety of sources, but primarily published DOE reports, including previous performance assessments for the Yucca Mountain and other repositories. Many of the data are highly uncertain. Nevertheless, the inputs represent the best data available to the staff at the present time. Sensitivity analyses performed following the calculations point out areas where improvement in data would be important in narrowing the ranges of calculated performance. Table 9.4.2 shows the input ranges and distributions of parameters for the NEFTRAN and other analyses as generated by the Latin Hypercube Sampling program LHSVAX. The following sections describe the basis for choosing the ranges appearing in the Table.

Table 9.4.2 - Input to Latin Hypercube Sampling Program

DISTRIBUTION	RANGE	LABEL
NORMAL	100 TO 1000	Engineered Barrier lifetime, years
UNIFORM	1.0E-04 TO 1.0E-03	Solubility of matrix, gm/gm water
NORMAL	0.10 TO 10	Dispersivity, ft
		Infiltration Rate, Ft^3/day
UNIFORM	0.5E+02 TO 0.25E+04	Base Case scenario
UNIFORM	0.25E+04 TO 0.5E+04	Pluvial scenario
UNIFORM	1.0E-04 TO 1.0E-02	Fraction of water contact
		Porosity of Matrix
UNIFORM	0.10 TO 0.18	TSw
UNIFORM	0.04 TO 0.14	CHv
UNIFORM	0.28 TO 0.36	CHz
UNIFORM	0.26 TO 0.31	PPw
UNIFORM	0.10 TO 0.18	PPnw
UNIFORM	0.13 TO 0.28	BFw
		Log k_s, mm/yr
UNIFORM	-0.5 TO 0.25	TSw
UNIFORM	-1.4 TO 0.5	CHv
UNIFORM	-0.7 TO 1.2	CHz
UNIFORM	1.4 TO 2.2	PPw
UNIFORM	1.4 TO 2.2	PPnw
UNIFORM	1.5 TO 2.5	BFw
	Standard Deviation of log k_s, mm/yr of log ks, mm/yr	
UNIFORM	0.6 TO 0.75	TSw
UNIFORM	0.7 TO 1	CHv
UNIFORM	0.8 TO 1	CHz
UNIFORM	0.4 TO 0.6	PPw
UNIFORM	0.4 TO 0.6	PPnw
UNIFORM	0.5 TO 0.7	BFw

Table 9.4.2 - Input to Latin Hypercube Sampling Program

(continued)

DISTRIBUTION	RANGE			LABEL
				Retardation Coefficients
UNIFORM	100	TO	1.0E+04	Am
UNIFORM	3000	TO	3.0E+04	Cm
UNIFORM	3	TO	2000	Ni
UNIFORM	5	TO	100	Np
UNIFORM	10	TO	100.	Pu
UNIFORM	0.10E+04	TO	3.5E+04	Ra
UNIFORM	0.20E+04	TO	0.4E+04	Sn
UNIFORM	5	TO	10	Tc
UNIFORM	200	TO	0.50E+04	Th
UNIFORM	5	TO	30	U
UNIFORM	1	TO	1.0E+04	Zr
UNIFORM	20	TO	0.1E+04	Pb
				Solubilities, gm/gm water
UNIFORM	2.0E-10	TO	2.0E-07	Am
UNIFORM	1.0E-09	TO	2.0E-07	Cm
UNIFORM	2.0E-04	TO	1.0E-03	Ni
UNIFORM	2.0E-05	TO	3.0E-04	Np
UNIFORM	5.0E-08	TO	3.0E-06	Pu
UNIFORM	1.0E-08	TO	1.0E-07	Ra
UNIFORM	5.0E-12	TO	5.0E-10	Sn
UNIFORM	0.5	TO	1.0	Tc
UNIFORM	1.0E-11	TO	5.0E-10	Th
UNIFORM	2.0E-11	TO	1.2E-10	Zr
UNIFORM	1.0E-04	TO	2.0E-03	Pb
UNIFORM	20.0	TO	50.0	Correlation length, ft.

9.4.2.1 Waste Package Lifetime

There were no readily available models accessible to the staff to assist us in the choice of the waste package lifetime in the unsaturated zone. The NEFTRAN code is simplistic, and able to accept only a single value of lifetime for each run, even though it is likely that waste package failure would occur in a highly distributed manner.

Waste package lifetime will affect the source term in several ways. First, thr package must fail in order for anything to be released at all (although failur does not alone imply that there will be contact between the waste and the water). Second, if the package fails in an essentially dry environment, oxygen from the unsaturated zone will enter, which might allow oxidation of the UO_2 to proceed for a fraction of the fuel rods that have defects. The more-oxidized uranium would have increased solubility over the less-oxidized form (Grambow, 1989). Furthermore, oxidation could cause an increase in volume of the pellets, causing splitting of the cladding and spallation of the pellets and thus possibly increasing surface area. Oxidation might also take place in some of the unfailed canisters because of the presence of small amounts of oxygen, or the dissociation of water caused by ionizing radiation (Reed, 1987). This radiation could form hydrogen peroxide or nitric oxide which are powerful oxidants. The time to failure of the canister would impact directly on fuel oxidation because the reactions involve temperature and radiation, both of which decrease with time.

For the initial phase of this study, we assumed that the fuel solubility is fixed and not a function of time and temperature. Refinements to account for time-dependent oxidation state and temperature may be incorporated into the model in later phases of this study. A possible subject for further study would be the potential isolation afforded the waste by the drying out of the rock.

The staff chose the waste package failure for the liquid pathway analyses as normally distributed with a 0.001 to 0.999 fractiles range for 100 and 1000 years, respectively. For the gas pathway, the staff chose two distributions in order to demonstrate the sensitivity of release of C-14 to waste package lifetime (see Appendix D)

9.4.2.2 Solubility of uranium matrix

Assuming the canisters and cladding have failed and water penetrates the canister, the bulk of the radionuclide release is likely to be from the dissolution of the uranium dioxide waste matrix. The solubility of the waste will be controlled by several factors. Among the more important factors will be the oxidation state of the fuel, which is in turn a function of temperature, oxygen availability and time. The staff assumes that the dissolution rate of the waste is controlled by the rate of disintegration of the uranium dioxide matrix as characterized by a solubility limit (The disintegration of the fuel matrix may not actually be limited by solubility, but by the rate of oxidation). For the present case, the solubility has been chosen to be independent of waste package failure time and temperature and uniformly distributed between 0.0001 and 0.001 grams UO_2 per gram of water.

9.4.2.3 Dispersivity

The dispersivity is a measure of the spatial variance in the transport speed, particularly that caused by variability in material properties, which causes the arrival time distribution to spread. It is not likely to be an important consideration in most analyses for cumulative releases. We have chosen the dispersivity to be normally distributed between 0.1 and 10 feet for the 0.001 and 0.999 fractiles respectively.

9.4.2.4 Infiltration Rate

One of the key variables in the analysis is the rate of infiltration which is the main influence on the speed of water movement in the vertical column as well as the amount of water coming into contact with the waste.

Base Case Infiltration

At this time there are no direct measurements of infiltration at Yucca Mountain. Estimates of present day infiltration rates have been calculated from (1) heat flow measurements, (2) precipitation and elevation data, and (3) hydrologic parameters measured from core and in situ in site boreholes. Table 9.4.3 contains a summary of infiltration estimates cited in the literature. Estimates of infiltration rates range from less than 0.1 mm/yr to 10 mm/yr.

Most of the previous DOE analyses have employed infiltration rates in the range of 0.1 and 0.5 mm/year. However, because of the considerable uncertainty in the estimates presented in Table 9.4.3, we have chosen a considerably wider range of infiltration rates than previous DOE analyses. For the base case scenario, infiltration rate is considered to be uniformly distributed between 0.103 and 5.14 mm/year (500 to 2500 cubic feet per day over the total repository area). This range was considered to be a sufficient representation of available data for the purposes of this demonstration.

Pluvial Scenario

Czarnecki (1985) estimated infiltration for a future pluvial climate scenario for the purpose of calculating the potential rise in the water table. Estimates of future precipitation were based on descriptions of paleoclimates where annual precipitation 12,000 to 9,000 years before present in the modeled area may have been 100 percent greater than modern day annual precipitation. This 100 percent increase with respect to modern-day precipitation was assumed to be the probable maximum increase in the next 10,000 years. Czarnecki doubled the rainfall estimate of Rush (1970), and then multiplied by the percentage of precipitation occurring as recharge that is associated with that higher precipitation range. He assumed that the increased flux across the northern boundary of the modeled area occurred because of the increased precipitation in recharge areas to the north. Vertical infiltration into Fortymile Wash increased because of surface-water runoff from its drainage basin. Czarnecki calculated that increased recharge from a 100 percent increase in annual precipitation would be 13.7 times greater than estimates of modern day recharge, corresponding to about 7 mm/year infiltration. He also predicted a rise in the water table of 130 meters.

Table 9.4.3 - Infiltration Estimates

Estimate	Location	Methodology	Source
4 mm/yr	Yucca Mt.	precipitation and elevation data	Rice, 1984 Rush, 1970
1-10 mm/yr	Yucca Mt.	drill hole thermal data	Sass, 1982
2 mm/yr	Yucca Flat	hydrogeologic parameters	Winograd, 1981
0.5 mm/yr	Yucca Mt.	precip. and elevation data	Czarnecki, 1985
<0.5 mm/yr	Yucca Mt.	core and insitu hydrogeologic parameters	Wilson, 1985
0.5 mm/yr	Yucca Mt.	maximum for matrix k_s data	Sinnock, 1984
0.1 - 0.5 mm/yr	USW UZ-1	core and insitu hydrogeologic parameters	Montezar, 1985
10^{-7} - 0.2 mm/yr	USW UZ-1	core and USW UZ-2 insitu hydrogeologic parameters	Montezar, 1984

For the purpose of the present study, we estimate the range of infiltration for the pluvial scenario as 5 to 10 mm/year, with an increase in the water table height of 100 meters.

9.4.2.5 Fraction of water contacting waste

The staff characterizes the ratio of water infiltrating the site to the water actually coming into contact with the waste as a constant. The staff performed simple calculations to estimate the fraction of the waste canisters exposed to purely vertical infiltration by taking the ratio of the cross-sectional area of the canisters to the total area of land surface projected by the repository. This ratio is approximately equal to 0.00078. In most cases, infiltrating water could flow around the canisters because of the matrix suction of the unsaturated rock, so this figure derived from this simple approach does not capture the true nature of water contact.

DOE plans to emplace the canisters in the host rock in a manner that they believe would reduce the likelihood of water coming into contact with the waste. These precautions includes vertical storage and an air gap between the canister and the rock walls. Furthermore, DOE believes that the heat generated by the waste may create a significant zone of dry rock around the canisters, isolating them until cooling of the rock at a later time allows water to rewet the rock (SCP, Section 8.3.5.9). Water may still come into contact with the canisters by several mechanisms:

1. Infiltrating water flowing through fractures and dripping onto the canisters.

2. Loss of the air gap caused by failure of the emplacement holes through mechanical and thermal stresses, or mineral and sediment infilling.

Two additional and potentially important sources of water could be (1) lateral inflows from areas of perched water and (2) liquid water circulation caused by heat-driven evaporation and condensation. We assumed that lateral inflows are unlikely to affect more than a few of the canisters, since the water necessary for this phenomenon to be viable would be diverted from the vertical infiltration available for all canisters. If such a diversion was possible, some canisters might get a greater share of the overall infiltration at the expense of the remaining canisters being exposed to less water. Liquid water circulation caused by heat is potentially important, and is discussed further in Section 5, Source Term.

For this preliminary analysis, we have chosen the water contact fraction to be 0.002 to 0.01, based on the assumed wetting of a small fraction of the canisters.

9.4.2.6 Saturated Hydraulic conductivity

Water flow in the unsaturated fractured rock could proceed through both the matrix of the rock at low rates of infiltration or through the fractures and the matrix at higher rates of infiltration. The switchover from matrix flow to flow in the fractures may be related to the saturated hydraulic conductivity of the rock matrix. Statistical evaluation of the data presented in Appendix F indicates that k_s is lognormally distributed. Table 9.4.4 summarizes the available data on saturated hydraulic conductivities from rock cores at the Yucca Mountain site in terms of its log means and standard deviations where there are sufficient data available.

9.4.2.7 Spatial Correlation of Saturated Hydraulic Conductivity

Geostatistical analyses of the k_s data presented in Appendix F indicate that there is no apparent spatial correlation of the core data on saturated hydraulic conductivity of the matrix above the minimum separation distance of 10 meters used in the analysis. Since larger correlation scales are conservative, we assumed that there is a correlation scale between 20 and 50 feet. There are insufficient data to determine the distribution of the mean and standard deviation of k_s for, so we assumed that it is uniformly distributed from the values calculated for each unit and each borehole. The mean, standard deviation and correlation length of k_s were used to choose representative hydraulic coefficients for each hydrogeologic unit as described in Section 9.3.1.

Table 9.4.4 - Log mean and standard deviation of k_s

Unit	Mean of log k_s mm/yr	S.D. of log k_s mm/yr
BFnw	2.22	
	1.38	
	1.71	0.59
BFw	2.08	
CHnv	-1.32	
	0.47	
	0.07	
CHnz	1.16	
	-0.65	0.87
PP	1.44	
	2.09	

ISw	0.22	0.72
	-0.45	0.61

9.4.2.8 Porosity

There are probably more porosity data available from core taken at the Yucca Mountain site than any other type of data used in this study. As used in this study, water velocity and radionuclide transport speed in the matrix are tied closely to the average value of porosity for the columns. We chose the porosity ranges from available data averaged over each unit. There were insufficient data to determine the distributions of the average properties, so the averages were assumed to be uniformly distributed. Representative values of porosity for each hydrogeologic unit were sampled from the distribution of arithmetic mean porosities shown in Table 9.4.5.

Table 9.4.5 - Mean Porosity for Units

Unit	Arithmetic Mean Porosity
BFnw	0.2
	0.22
	0.25
BFw	0.13
	0.28
CHn	0.36
	0.2
	0.28
	0.34
	0.29
PPn	0.29
PPw	0.31
	0.31
	0.26
TSw	0.11
	0.13
	0.1
	0.11
	0.18

9.4.2.9 Brooks-Corey Coefficients

The Brooks-Corey Coefficients are used to determine the fraction of saturation for a given infiltration rate, as described in Section 9.3. The values used in the present study were taken from Lin and Tierney (1986) and are presented in Table 9.4.6.

Table 9.4.6 - Brooks-Corey Coefficients

Unit	Brooks-Corey Coefficient
TSw	5.9
CHnv	4.2
CHnz	7.0
PPw	4.0
PPn	5.2
BFw	4.6
BFn	5.2

9.4.2.10 Retardation coefficients

The staff chose values of retardation coefficients for the matrix to reflect reported values for batch and column tests performed. For the key radionuclides plutonium and americium, values were chosen at the low end of the range in order to account partially for data that indicate that these substances do not behave simply, tend to form colloids, and may be difficult to predict under repository conditions (Thompson, 1989). We should hasten to add however that much of the data in column experiments that indicated low retardation for some elements was collected for flow rates 3 to 4 orders of magnitude greater than we are using in the present study, and therefore may be pessimistic. Furthermore, sensitivity studies presented in Section 9.5 indicate that retardation coefficients for plutonium and americium in the present study are relatively unimportant, indicating that factors such as low solubility and long half life may be more important than retardation for these nuclides. Values used in this study are typical of those used previously in Yucca Mountain performance studies (Lin, 1986). While most of the retardation coefficients are sampled by LHS from the distributions presented in Table 9.4.2, the retardation coeffients for a few of the elements were taken to be constants. These retardation coefficients are 1.0 for iodine, 10,000 for cesium, 1,000 for strontium and 1.0 for carbon.

Retardation coefficients for the fractures were taken from the study by Lin (1986), and are orders of magnitude smaller than the matrix retardation coefficients. The values of retardation coefficients for fractures were not sampled, but remain fixed for all realizations. The values used are given in

Table 9.4.7. In both the matrix and fracture cases, there was no distinction made for retardation coefficients between different hydrogeologic units. Those units that have low values of saturated hydraulic conductivity however will tend to have lower values of effective retardation coefficients because of the greater proportion of the flow to be expected in the fracture zone (as calculated by the procedure presented in Section 9.3.1.5).

Table 9.4.7 - Retardation Coefficients for Fractures

Element	R_{df}
Cm	1.4
Pu	1.1
U	1.0
Am	1.4
Np	1.0
Th	2.2
Ra	2.8
Pb	1.0
Cs	100
I	1.0
Sn	1.3
Tc	1.1
Zr	2.0
Sr	10.0
Ni	1.2
C	1.0

9.4.2.11 Solubilities

We have taken the solubilities of radionuclides primarily from DOE references, including several preliminary performance assessments. Values used reflect those reported in previous performance assessments from Yucca Mountain (Lin, 1986).

9.4.3 Direct (Drilling) Pathway

The drilling program was developed to calculate the consequences from the expected number of boreholes intercepting the repository (see Appendix H). The following values were needed: drilling rate, size and number of waste packages, area of repository, time of drilling, and the radius of the borehole. Additionally, the following values from the liquid pathway were used: time of waste package failure, volumetric flux, water contact fraction, and solubility limits (these values were discussed in the above Section and will not be discussed here).

Based on conceptual repository designs the dimensions of the repository system were set as follows: area of repository = 5.1 square km, number of waste packages =18,000, borehole radius = 6 cm, waste package radius =0.34 m, and waste package length = 4.8 m. The time for commencement of drilling was set to a arbitrary value of 100 years and the drilling rate was set to .0003 drillings per square km per year based on EPA average drilling rates (EPA,1985).

9.5 Sensitivities and Uncertainties for Liquid Pathway Analysis

9.5.1 Introduction

This section covers the sensitivity and uncertainty analyses of the liquid pathway calculations on a scenario by scenario basis. It does not cover either the drilling or gas pathway analyses. We present the complimentary cumulative distribution functions (CCDF's) for the Base Case and Pluvial scenarios which take into account the uncertainty in the values of the coefficients for each scenario, but not the scenario probabilities. We also present the sensitivity to variations in parameters using rank regression and ad hoc variations of single parameters, including those parameters relating to the NRC guidelines of 10CFR60.113. Total system results, which also take into account the scenario probabilities, are covered in Section 9.6, but we have not performed formal sensitivity and uncertainty analyses on these results.

9.5.2 Statistical uncertainty analysis

An important part of conducting a performance assessment of a waste repository for high level waste is quantifying the uncertainties associated with the probabilities of occurrence of credible scenarios and those associated with the offsite and onsite consequences (both radiological and nonradiological).

Many risk and environmental impact assessments apply single or best-estimate values for model parameters and assert that these valuations are reasonable and conservative (i.e., lead to overpredictions) without quantifying the degree of conservatism inherent in the assessments. A variety of techniques is available to quantify the uncertainty in complex models for assessing radiological impact upon man and the environment that may include nonlinearities and time-varying phenomena (1,2). These include: the Monte Carlo (Helton, 1961), fractional factorial design (Cochran, 1963), Latin hypercube sampling (Cranwell, 1981, Iman, 1979, McKay, 1979), response surface (Meyers, 1971), differential sensitivity analysis, (e.g., adjoint (Baybutt, 1981, Oblow, 1978, Cacuci, 1980)) and Fast Probabilistic Performance Assessment (CNWRA, 1988) methodologies. A preferred technical approach would be flexible, economical to use, easy to implement, provide a capability to estimate an output distribution function and rank input variables by different criteria.

9.5.2.1 Latin Hypercube Sampling

In this study the Latin hypercube sampling (LHS) scheme was chosen to be implemented on the flow and transport model in the performance assessment of the high level waste repository. The advantages and properties of the Latin hypercube sampling techniques are:

o The full range of each input variable is sampled and correlation coefficients between all pair-wise input variables can be specified.

- It provides unbiased estimates of the parameters (means and variances) of cumulative distribution functions and means for model output under moderate assumptions.

The LHS method is a member of the class of sampling techniques which include Monte Carlo and stratified random sampling. Several risk assessments for nuclear waste repositories (Campbell, 1979) have applied LHS techniques. Furthermore, LHS has been applied to the model for atmospheric transport of reactor accident consequences and recently used for the severe reactor accident calculations in NUREG-1150 (NRC, 1989). We remark that one may wish to distinguish between different types of uncertainty associated with modelling of physiochemical processes - in particular:

- The statistical uncertainty due to inherent random nature of the processes, and

- The state of (perhaps "lack-of") knowledge uncertainty.

This latter state-of-knowledge uncertainty may be further subdivided into model and parameter uncertainty. The parameter uncertainty is due to insufficient knowledge about what the input to the code should be. The modeling uncertainty is due to simplifying assumptions and the fact that the models used may not accurately model the true physical process. This study deals primarily with parameter uncertainty.

As shown in Table 9.5.1, first a set of key parameters in the model under study needs to be identified. For each chosen variable, a set of quantitative information is developed regarding the range of variation, probability distribution, as well as correlations among the variables. For our study, we did not use any correlations between input variables. The data input to the LHS program is given in Table 9.4.2., which shows the distribution and range of input for each variable. The basis for choosing these inputs is discussed in Section 9.4. This information is used as input to the Latin hypercube sampling code (Iman, 1984a,b). LHS is used to generate what is called a design matrix. Specifically, if N computer runs are to be made with k parameters under study, the design matrix has dimensions N x k. Each row of this matrix contains the input valuations of each of the chosen k parameters (independent variables) for the N computer runs. The sample size N is specific to the problem being investigated (Iman, 1980). Appendix D presents a sensitivity study on the sample size for one scenario.

9.5.3 Ad Hoc Sensitivities

In this section, we present results of the NEFTRAN runs for the base case and pluvial liquid pathway scenarios with the intent of demonstrating the effects of individual variables on the resultant cumulative radionuclide releases to the accessible environment.

The NEFTRAN computer code as modified for the Yucca Mountain case was run for the base case scenario to calculate cumulative releases for either 10,000 years or 100,000 years, and the pluvial scenario for 10,000 years. For each simulation, we generated a list of 47 variables using Latin Hypercube Sampling. The list of variables for each simulation is called a "vector". The input constants, ranges and distributions for generating the vectors are presented in Tables 9.4.2.

9.5.3.1 Sensitivity to Infiltration

Figures 9.5.1 and 9.5.2 show the resultant conditional CCDF's for the base case scenario at 10,000 and 100,000 years, respectively. Also plotted on these figures are CCDF's composed only from vectors having infiltration rates less than limits set at 2.0 or 1.0 mm/yr in order to demonstrate the particular significance of this parameter to repository performance.

The great sensitivity to infiltration rate can be partially explained by the next two figures. Figures 9.5.3 and 9.5.4 show the CCDF's for the base case scenario at 10,000 and 100,000 years respectively, comparing the contribution of column D to the contribution from all 4 columns. Column D contains just 10% of the waste, but has the shortest pathway to the water table. In addition, column D contains just two units; the Topopah Springs welded and Calico Hills zeolitic. Both of these units have relatively low saturated hydraulic conductivities, k_s, which would make them prone to fracture flow for higher infiltration rates. Fracture flow leads to both short travel times for liquid water and low retardation coefficients. Figure 9.4.3 shows the effect most dramatically, where virtually all of the contribution to the high-impact portion of the curve would be caused by Column D alone. Retarded radionuclides have not yet started to arrive from the other columns. Travel times through the other three columns would be too long to contribute much to the CCDF within 10,000 years. Figure 9.4.4 shows that more of the contribution to the CCDF comes from the other three columns over the 100,000 year period, because the long-lived radionuclide start arriving.

Figure 9.5.5 shows the CCDF for the pluvial scenario. In this case, the water table is shallower and infiltration rates are higher than the base case scenario, so travel times are shorter for all columns. Relatively more of the cumulative EPA ratio comes from column A, B and C than was the case for the base case scenario. These scenarios are not directly comparable however, because long computer run times led to the necessity of reducing the number of vectors from 500 to 98 for the pluvial scenario. It should also be pointed out that the 98 outputs in the pluvial case were generated from a truncated run that was intended to contain 200 vectors. The desirable property of statistical independence in the LHS procedure can only be assured when the sample size matches the intended sample size. Statistical independence in the pluvial case was lower than desired, as indicated by the relatively high values of the off-diagonal elements in the correlation matrix as compared to the correlation matrix for the 500-vector base-case scenario.

9.5.4 Sensitivity Analysis using Regression

The next step in the process involves performing a sensitivity analysis on the calculated results. The aim is to determine and quantify the relative contributions of a particular variable toward the output variability. Sensitivity analyses can be very fruitful in preliminary studies such as this one, since sensitivity analyses can help to identify which parameters and models should be refined in future studies. In addition, sensitivity analyses may allow the analyst to check his intuition about the importance of the parameters and phenomena of the model.

Sensitivity can be determined by performing step-wise linear regression analyses on either the raw results of the model analysis (i.e., the EPA ratios) or the ranks of the raw results (i.e., replacing the "raw" data values by their ranks). Ranks may be preferred when highly nonlinear relationships are present between the model outputs and inputs, but the correlations obtained have less significance than those using the raw data. Both graphical analyses and statistical distribution fitting procedures may also be useful in identifying patterns in the data. The present report shows only the regression analyses on raw results; i.e., EPA release ratios.

The staff analyzed the sensitivity of the cumulative release for several cases using a modified version of the STEPWISE program from Sandia National Laboratories (Iman, 1980). We modified the STEPWISE program to read the data file of input vectors generated by the LHS sampling procedure and the combined results for columns A through D generated by NEFTRAN for those inputs. The regression coefficients are presented in Table 9.5.2 for the base case and pluvial scenarios. There were 500 vectors for the base case scenario, but because of excessively long run times, there were only 98 vectors for the pluvial scenario. The paucity of vectors led to more equivocal results for the pluvial scenario. We chose to show only the most significant regression coefficients or in some cases those regression coefficients pointing to an apparent lack of sensitivity to particular parameters.

The sensitivity analyses proved to be very revealing, both for the sensitivities to some parameters and apparent lack of sensitivities to others. The parameters consistently influential to the EPA ratio were contact fraction, infiltration rate, solubility of the matrix, and the saturated hydraulic conductivity of the Calico Hills vitric unit. Of these, high values of infiltration rate and saturated hydraulic conductivity lead to fast fracture flow pathways and low retardation in Column D, which contributes most of the high-impact releases in the base case scenario.

9.5.5 Average Importance of Radionuclides

We also evaluated the average contribution of the radionuclides to the EPA ratio for the scenarios. This parameter was calculated by taking the average contribution by radionuclide to the EPA ratio for all vectors. We present the average contribution by radionuclide in Table 9.5.3 for the base case scenario at 10,000 and 100,000 years, and the pluvial scenario at 10,000 years. In addition, we present further results for the base case scenario including only those vectors that have infiltrations less than 1.0 mm/yr or 2.0 mm/yr to demonstrate sensitivity of the result to infiltration. The isotopes Pu-239 and Pu-240 stand out as the most important contributors to the EPA ratio because of their large inventory in the source term, long half lives and potentially low retardation in the rock. Nearly all of the contribution of these radionuclides comes from inventory in the source term rather than from chain decay of heavier radionuclides (e.g., Am-243). Other radionuclides are important in a few cases. I-129 appears for the 100,000 year case with infiltration of less than 1.0 mm/yr because of its exceedingly long half life. The isotopes I-129, C-14 and Tc-99 would take on high relative importance if the groundwater flow were always restricted to matrix rather than fracture flow. This would have been the case except for column D for the base case scenarios, as the saturated k_s of most of the units in the other columns was sufficient to assure retention of most of the significant but retarded radionuclides.

9.5.6 Sensitivity to NRC Performance Criteria

NRC defines a set of performance criteria for particular barriers in 10CFR60.113:

"60.113(a)1(ii)(A) Containment of HLW within the waste packages will be substantially complete for a period to be determined by the Commission.....that such period shall not be less than 300 years nor more than 1,000 years after permanent closure of the geologic repository...."

"60.113(a)1(ii)(B) The release rate of any radionuclide from the engineered barrier system following the containment period shall not exceed one part in 100,000 per year of the inventory of the radionuclide calculated to be present at 1000 years following permanent closure......."

"60.113(a)2 The geologic repository shall be located so that the pre-waste-emplacement groundwater time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment shall be at least 1000 years......."

These limitations imposed by NRC have the intent of providing a set of criteria for the repository independent of the EPA release limits specified in 40CFR191, and prevent reliance on a single barrier to the release of radionuclides to the accessible environment.

9.5.6.1 Effects of NRC Performance Criteria on CCDF

We examined how compliance with the NRC standards relate to the outcome of the performance assessment calculations in terms of compliance with the cumulative release limits. This was not intended to be a demonstration of the effectiveness or lack of effectiveness of the NRC subsystem performance criteria, but was instead a demonstration of the usefulness of the performance assessment modeling to making future decisions on regulations. The conditional CCDF for the base case scenario was recalculated by using the original set of 500 input vectors and output releases, but screening out those vectors which did not comply with the NRC criteria stated above. The subset of vectors that "passed" the criteria were then used to plot a CCDF and compared to the CCDF plotted from all of the vectors for the base-case scenario unconditionally. The screening procedure is described below:

Substantially complete containment - Vectors with engineered barrier lifetime less than a specified time were screened out. For the sake of this demonstration, we chose only a single representative cutoff time of 500 years.

Release rate limitation - The release rate model in NEFTRAN accounts only for the congruent release of radionuclides contained in the uranium dioxide fuel. The maximum rate is controlled by the dissolution rate of the matrix. For this demonstration, we assumed that the release rate was equivalent to the dissolution rate of the matrix. Releases of some of the radionuclides might actually be smaller than the congruent dissolution rate because they are solubility limited, so the screening criterion might be slightly overrestrictive. The dissolution rate calculated in NEFTRAN is a function of uranium solubility, infiltration and water contact fraction. We should note for this demonstration that the assumptions used do not correspond precisely to the rule. Specifically, the rule states a limit of "one part in 100,000 per year of the inventory of that radionuclide present at 1,000 years", with a limitation on those radionuclides that might have decayed to very low levels at 1000 years. The present demonstration is therefore only an approximate comparison to the limitations of this subsystem requirement.

Groundwater travel time limitation - The model is based on the assumption that transport occurs in four separate pathways, columns A, B, C and D, partly in order to simulate the spatial variability inherent in the Yucca Mountain repository. Clearly, column D is both the shortest pathway and the one most likely to saturate, with correspondingly faster flow and lower retardation. Therefore we take "groundwater travel time along the fastest pathway of likely radionuclide travel" as the mean travel time along column D. In this demonstration, groundwater travel time is defined as the average time for plug flow through the column and is a function of infiltration rate, porosity, saturated hydraulic conductivity and correlation length.

Figure 9.5.6 shows the conditional CCDF for the base case scenario for unrestricted vectors, and vectors limited by either waste package lifetime release rate or groundwater travel time. It assumes no relationship between waste package lifetime and engineered barrier system release rate. For the present case, all 500 vectors had release rates less than 10^{-5}/yr, so that CCDF curve is coincident with the unrestricted curve. The CCDF is shifted toward lower releases for an engineered barrier lifetime of 500 years or greater, but only for the low-probability, high-impact releases.

The most dramatic effect is for the screening on the basis of groundwater travel times. All of the high-impact release were essentially eliminated when travel times shorter than 1000 years were eliminated from the CCDF. The explanation for this effect is that flow along column D is controlled by fractures for infiltration rates higher than the saturated hydraulic conductivity. Fracture flow is both faster and leads to conditions of lower radionuclide retardation. Eliminating the cases leading to saturation allows only releases through the rock matrix under unsaturated conditions, with commensurately greater retardation.

9.5.6.2 Average Contributions by Radionuclide

Table 9.5.4 illustrates the average contribution by radionuclide for the unrestricted releases and the releases complying with the NRC performance criteria. All cases except the one restricted by groundwater travel time show the main contributions coming from isotopes Pu-239 and Pu-240, which would be expected to be retarded in the matrix and greatly attenuated. For the releases restricted by the 1000 year groundwater travel time however, the main contributors are the radionuclides C-14 and I-129, which are unretarded and can therefore move relatively quickly through the matrix.

Table 9.5.4 - Fractional Contribution by radionuclide to EPA Release Ratio for Unrestricted Vectors and those Restricted by NRC Performance Criteria

Radionuclide	Unrestricted vectors	Restricted to 500 yr W.P. Lifetime	Restricted to 1000 yr. GWTT
Pu-240	0.41	0.40	0
Pu-239	0.39	0.37	0
C-14	0.094	0.13	0.94
Am-241	0.077	0.062	0
Am-243	0.014	0.014	0
I-129	0.005	0.007	0.05

9.5.6.3 Ad Hoc Sensitivities to NRC Criteria

We plotted the results of the 500 runs versus the values of the individual NRC criteria of groundwater travel time, waste package lifetime and release rate from the engineered barrier. The results, shown in Figures 9.5.7, 9.5.8, and 9.5.9 all demonstrate that imposing the NRC criteria would have a favorable impact on the total releases to the accessible environment. For the scenarios considered, imposing the 1000 year groundwater travel time limitation virtually eliminates any non-compliance with the EPA containment requirement. None of the vectors yielded release rates from the engineered barrier that exceeded 10^{-5}/yr, but the EPA release increases with increasing engineered barrier release. There was also a noticeable decrease in EPA release with increasing engineered barrier lifetime.

Table 9.5.1
Steps to Perform Uncertainty and Sensitivity Analysis

- o Specify Maximum-Minimum Ranges of Probabilities
- o Specify Correlation Matrix

2. Run Latin Hypercube Sampling Code

3. Run Source Term and Flow and Transport Models

4. Statistical Analysis

   Fitting Distributions
   Regression Analysis
   Graphical Display and Analysis

Table 9.5.2
Regression of Liquid Pathway Cumulative Releases
(Raw data correlations)

Variable	Base Case 10,000 yrs	Base Case 100,000 yrs	Pluvial 10,000 yrs
W.P. LIFETIME	-.045	-.049	-
SOLUBILITY UO_2	0.09	0.13	0.32
INFILTRATION	0.1	0.31	0.23
CONTACT FRACTION	-	0.18	0.44
MEAN LOG K_S TSW	-	-.11	-
MEAN LOG K_S CHNZ	-.14	-.22	-.28
RD CM	-	-	-.2
RD PU	-	-0.23	-.22
RD RA	-	-	0.18
SOL. CM	-	-	0.17
SOL. PU	-	-	-.27
CORR. LENGTH	0.11	-	-

ADDITIONAL REFERENCE

IMAN, R, W.J. CONNOVER, J.E. CAMPBELL, "RISK METHODOLOGY FOR GEOLOGIC DISPOSAL OF RADIOACTIVE WASTE: SMALL SAMPLE SENSITIVITY ANALYSIS TECHNIQUES FOR COMPUTER MODELS, WITH AN APPLICATION TO RISK ASSESSMENT", NUREG/CR-1397, U.S. NUCLEAR REGULATORY COMMISSION, MARCH, 1980.

Table 9.5.3 - Average Importance of Radionuclides to EPA Release Limits
(Only if greater than 0.01 contribution, bold if greater than 0.05)

Radionuclide Time Infilt.	Base Case 10^4 yr <5.14 mm	Base Case 10^4 yr <2.0 mm	Base Case 10^4 yr <1.0 mm	Base Case 10^5 yr <5.14 mm	Base Case 10^5 yr <2.0 mm	Base Case 10^5 yr <1.0 mm	Pluvial Case 10^4 yr
Am-241	0.077	0.061	0.069		0.014	0.017	0.069
Am-243	0.014	0.016	0.016			0.013	
C-14	0.094	0.013		0.015	0.031	0.061	
I-129	0.05				0.037	0.229	
Np-237	0.01			0.015	0.014		
Pu-238	0.010						
Pu-239	0.39	0.438	0.438	0.726	0.589	0.183	0.443
Pu-240	0.41	0.463	0.465	0.069	0.181	0.442	0.459
Pu-241	0.02						
Pu-242				0.024	0.011		
Tc-99				0.016	0.022	0.013	
Th-230					0.011	0.011	
U-233				0.012			
U-234	0.02			0.048	0.034	0.010	
U-236				0.026	0.018		
U-238				0.024	0.018		

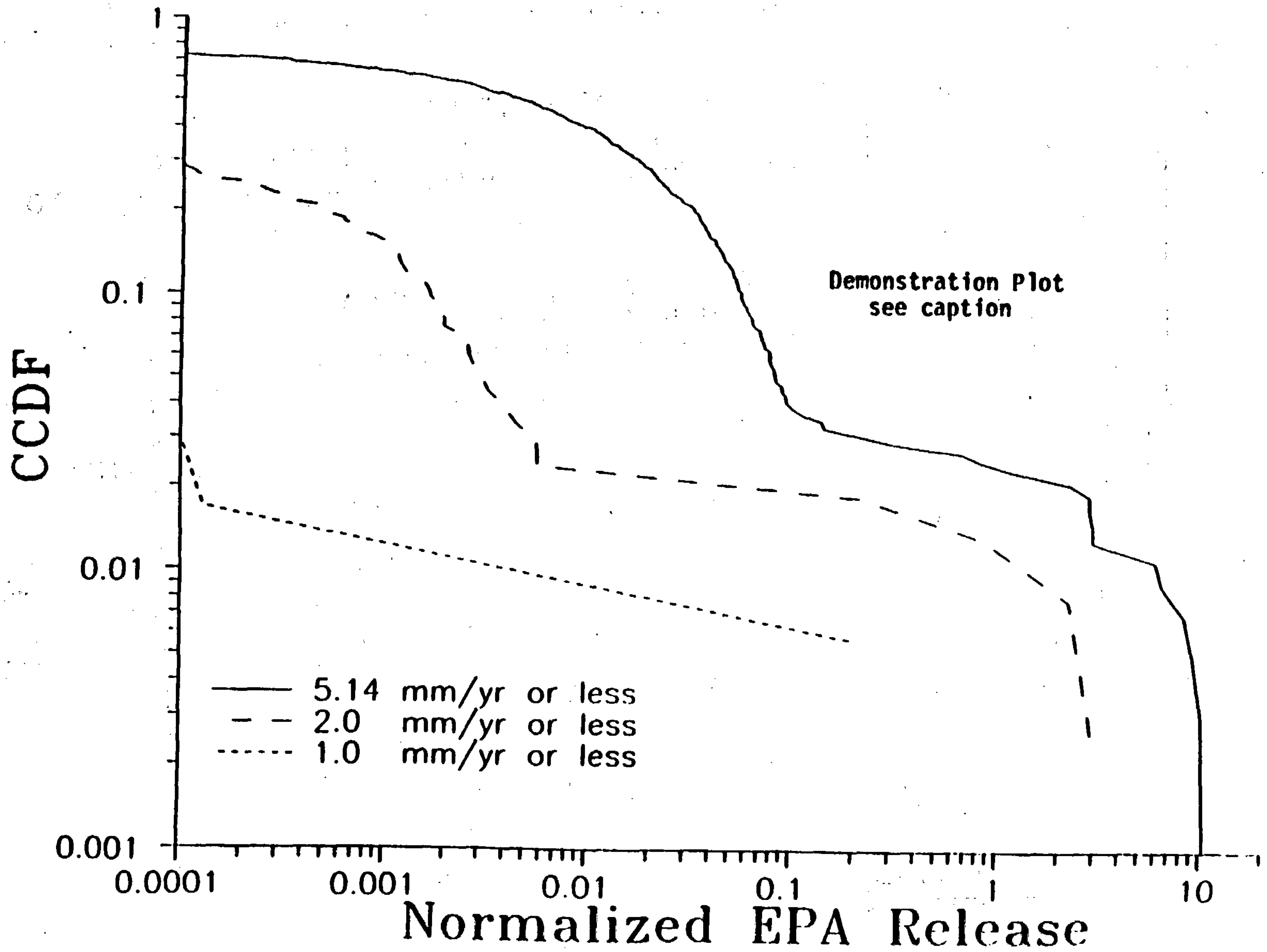


Figure 9.5.1 CCDF for Base Case; 500 Vectors, 10,000 Years. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

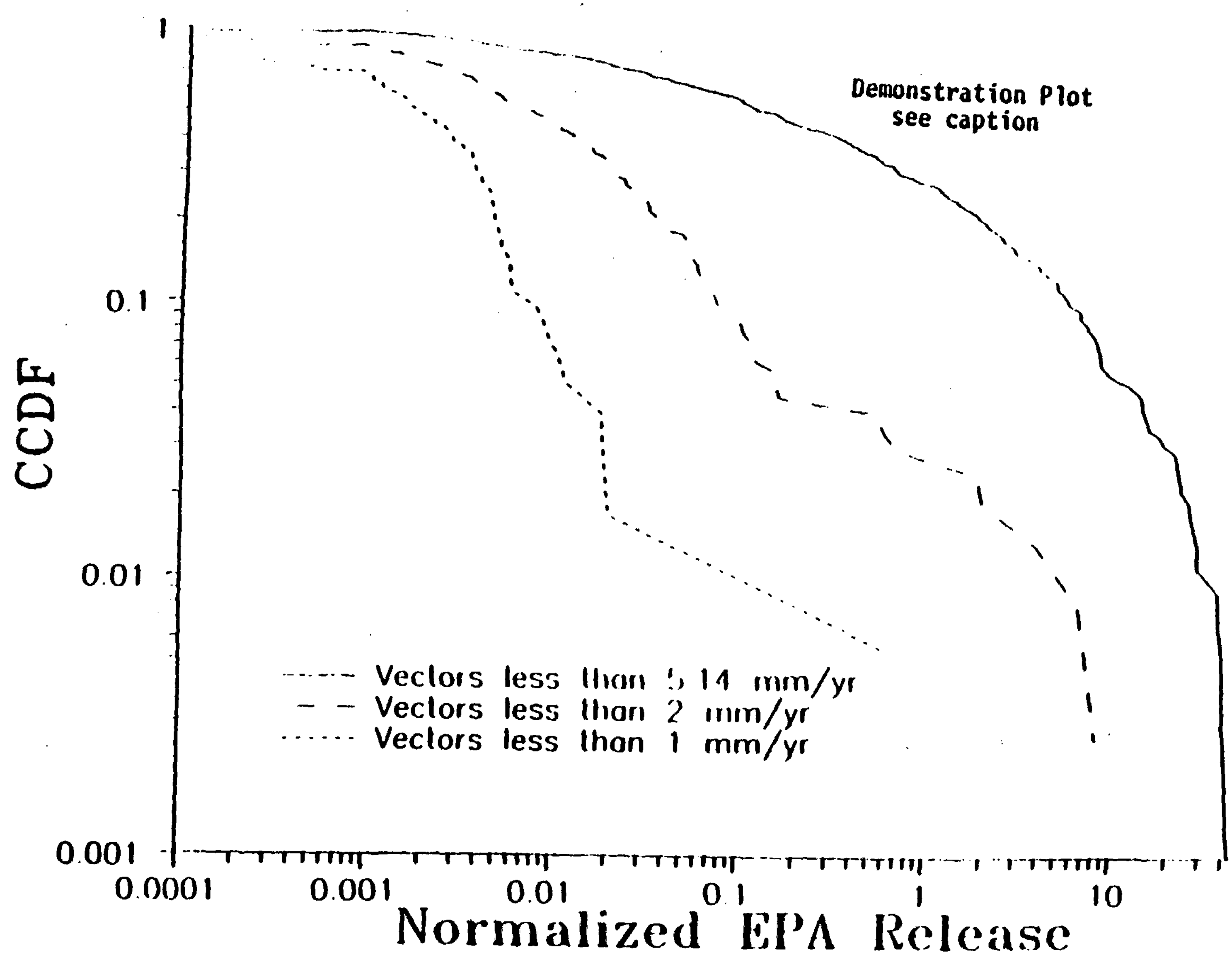


Figure 9.5.2 CCDF for 100,000 Years, 500 Vectors. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assu--tions and sparse data.

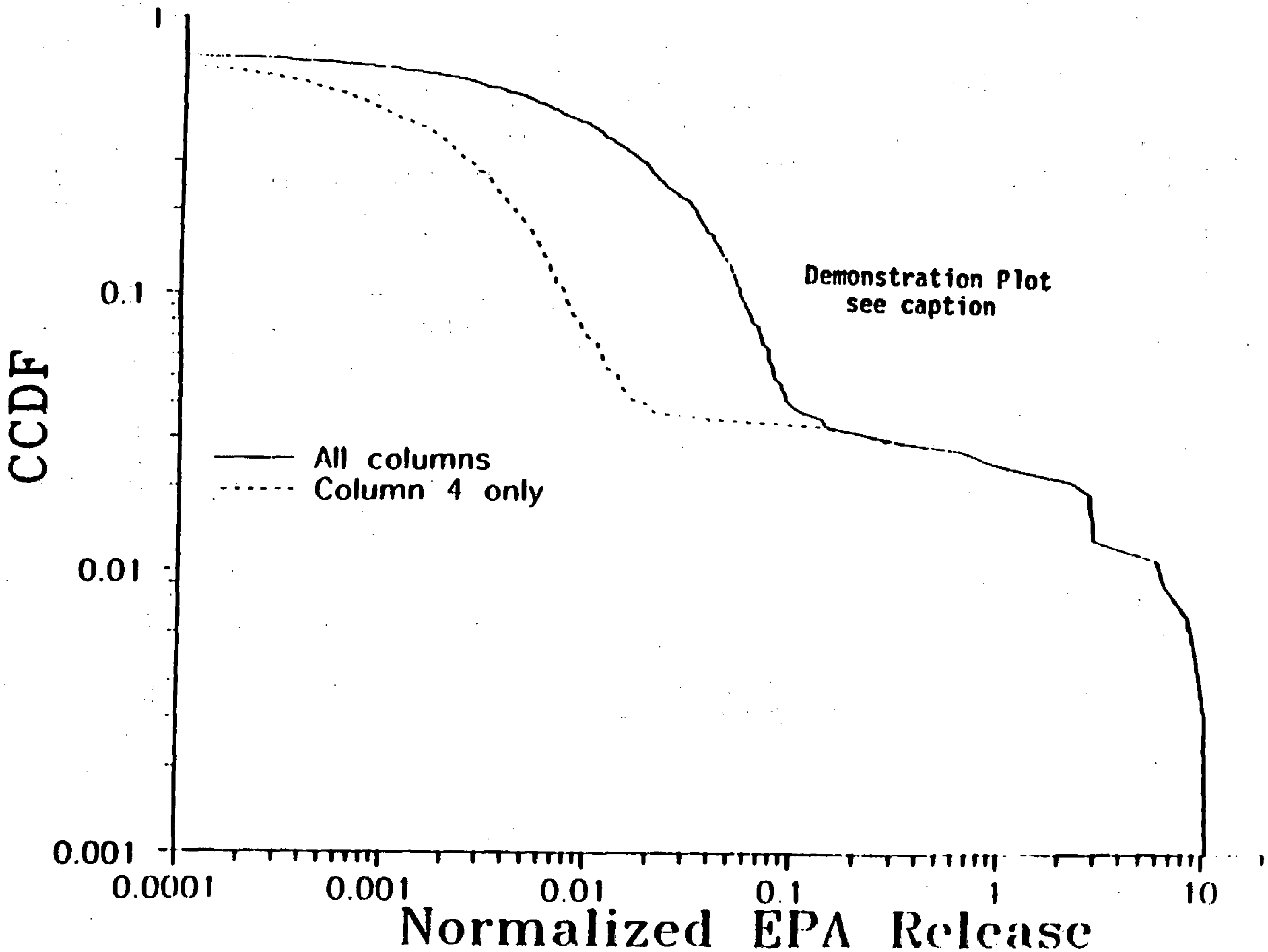


Figure 9.5.3 CCDF for Base Case; 500 Vectors, 10,000 Years. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

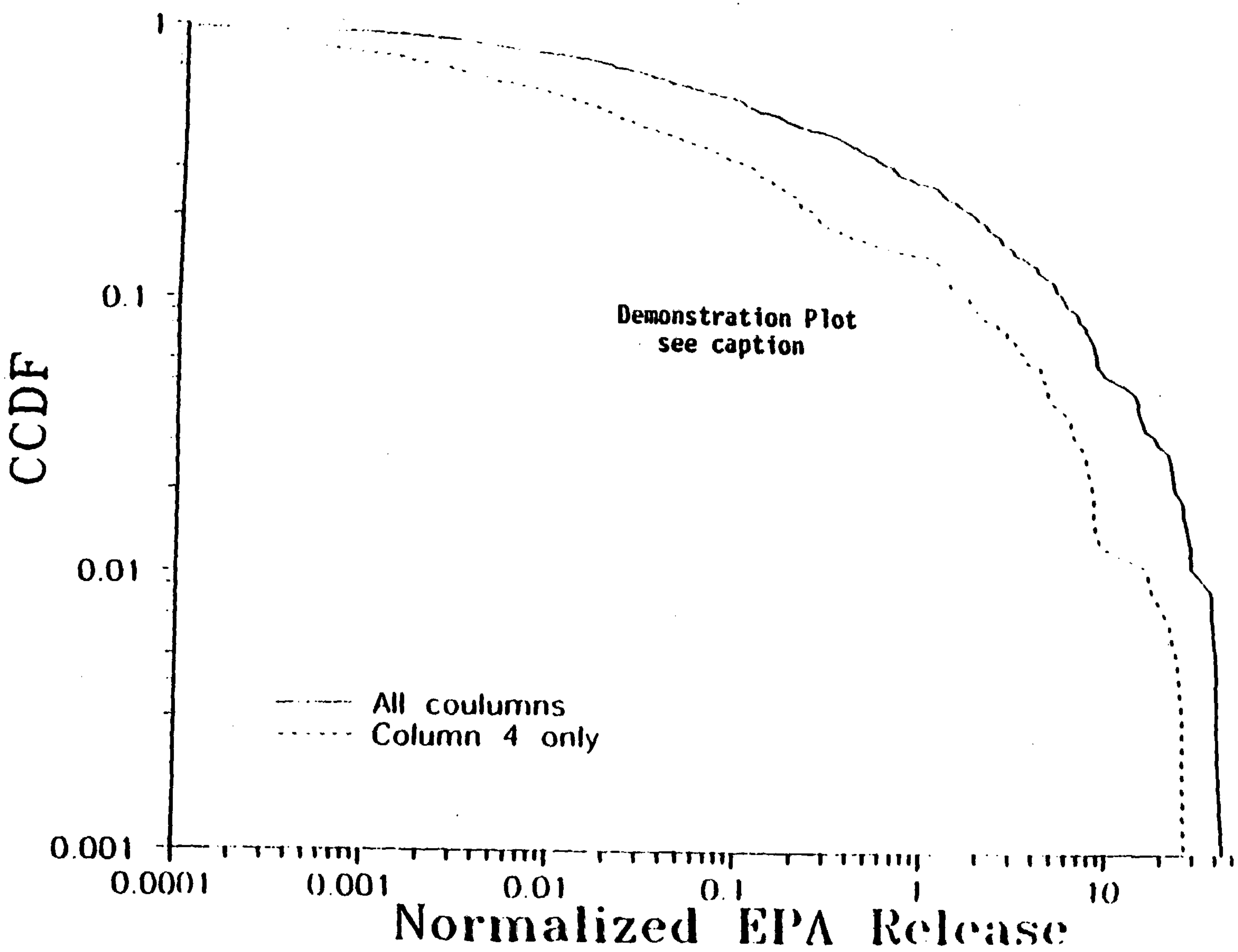


Figure 9.5.4 CCDF for 100,000 Years, 500 Vectors. Compare column 4 to all. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse data

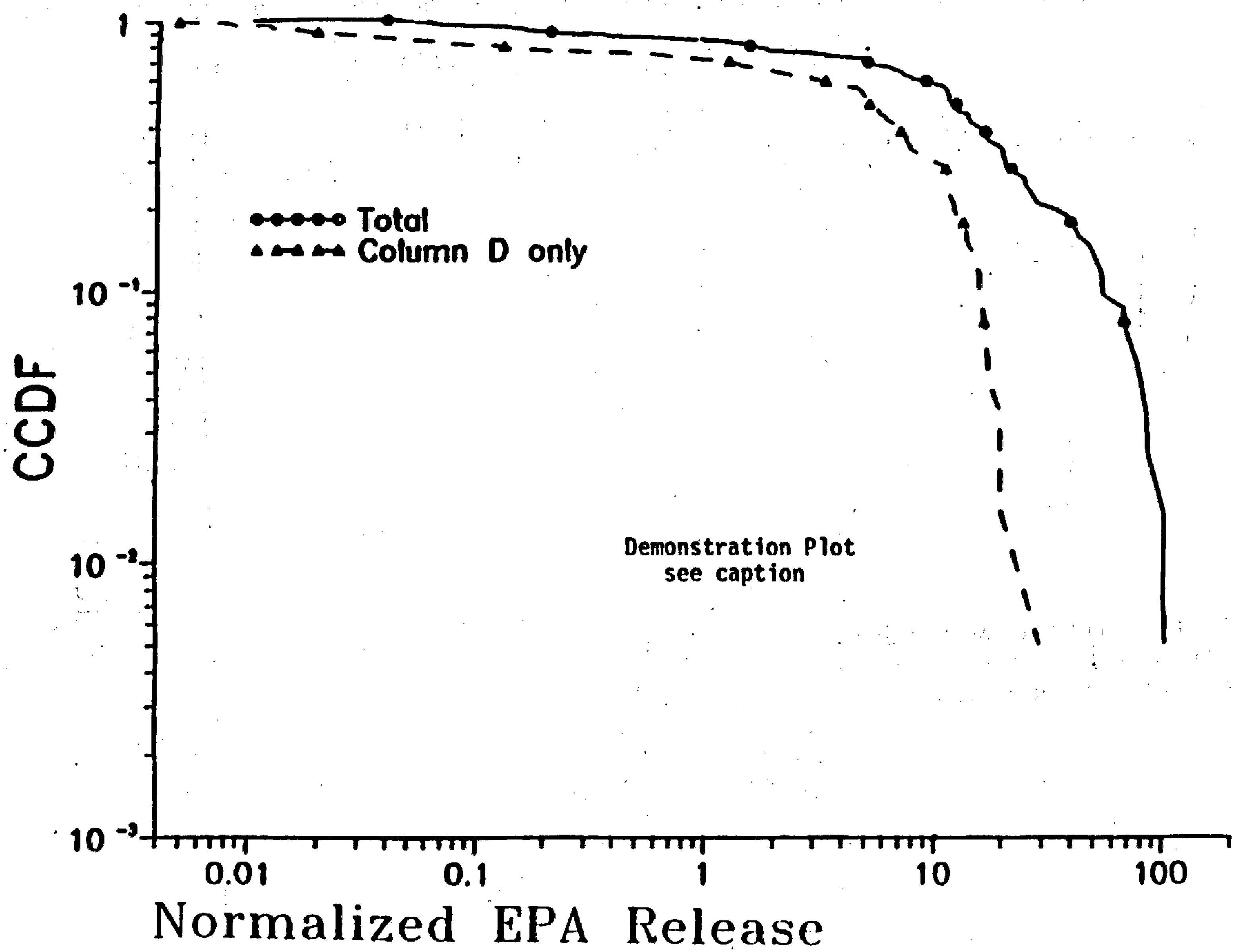


Figure 9.5.5 CCDF for Pluvial Scenario; 98 Vectors Only. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

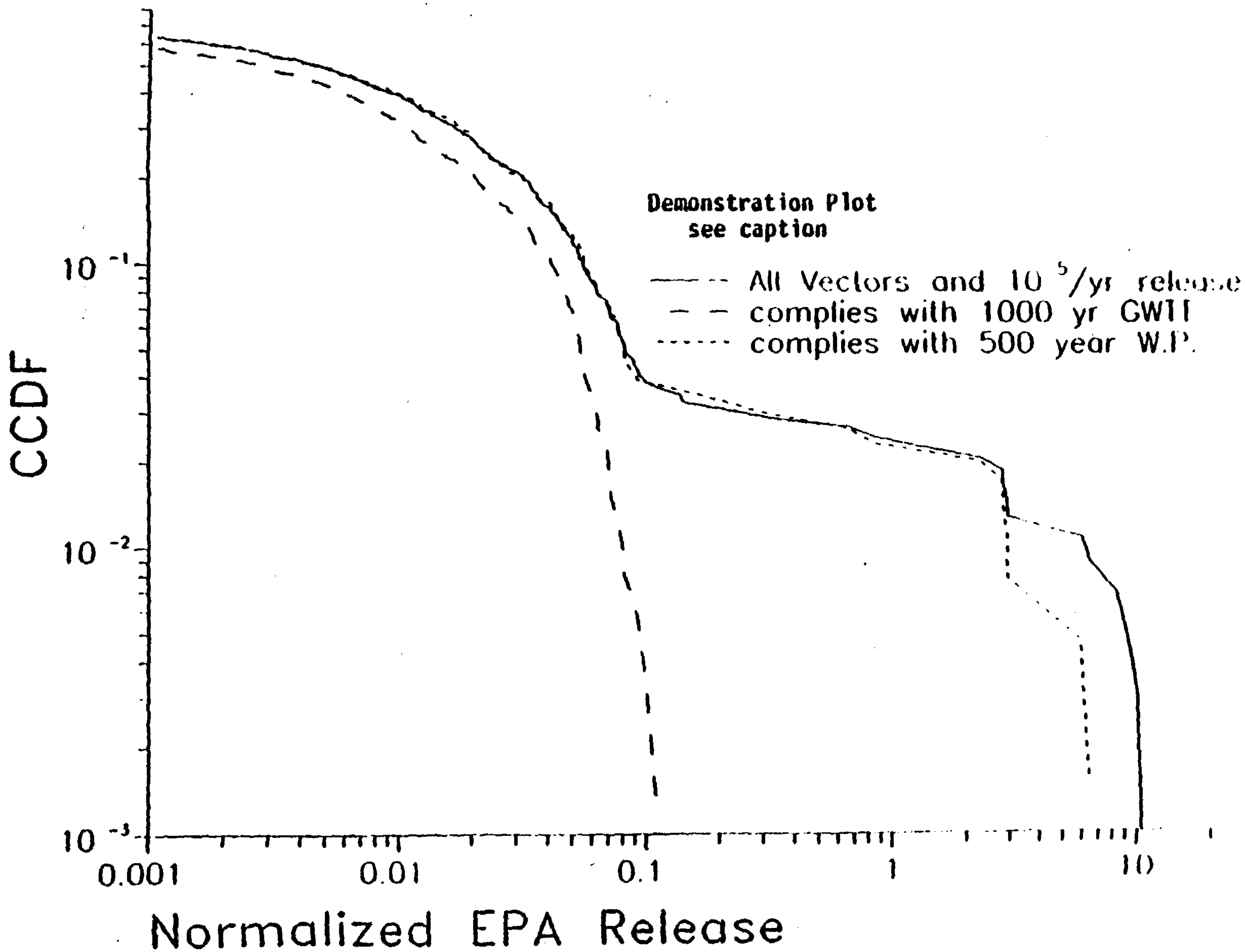


Figure 9.5.6 Base Case Conditional CCDF; 10,000 Years. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of ·y simplifying assumptions and sparse data.

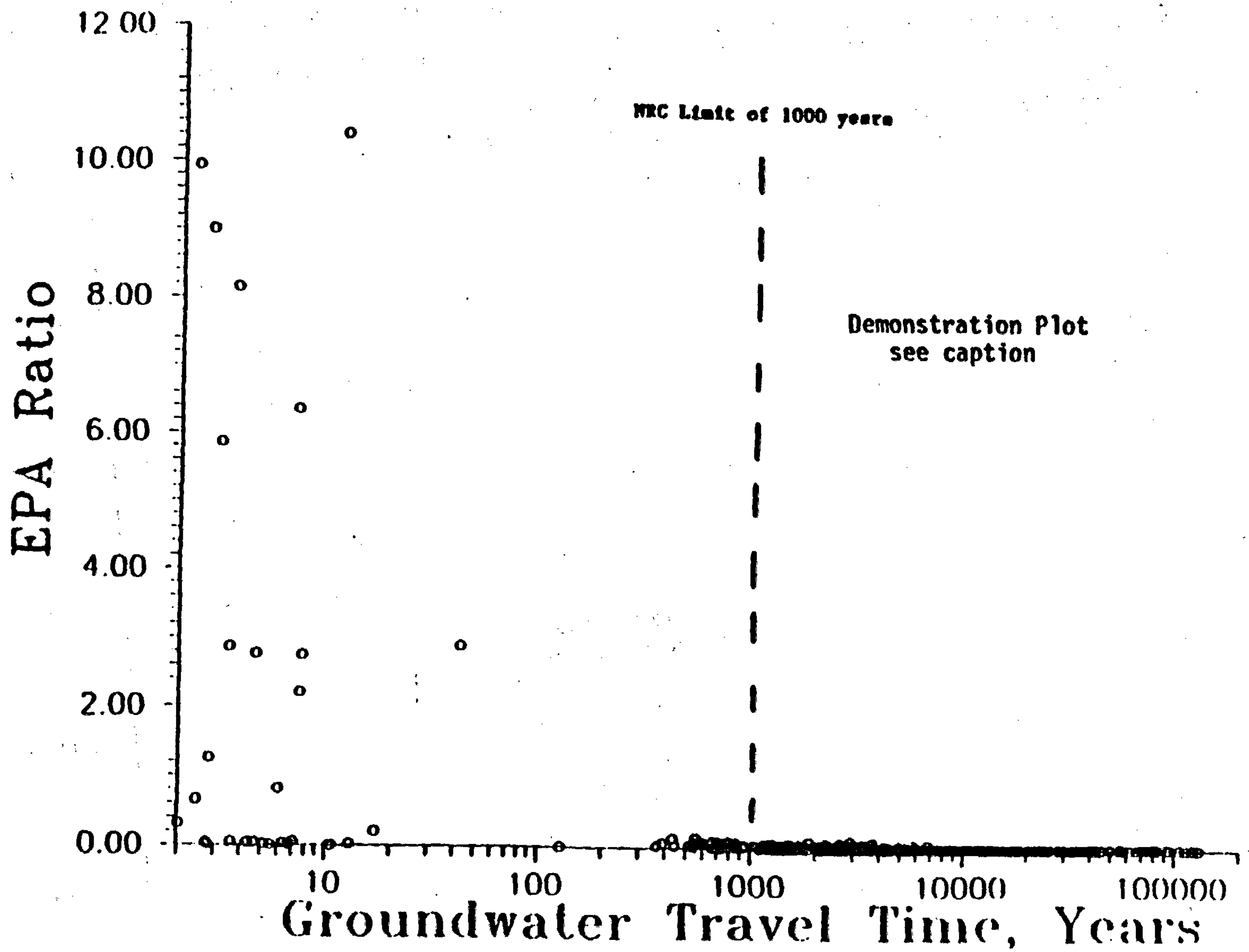


Figure 9.5.7 Base Case Liquid Pathway Scenario; 10,000 Years. Effects of Groundwater Travel Time on EPA Release. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

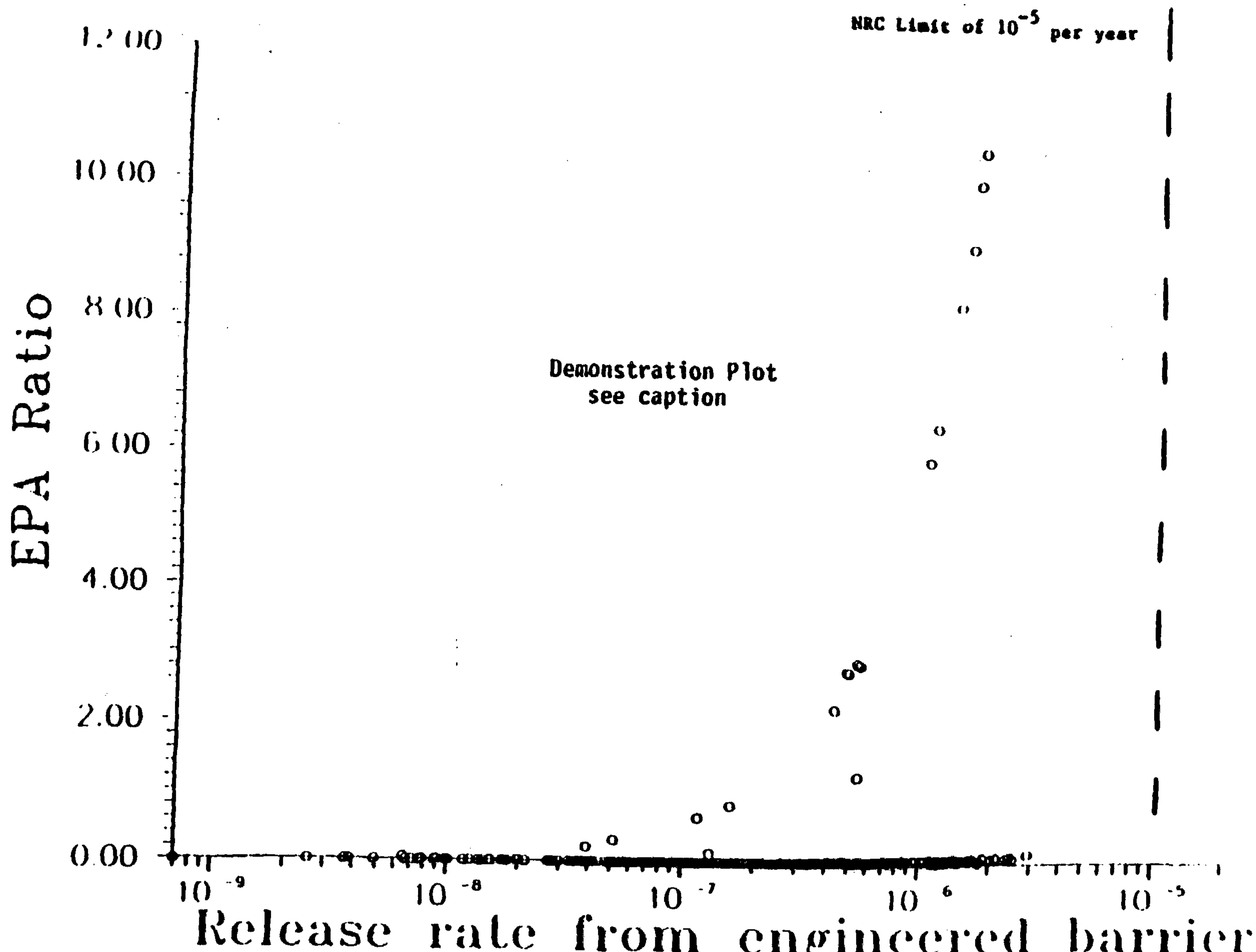


Figure 9.5.8 Base Case Liquid Pathway Scenario; 10,000 Years. Effects of Release Rate from Engineered Barrier. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like t' demonstration, is limited by the use of many simplifying assumptions and sparse data.

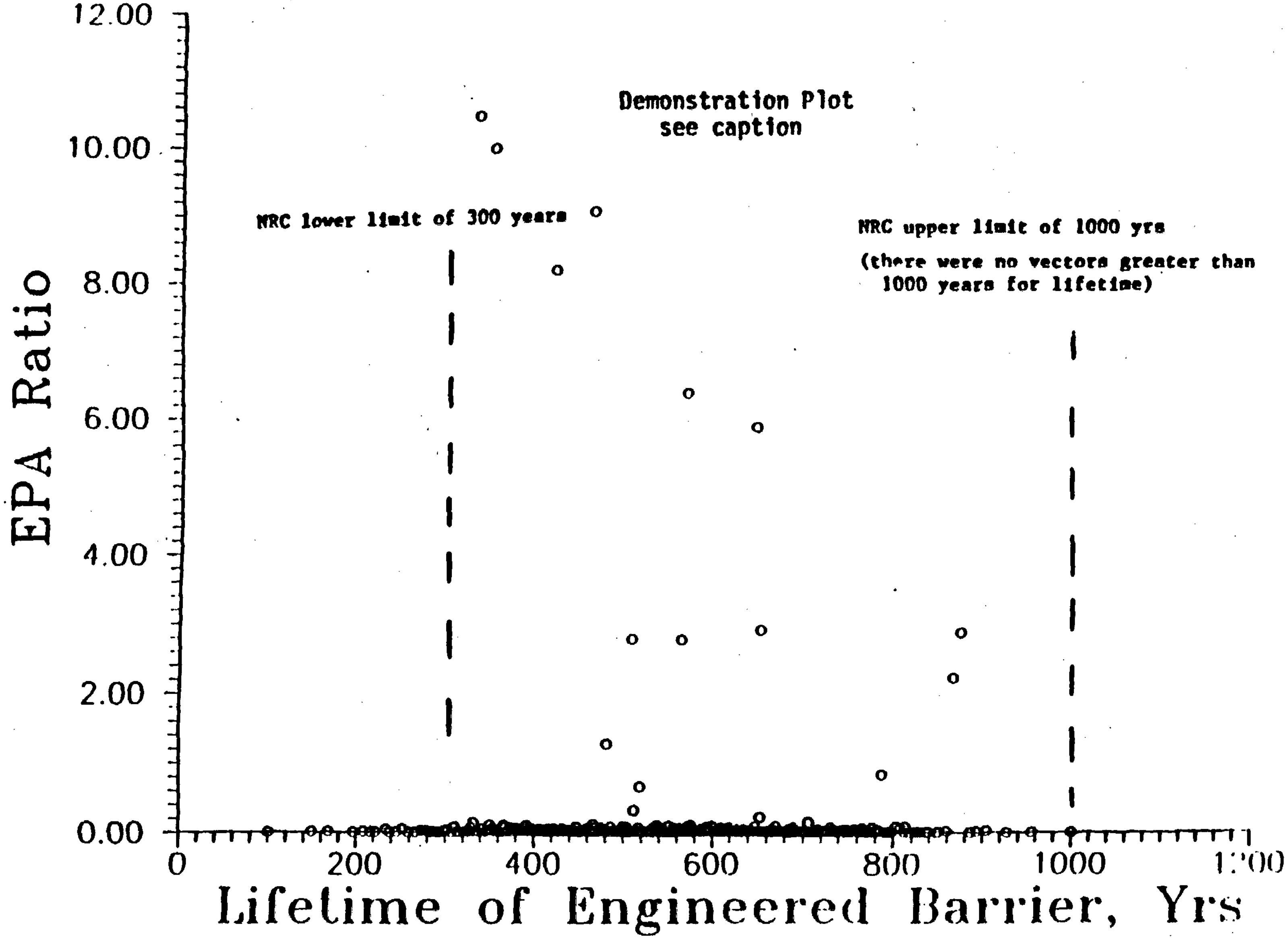


Figure 9.5.9 Base Case Liquid Pathway Scenario; 10,000 Yrs. Effects of Engineered Barrier Lifetime. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

9.6 Total CCDF

9.6.1 Introduction

The results presented here can only be considered as a demonstration of a performance assessment capability and should not be taken as representative of the performance of a repository at Yucca Mountain, Nevada. Among the most important limitations of the study are:

1) the lack of sufficient site data,
2) the large uncertainties in the data now in use,
3) the use of only four scenarios to characterize future states at the site,
4) uncertainties in the site conceptual model, and
5) uncertainties in modeling the physicochemical processes leading to radionuclide release and migration in the geosphere.

For this demonstration, the staff considered four scenario classes:

1) an undisturbed or base case,
2) pluvial conditions,
3) drilling under undisturbed conditions, and
4) drilling under pluvial conditions.

As shown in Figure 9.6.1, these particular scenarios arise from the possible combinations of two fundamental events: a pluvial period (or not) and drilling at the site (or not). Probabilities for each of the scenario classes are determined by multiplying the probabilities of their independent constituent events. The likelihood of each event is based upon staff judgment in the case of the pluvial/nonpluvial events, and 40 CFR Part 191 Appendix B for the human intrusion events. 40 CFR 191 assumes a likelihood of drilling at the site as a set number of boreholes per unit area over 10,000 years based upon the geologic formations in which the repository is located.

There are two important points to note in Figure 9.6.1. First, the case in which conditions at the repository over the next 10,000 years remain as they are today appears highly unlikely. Secondly, the two human intrusion scenario classes have probabilities orders of magnitude greater than the base case and pluvial scenarios which do not incorporate the possibility of drilling events. This difference is due to the high probability of drilling as opposed to not drilling as shown in the figure.

The consequences of each scenario and of all scenarios combined can be expressed in terms of normalized cumulative releases of radionuclides to the environment over a specified period of time. These results, displayed as a curve of consequences versus the probability that such consequences will be exceeded (i.e. a CCDF), can in turn be compared with the curve of the EPA containment requirements in 40 CFR Part 191 (Figure 9.6.2a). The EPA standard requires normalized cumulative releases to the environment of (1) 1.0 not to exceed a probability of 0.1, and (2) 10.0 not to exceed a likelihood of 0.001.

Compliance with the containment requirements cannot be determined solely on the basis of the strict numerical results of a performance assessment. As recognized in 40 CFR Part 191, substantial uncertainties are inherant in projecting future disposal system performance, and thus the bias towards this uncertainty in component performance must also be taken into account. For example, in Figure 9.6.2b, a portion of the empirical CCDF lies above the EPA containment requirement and is therefore labeled a "possible violation". If the bias in component performance was consistently towards more pessimistic performance, then the results expressed in the CCDF may be too conservative, and thus this portion of the curve may be judged to be not a violation. If on the other hand, component performance was viewed optimistically, the CCDF may well be found to be in violation of the EPA standard. Since definitive proof of future system performance cannot be provided, 40 CFR Part 191 only requires a "reasonable expectation" that compliance will be achieved.

The partial CCDFs for each of the scenario classes are shown in Figures 9.6.3 through 9.6.6. These curves differ from the distribution of consequence figures shown earlier in Section 9.5 in that the partial CCDFs incorporate the probabilities of the scenarios themselves. For this reason, the cumulative probability of any single scenario presented here never reaches 1.00, as it will for the total CCDF, which is a composite of all four scenario classes.

9.6.2 Partial CCDF Results

9.6.2.1 The Undisturbed Case

The log-log plot of summed normalized EPA release versus cumulative probability for undisturbed conditions (Figure 9.6.3) shows the characteristic concave downwards shape for a CCDF. As will be the case for each CCDF, the curve intersects the y-axis at the likelihood of the scenario; here the likelihood is equal to 2.3×10^{-7}. For this scenario, EPA ratios of 1.0 and 10.0 have corresponding cumulative probabilities of approximately 4.9×10^{-9} and 4.1×10^{-10}, both of which are well below the EPA critical point likelihoods of 0.1 and 0.001 for these same EPA ratios.

9.6.2.2 Pluvial Conditions

Consequences from the pluvial case (Figure 9.6.4) equal to an EPA ratio of 1.0 have an aggregate probability of 1.9×10^{-8}, while an EPA ratio of 10.0 has a cumulative likelihood of 1.3×10^{-8}. These results combined with an overall scenario probability of 2.0×10^{-8} leave the CCDF for the pluvial case orders of magnitude below the EPA containment requirement.

Note: An inordinate amount of computer time required on the CRAY supercomputer limited the pluvial and drilling under pluvial conditions scenarios to only 98 vectors. Furthermore, because a sample of 200 input vectors was planned and generated with the LHS sampling routine to represent this pathway and scenario class, a subset of 98 vectors might have led to spurious correlations and an inadequate representation of the partial CCDFs.

9.6.2.3 Drilling Under Undisturbed Conditions

The CCDF for drilling under undisturbed conditions (Figure 9.6.5) shows a slight step, which is attributable to consequences from the drilling, in the low consequence/high probability end of the curve. The rest of the CCDF curve is dominated by releases via the liquid pathway.

More importantly though, with the addition of drilling events to the base case, the overall probability of the scenario is increased to 0.9. Thus, for this scenario, although the sum probability of an EPA ratio of 1.0 is below the EPA standard at 0.022, the EPA ratio/cumulative probability pair of 10.0 and 0.0036 falls above the standard, which appears as a step function in this and the following figures.

9.6.2.4 Drilling Under Pluvial Conditions

The shape of the partial CCDF for drilling under pluvial conditions (Figure 9.6.6) does not exhibit the effects of the drilling. This is because the consequences due to drilling are in the range of .0001, and are therefore negligible when factored into overall scenario consequences of .01 to 100.

With the overall likelihood of drilling under pluvial conditions equal to 0.1, the 1.0/0.082 consequence/aggregate probability pair falls just below the EPA containment requirement, while an EPA ratio of 10.0 for this scenario has a cumulative probability of approximately 0.06, which lies above the standard.

9.6.3 Results for the Total CCDF

Figure 9.6.7 demonstrates how each of the four individual scenarios contributes to the total CCDF. It is readily apparent that releases from the two human intrusion scenario classes dominate the CCDF under the given probabilities and conditions. Contributions to the total consequences from the undisturbed and pluvial scenarios are negligible, because their respective scenario probabilities are too low.

The total CCDF for the four scenario classes modeled is plotted against the EPA standard in Figure 9.6.8. This comparison shows that for this demonstration, the empirical CCDF lies above the EPA standard at both containment requirement break points, with cumulative probabilities of approximately 0.104 and 0.06 for EPA ratios of 1.0 and 10.0 respectively.

The results of this demonstration should not be taken as representative of the performance of a repository at Yucca Mountain, Nevada. Rather, they should be used to indicate the importance of (1) the assumptions in modeling phenomena, such as fracture/matrix interactions, (2) the data used in the total system modeling, e.g. infiltration rate, and (3) the consistency of the bias, whether pessimistic or optimistic, towards the performance of the various disposal system components.

DETERMINATION OF SCENARIO PROBABILITIES FROM THE PROBABILITIES OF FUNDAMENTAL EVENTS

	$\bar{P}$ 0.9	P 0.1
$\bar{D}$ 2.3×10^{-7}	scenario class # 0 probability $= 2.0 \times 10^{-7}$	scenario class # 1 probability $= 2.3 \times 10^{-8}$
D = 1.0	scenario class # 2 probability = 0.9	scenario class # 3 probability = 0.1

$\bar{P}$ is not pluvial

P is pluvial

$\bar{D}$ is no drilling

D is drilling

scenario class # 0 is no drilling, not pluvial

scenario class # 1 is no drilling, with pluvial

scenario class # 2 is drilling, not pluvial

scenario class # 3 is drilling and pluvial

Note: Probability combinations assume that fundamental events have independent probabilities of occurence; this is not a general restriction.

Figure 9.6.1 Determination of scenario probabilities from probabilities of fundamental events. This figure presents results from an initial demonstration of staff capability to conduct a performance assessment. The figure, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

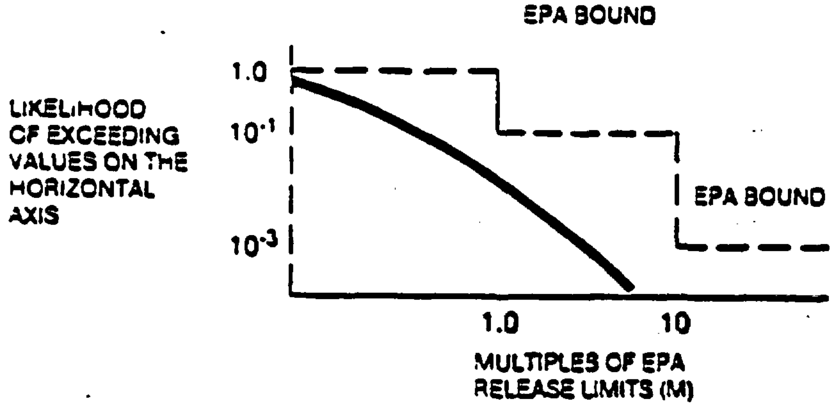


Figure 9.6.2a Graphical representation of hypothetical CCDF with the EPA containment requirements (DOE, 1988).

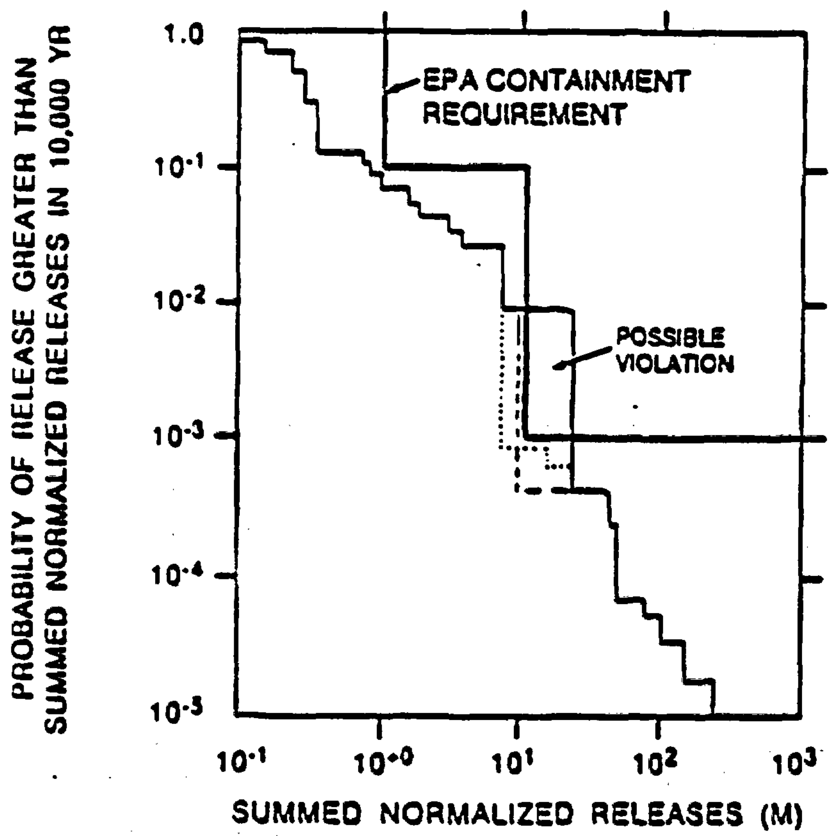


Figure 9.6.2b Plot of an empirical CCDF against the EPA containment requirements (DOE, 1988).

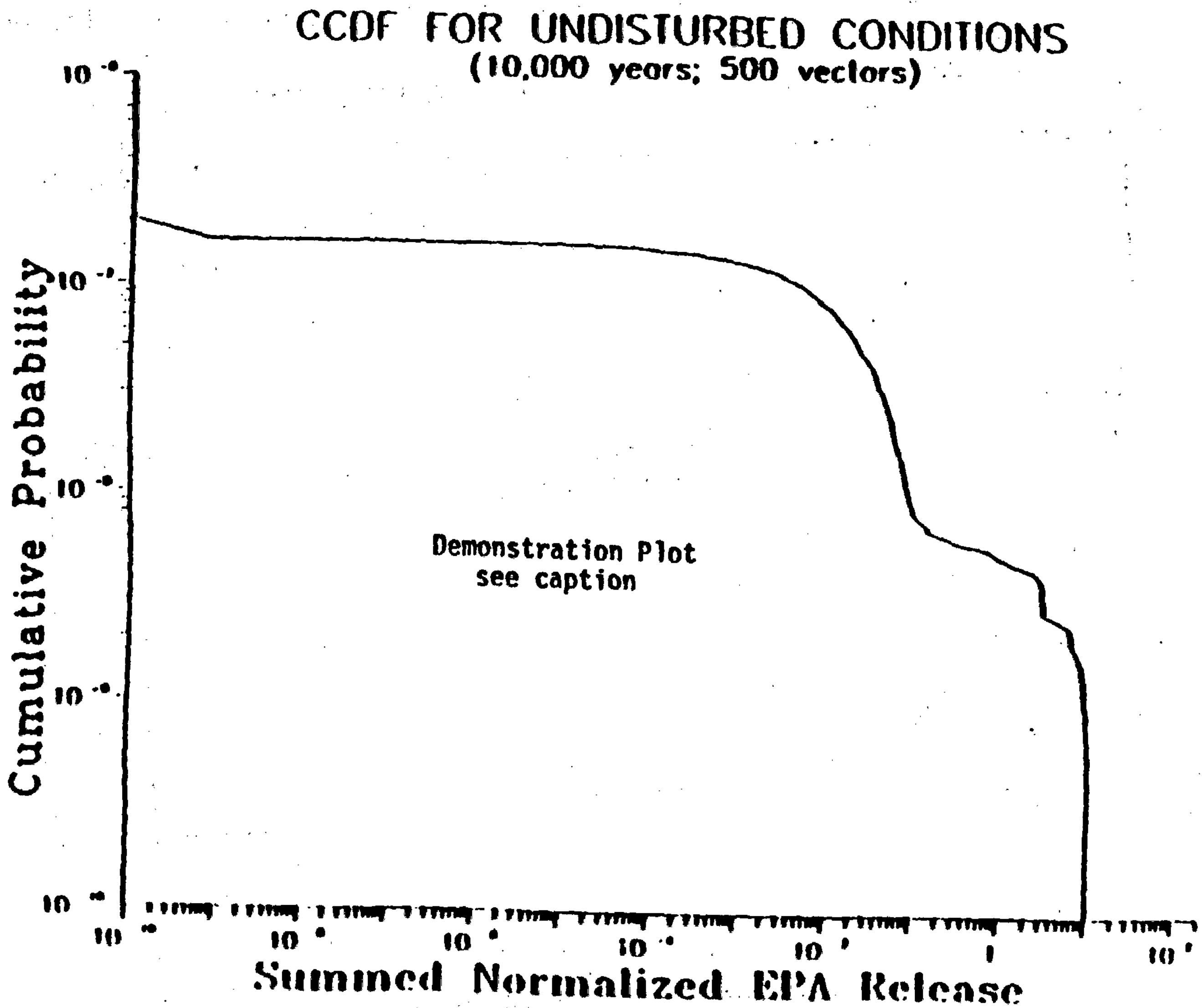


Figure 9.6.3 Partial CCDF for Undisturbed Conditions. Phase 1 of the Iterative Performance Assessment. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

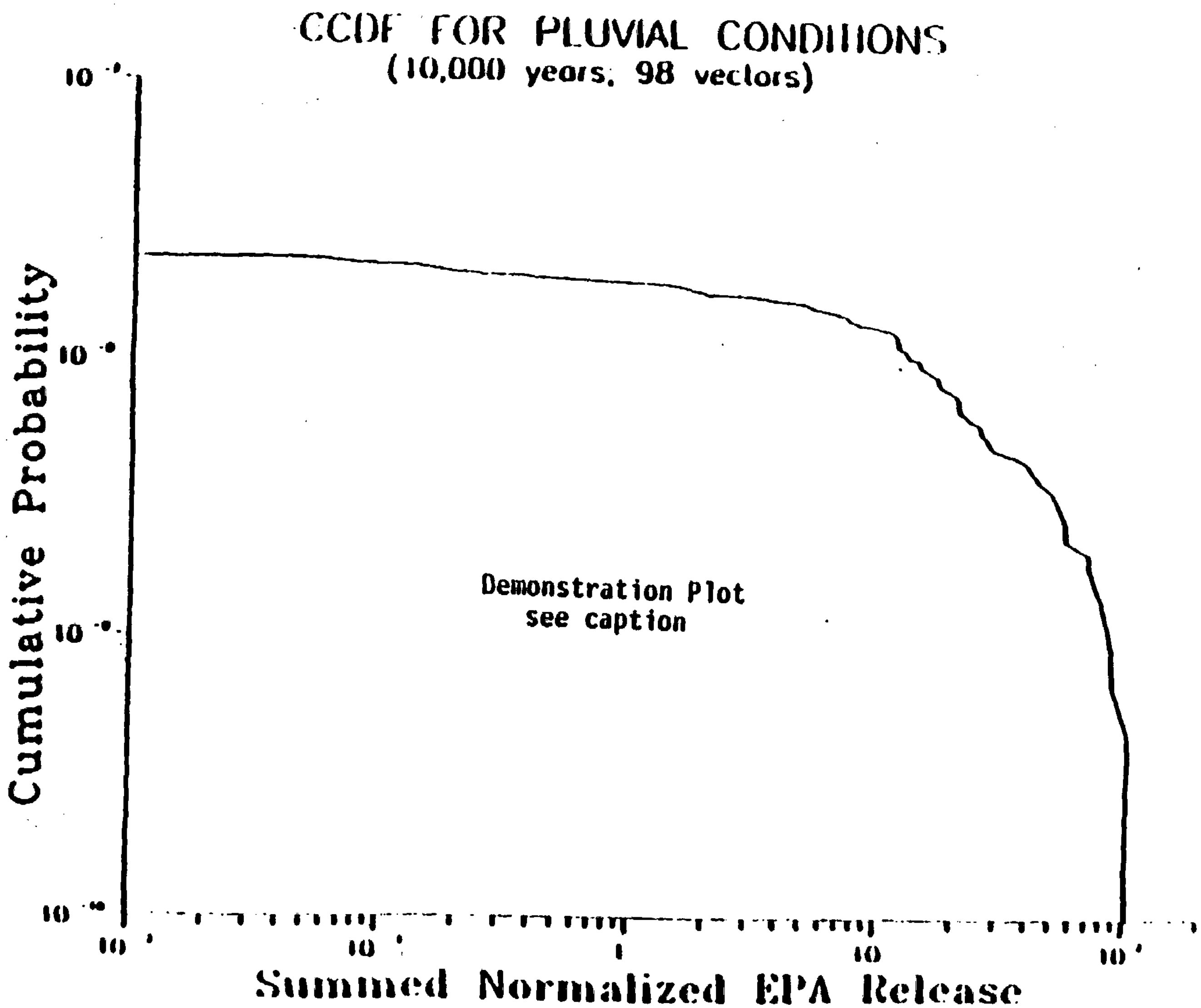


Figure 9.6.4 Partial CCDF for Pluvial Conditions. Phase 1 of the Iterative Performance Assessment. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

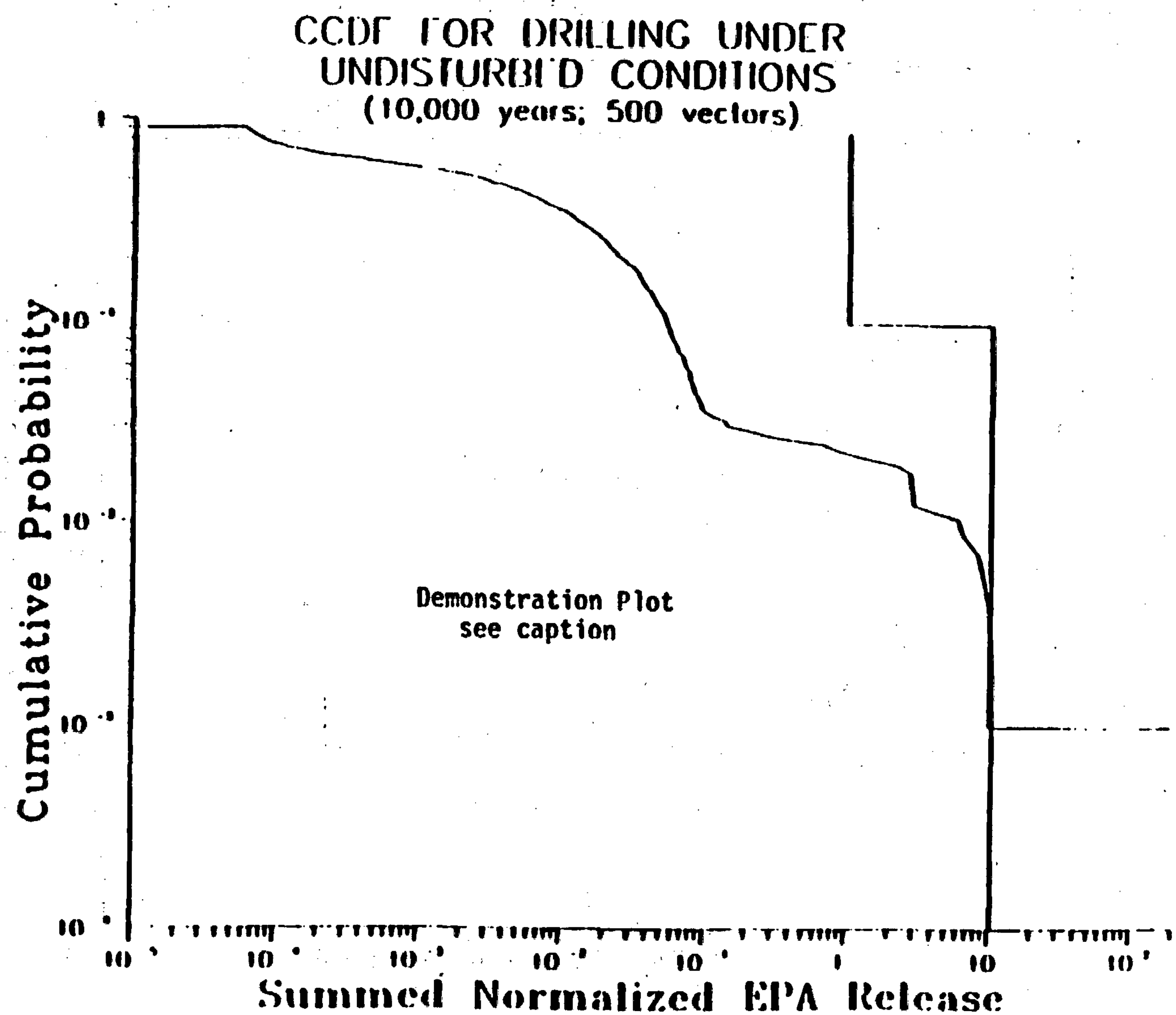


Figure 9.6.5 Partial CCDF for Drilling Under Undisturbed Conditions. Phase 1 of the Iterative Performance Assessment. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

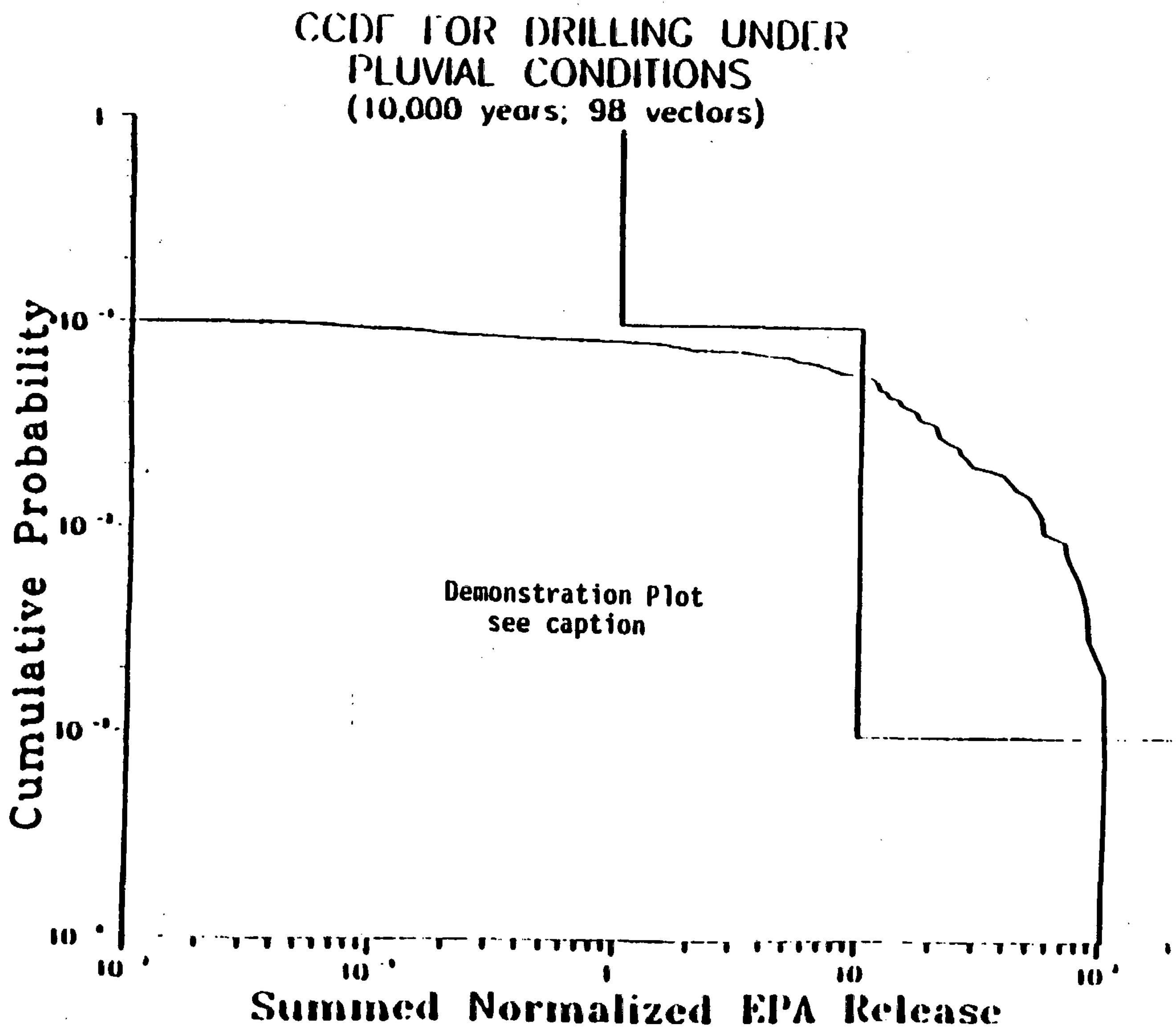


Figure 9.6.6 Partial CCDF for Drilling Under Pluvial Conditions. Phase 1 of the Iterative Performance Assessment. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse `a.

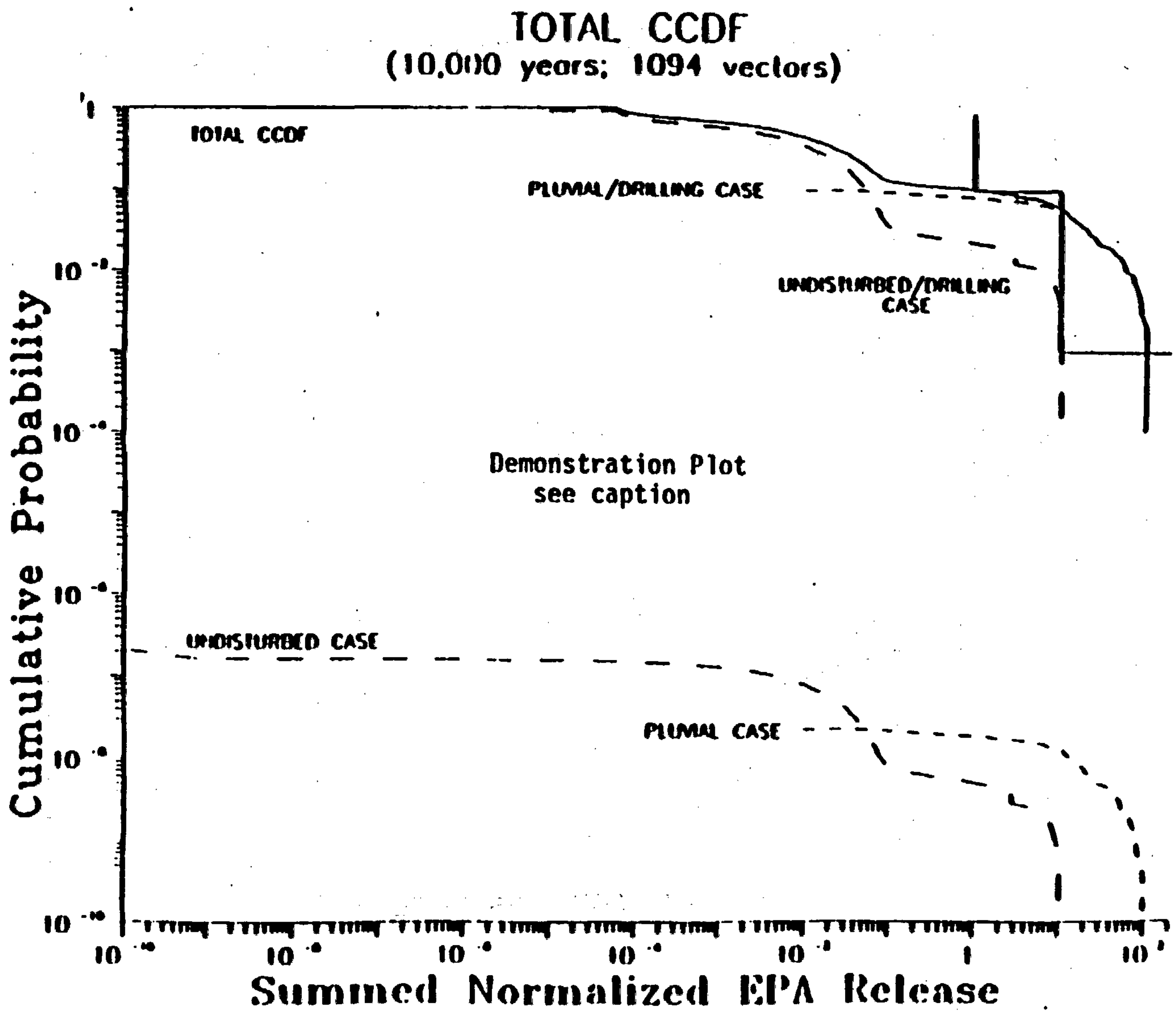


Figure 9.6.7 Composite CCDF curve for the scenario classes considered in Phase 1 of the Iterative Performance Assessment. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

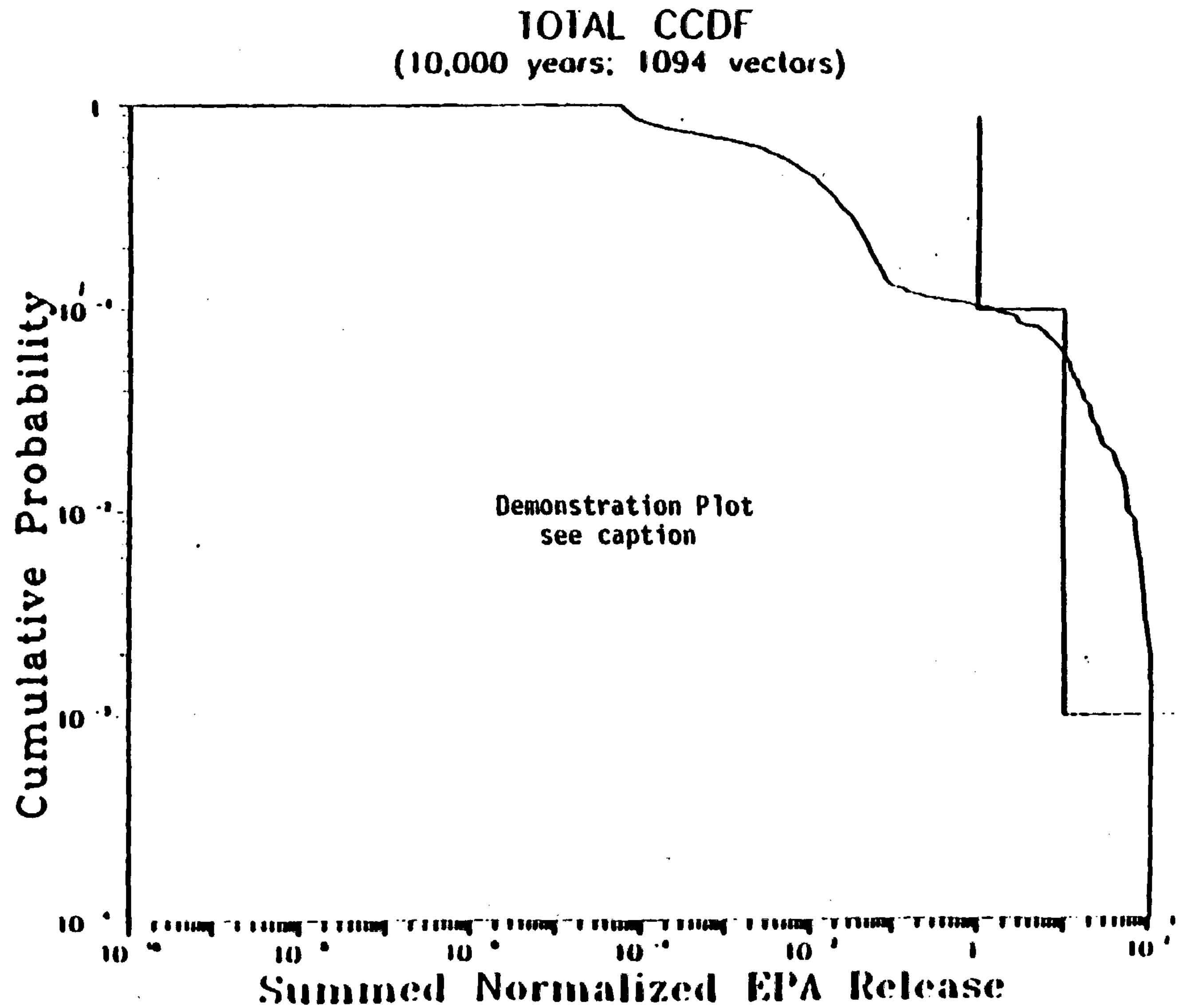


Figure 9.6.8 Total CCDF for Phase 1 of the Iterative Performance Assessment. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the ot many simplifying assumptions and sparse data

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10.0 PRELIMINARY SUGGESTIONS FOR FURTHER WORK

Based on this preliminary analysis and the limitations noted, the staff has some preliminary recommendations regarding the directions for further technical work. These suggestions are based on insights gained during the Phase 1 effort. Although these suggestions derive from this work, they are not necessarily unique to this work, are generally consistent with scientific intuition, and are largely consistent with planning documents such as the DOE SCP. The suggestions relate to this report and are not intended to indicate an evaluation of the DOE program outlined in the SCP. These recommendations have all the limitations inherent in the analyses on which they are based. These suggestions presented are in the spirit of providing some ideas to guide further work and are not intended to be definitive. Some of this suggested work is clearly the responsibility of DOE; other items could be performed by NRC, DOE, or a third party. Most of the recommendations of this type reflect the general lack of data available for executing an analysis of this type. The suggestions for technical improvements can be grouped into three categories:

1. suggestions to improve or extend the modeling used to obtain preliminary estimates of performance;
2. suggestions for refining or for additional auxiliary analyses to help better evaluate the performance estimates obtained;
3. suggestions for refiniements to or additions to the scientific basis, including the methodologies available, for arriving at estimates of repository performance.

Improvements and Extensions to Modeling

The following are recommended improvements to modeling of performance. These are considered to be ideas for further work that could improve the current preliminary assessment and might be suitable first steps in generally upgrading the methodology.

General

1. Add the capability for modeling additional scenario classes.

   In this Phase 1 demonstration the staff made use of a readily available computer code, NEFTRAN, to model the release of radionuclides by the groundwater pathway. This code was able to treat both the "base case" for current climate conditions and the "pluvial case" for a wetter climate. A simple model and computer code were developed to treat the release of radionuclides directly to the environment through exploratory drilling. However, there did not appear to be any readily available models and computer codes to estimate consequences from volcanism, faulting, subsidence, uplift, and other tectonic events and processes and other types of scenarios. The consequences from these scenarios do not appear to be readily treatable by extensions of models currently in use (such as the way the pluvial case was treated by extending the base case treatment). Therefore, the capability for modeling the consequences of additional scenario classes must be added to the methodology, if such scenario classes are to be treated explicitly in the CCDF.

2. Test the system code using the consequence codes as subroutines, instead of generating data sets external to the system code.

   In the Phase 1 effort the consequence modules were run separately from the system code and the resulting files were manipulated to generate the total system CCDF. An attempt to run the consequence modules as subroutines of the system code was not made. Such an attempt would indicate whether such an approach may be practicable and would provide an important insight into the direction for further development of the NRC independent performance assessment capability.

3. Acquire, test, and evaluate codes developed by Sandia National Laboratories (SNL) for a repository in the unsaturated zone.

   While this Phase 1 effort was being performed by the NRC staff, Sandia National Laboratories, under contract to RES, has been developing an extension of the SNL performance assessment methodology to treat a HLW repository in partially saturated tuff. At the beginning of this effort it was recognized that the SNL tuff methodology would not be available for use in the Phase 1 effort. In addition, the tuff methodology will incorporate the ability to treat transient conditions by a multiple steady-state approximation. Because this methodology was developed specifically for the NRC waste management program, it can potentially make great improvements to the accuracy and adequacy of the performance assessment capability. However, by acquiring and evaluating this methodology, the NRC staff can determine what improvements or additions, if any, may be needed.

4. Evaluate additional codes, which could not be acquired and evaluated during this short-time effort, to determine whether existing codes can meet the NRC modeling needs or whether additional code development is needed.

   Several computer codes, which appeared to be promising in terms of providing missing parts of the analysis or which might offer improved treatment of certain aspects of modeling, were not available for the Phase 1 demonstration. Several of these codes should be evaluated in subsequent iterations to determine how relevant and useful these codes are for the NRC iterative performance assessments. Some of the codes that might be worthwhile investigating are: TOSPAC, AREST, NEFTRAN 2, EBSPAC.

5. Explore, with the Center for Nuclear Regulatory Analysis (CNWRA), the adaptation of the FPPA (Fast Probabilistic Performance Assessment) methodology to generate the total system CCDF.

   During this Phase 1 demonstration, questions were raised regarding the number of vectors required for adequate representation of the distribution of consequences for a given scenario class. This question usually arises in studies of this type where performance is estimated using an "empirical distribution" derived from models of system performance using multiple samples of input data. Appendix E discusses some of the concerns with assuring that enough samples are used to obtain a sufficiently accurate representation of performance. A concern in this study is that several vectors yield zero cumulative releases; although this outcome increases confidence in the probability estimates of the low-consequence/high-probability end of the CCDF, less confidence is available for the high-consequence/low-probability end of the CCDF, which may be the critical region for assessing regulatory compliance. Therefore, the use of an importance sampling technique, such as the FPPA methodology, if it can be made applicable for the total CCDF, may permit an increase in accuracy and confidence in results with a saving in computational cost and time.

6. Perform a sensitivity analysis using both drilling and groundwater transport parameters.

   During the Phase 1 analysis the sensitivity analysis was performed only on the liquid pathway model (because the drilling model and code were not available at the time the sensitivity analysis was done), using the variables and distributions germane to that model. Some of these same variables are important for the model of direct releases by drilling. However, some of the variables that could have a significant effect on the consequences of drilling were not included in the sampling procedure used to perform the sensitivity analysis, but were fixed in the model. As a consequence, the variability in the output of the drilling model may have been inappropriately kept small and the importance of some of the variables was not revealed by the sensitivity analysis.

<u>Flow and Transport</u>

1. Refine groundwater modeling (e.g., by considering more dimensions).

   The assumptions used as the basis for flow modeling, which is then the basis for transport modeling, greatly simplify the complexity of the structure, boundary conditions, and physical processes considered in modeling flow at Yucca Mountain. Among the more significant simplifying assumptions are: the flow is one dimensional and vertically downward; the flow is steady; the important boundary condition is the infiltration on the surface, which is assumed constant in time; fracture flow is initiated, when the infiltration rate exceeds the saturated hydraulic conductivity of the matrix. A more precise and complete treatment of the hydrology at the site could treat some of these aspects by using two or three dimensional models, incorporating a better treatment of fracture flow, considering the coupling to regional hydrology, and removing additional simplifying assumptions. Additional site hydrologic data could be incorporated, if available.

2. Incorporate a model of gas-pathway transport in the calculation of the CCDF.

In Phase 1 of this demonstration the only release pathways implemented in the model used to generate estimates of performance were the liquid pathway and direct release by exhumation of waste or contaminated rock. A more complete treatment would explicitly use the concepts discussed in Appendix D - Gaseous Releases of C-14 to formulate a model that quantitatively estimates releases by this pathway and then to incorporate these estimates into the estimate of total system performance, as discussed in Section 4, "System Code". In addition, it might be necessary to couple the liquid pathway and direct pathway calculations of releases to the gaseous pathway to assure conservation of mass (currently the models assume all C-14 is released in dissolved groundwater) and to characterize the interactions between the various pathways correctly.

3. Include flow ana transport through the saturated zone.

   In the Phase 1 demonstration flow and transport of radionuclides in the saturated zone were not incorporated in estimating the performance of the total system. Instead, the radionuclide releases were calculated at the groundwater table (the boundary between the unsaturated and saturated zone). Although estimating consequences in this manner is probably conservative, because the travel time and retardation that may occur in the saturated zone are neglected. Adding consideration of transport in the saturated zone is recommended because (1) a more realistic model of system performance will result and (2) synergistic effects will be portrayed with increased confidence (e.g. the impact of releases from the vertical columns used in Phase 1 to describe the geometry of the repository may be substantially different when the effect of transport through the saturated zone on those releases is included in the model).

4. Instead of the indirect, approximate representation used in Phase 1, use a more sophisicated computational model for transport through a partially saturated, fractured rock.

   The NEFTRAN code was used to calculate transport in the Phase 1 demonstration. The NEFTRAN code was developed to simulate radionuclide migration in saturated rock. The following analytical steps were used to simulate radionuclide migration in partially saturated rock using the NEFTRAN code:

   i. The saturated flow solver incorporated in the NEFTRAN code was bypassed and the flow was calculated assuming partially saturated flow in four one-dimensional columns.

   ii. If the calculated conductivity of any segment of a column was less than the saturated hydraulic conductivity for that segment, then the porosity was multiplied by the degree of saturation (to account for partially saturated conditions), and this modified porosity was used in the NEFTRAN code to calculate radionuclide migration.

iii. If the calculated conductivity of any segment of a column was greater than the saturated hydraulic conductivity for that segment, then all the transport was assumed to occur in the fracture and the properties of the fracture were used in the NEFTRAN code to calculate radionuclide migration.

Improvement in the transparency, accuracy, and robustness of the modeling would be achieved by a more direct approach to modeling: flow in the partially saturated rock, the transition from matrix flow to fracture/matrix flow, transport in the partially saturated matrix, and exchage of mass between the fracture and matrix.

5. Explicitly model fracture/matrix coupling.

   In the Phase 1 demonstration the coupling between groundwater flow in the fractures and matrix was modeled by assuming the flow was entirely in the matrix, if the infiltration was less than or equal to the saturated conductivity for the matrix of that segment. If the infiltration of the segment was greater than the saturated conductivity for the matrix, then the excess flow was assumed to be carried by the fracture. Although the NEFTRAN code has the capability to treat matrix diffusion, this capability was not exercised to obtain estimates for the Phase 1 demonstration. A more complete, precise treatment of both the flow and transport coupling between the rock matrix and the fractures would improve the completeness of the model and would provide further insight into the importance of these couplings and the parameters influencing the couplings.

Source Term

1. Attempt to develop or use a previously developed mechanistic model of waste package failure.

   In the Phase 1 demonstration a distribution was assumed to describe the time of waste package failure and all waste packages were assumed to fail at the same time. This was an ad hoc assumption; the distribtion was not related to any of the parameters that are usually thought to influence waste package failure, such as repository temperature as a function of time, rate and manner of water contacting the waste packages, the geochemistry of the groundwater, and the stress field to which the packages are subject. A mechanistic model of waste package failure would relate the source term to these factors affecting it. These factors can be a function of the repository design, the evolution of repository conditions with time (primarilly thermal and hydrologic conditions), and the occurrence of substantially changed conditions produced by various scenarios. Incorporation of such a mechanistic model can help to reveal the interactions between the source term behavior and the behavior of other parts of the repository system.

2. Develop a mechanistic model of contact between groundwater and the waste.

   In the Phase 1 demonstration the fraction of groundwater contacting the waste (and thereby brought up to the appropriate limiting concentration for each radionuclide) is assumed to be a random variable, which is selected from an assumed distribution. A mechanistic model for the fraction of groundwater raised to the limiting concentration of radionuclides could relate the fraction to parameters generally thought to influence such mass transfer, e.g. the nature of the flow near the repository (including flow rate, degree of saturation, flow profile near the waste packages), the degree of mixing induced by the repository design, the thermal conditions in the repository and the potential for thermally driven flow. An even more direct approach would dispense with the concept of the fraction of groundwater contacting the waste and instead, would calculate mass transfer from the ensemble of waste packages to the geosphere based on the appropriate physical and geometrical parameters.

3. Treat the repository as a source of radionuclides distributed in time and space.

   In the Phase 1 demonstration the waste packages in the repository were not considered to have failures distributed in time; that is, at a single time-of-failure the repository was enabled to release the available inventory. Of course the release rate of the inventory was assumed to be limited further by its solubility. However, all the waste packages were assumed to fail at a single time, rather than the more likely aspect that the waste package failures will be distributed in time and, therefore, in space. Some of the spatially distributed nature of the repository was treated in Phase 1 by partitioning the waste into four groups of packages overlying four columns for radionuclide transport. Because all the groups of packages were assumed to fail simultaneously, the variance in radionuclide releases may have been underestimated. A more inclusive and mechanistic model of the repository distributed in space and time should provide a more realistic picture of the dependence of repository performance on various parameters and on various components. Improved modeling could be accomplished by extending some of the methods used in the Phase 1 demonstration.

<u>Auxiliary Analyses</u>

The following are recommended improvements to and extensions of the auxiliary analyses. These appear to be important aspects of a performance assessment, requiring more detailed study, which were not within the scope of Phase 1.

1. Perform detailed geochemical analyses to investigate:
   - use of K_D's (distribution coefficients)
   - effects of spatially varying saturation on radionuclide migration

- waste form, groundwater, tuff reactions
- waste package degradation
- oxidation of the spent fuel matrix
- plutonium behavior

o In the Phase 1 demonstration K_D's were used in estimating the transport of radionuclides. Because of the complex and time-consuming nature of detailed geochmical analyses, which are an alternative to the K_D approximation, additional modeling efforts are likely to use the K_D approximation. Therefore, an auxiliary analysis to show how good this approximation is and under what conditions it is more or less accurate would be useful.

o In the Phase 1 demonstration the effects of spatially varying saturation were assumed to be limited to changing the amount of groundwater available for advection and dispersion, as the groundwater moved through various units. The possibility of a more complex influence of the variation in saturation along the migration path on the transport of radionuclides was not considered. For example, some reactions, such as those that result in precipitation, may be dependent on the amount of water available. An auxiliary analysis to determine how well approximations useful in fully saturated flow can be extended to model partially saturated flow would be useful.

o In the Phase 1 demonstration the dissolution of the waste form was based on a simple model of the solubility of a particular radionuclide in the groundwater. A more complex, comprehensive, realistic treatment of the dissolution of the waste form that considers the complex interations of the waste form, the host rock, and the groundwater would help to determine the accuracy of the simpler modeling approaches.

o In the Phase 1 demonstration a non-mechanistic model of waste package degradation was used. An essential ingredient of of more realistic treatment is to consider the geochemical interactions among the canister, host rock, and groundwater. An auxiliary analysis of this type could indicate important parameters, outstanding questions regarding phenomenology, and the directions for additional work to take.

o In the Phase 1 demonstration oxidation of the spent fuel matrix was a phenomenon important in determining the behavior of the source term, especially the gaseous phase releases of C-14. Various empirical and semi-empirical approaches were employed to describe this phenomenon. Detailed geochemical analyses of the rate of spent fuel matrix oxidation and the dependence on temperature and geochemical conditions would help to determine whether this phenomenon is understood well enough and whether the modeling needs improvement.

o In the Phase 1 demonstration plutonium appeared to be a major contributor to the total system performance measure, the EPA ratio. An auxiliary analysis to evaluate the adequacy of the transport modeling of plutonium and to determine whether the geochemical data base for plutonium interactions with tuff is adequate, would be useful. The geochemical behavior of plutonium in the near field would also be a useful subject of study.

2. Evaluate heat effects at early times; estimate the thermal, hydrologic, and geochemical environment of the repository at early times.

   In the Phase 1 demonstration the calculated performance did not explicitly take into account the thermal, hydrologic, and geochemical conditions of the repository at early times and how such conditions might affect performance. Consequently, the design, environmental, and site conditions that influence these conditions were not explicitly modeled. An auxiliary analysis of these complex interactions could help to determine which phemomena and parameters to include in improved models of repository performance.

3. Evaluate importance of thermally and barometrically driven air flow on repository performance at Yucca Mountain.

   In the Phase 1 demonstration the flow of groundwater was calculated using a simple, one-dimensional flow approximation which did not include interaction was fluids in the gaseous phase. The SCP, SCA, and other documents (including several reviewed as part of the Phase 1 effort) indicate that the barometrically and thermally driven flow of air and water vapor at Yucca Mountain may have a significant impact on the movement of groundwater and, therefore, may have a potential impact on repository performance. An auxiliary analysis of the nature of such thermally and barometrically driven gas flows and their impact on the movement of groundwater at Yucca Mountain could indicate whether such effects should be included explicitly in models of repository performance.

4. Perform detailed hydrologic analysis for Yucca Mountain, to provide a better input to the transport analysis and to examine, in more detail, various alternative hypotheses regarding hydrology at Yucca Mountain.

   In the Phase 1 demonstration the hydrologic analysis consisted of a one-dimensional, steady approximation to the unsaturated flow conditions at Yucca Mountain. Detailed hydrologic analyses that evaluate the applicability of these and other assumptions (steady, one-dimensional vertical, fixed water table location) and that evaluate the effects of regional flow conditions could indicate the direction for improved modeling of repository performance.

<u>Additional Scientific Input</u>

The following are recommendations for additional scientific input (N.B.: some of these items could be performed by either the DOE or NRC, while others are clearly the responsibility of DOE). These suggestions were clearly beyond the scope of Phase 1, but were identified as gaps in knowledge on the work in Phase 1 was in progress.

1. Develop and demonstrate a mathematically rigorous, scientifically robust method for scenario analysis.

   In the Phase 1 demonstration an attempt was made to follow the methodology for scenario analysis developed by Sandia National Laboratories. Conceptual and logical problems were encountered when attempting to define, enumerate, and screen scenarios. A more mathematically rigorous, scientifically robust approach to scenario analysis would streamline the interactions between modelers and various scientific disciplines and would permit a more transparent, direct derivation and presentation of results.

2. Obtain geoscience input for modeling volcanism.

   During the Phase 1 demonstration some consideration and evaluation was given to the scientific basis available to model the occurrence and manifestation of volcanism. Although some information was found regarding the previous occurences of volcanism at Yucca Mountain, the physical mechanisms for predicting site-specific volcanism at Yucca Mountain appear to be poorly understood. Some information was also found regarding how different types of volcanic events might be manifested within or nearby a repository. It would be useful to perform a comprehensive review of potentially valuable literature , as well as to give consideration to additional general and site-specific information and original research needed to estimate the likelihood and consequences of volcanism at Yucca Mountain.

3. Obtain geoscience and hydrologic input to modeling faulting, uplift, and subsidence at Yucca Mountain.

   During the Phase 1 demonstration tectonic events and processes such as faulting, uplift, and subsidence were identified as potentially important fundamental events that should be considered in defining and selecting scenarios for a performance assessment of a Yucca Mountain repository. Although some substantial information has been compiled (e.g. see the SCP) on these processes and events in the tectonic province and in the immediate vicinity of Yucca Mountain, additional field data and other original research may be needed. A more comprehensive review of applicable literature and a definition of additional data needs would be useful.

4. Obtain laboratory chemical analysis to determine the partitioning of radionuclides in various compartments of the spent fuel waste form.

   During the Phase 1 demonstration an important issue regarding the behavior of spent fuel as a waste form was the quantity of various radionuclides in various compartments of this complex waste form. Spent fuel can be considered to consist of at least five different compartments (proceeding from outside in): (1) crud adhering to the outer surface of the cladding,

(2) the cladding, (3) the gap between the cladding and fuel pellets, (4) the intergranular spaces in the fuel matrix, and (5) the fuel matrix itself. The rate of release of a radionuclide depends on the compartment in which it is located, because of the physical and chemical form it may be in and because compartments closer to the geosphere may release their radionuclide inventory first. This consideration appears to be important in determining the rate and quantity of C-14 release. However, very little data on the inventory of various nuclides in these various compartments of spent fuel were found. This paucity of data limited the Phase 1 analysis.

5. Obtain field and laboratory data on phenomena important to the near-field behavior of the repository, especially the effects of heat.

   Although the Phase 1 demonstration explicitly took into account the thermal, hydrologic, and geochemical conditions in the near-field of the repository and hcw such conditions might affect performance, considerations of such complex, near-field interactions was limited to rudimentary, frequently nonmechanistic modeling. Although an auxiliary analysis of these complex interactions could help to determine which phemomena and parameters to include in improved models of repository performance, execution of such auxiliary analyses appears to be limited by the dirth of phenomenological information and data available for tuff. Additional field and laboratory experiments could provide needed data.

6. Obtain more data on plutonium geochemistry.

   In the Phase 1 demonstration plutonium appeared to be a major contributor to the total system performance measure, the EPA ratio. An expansion of the geochemical data base for plutonium interactions with tuff may be useful.

7. Obtain a better understanding of waste package corrosion in the unsaturated zone.

   In the Phase 1 demonstration an ad hoc distribution of waste package failure was employed, in large part because few data or analyses exist that treat the corrosion of waste packages in a partially saturated repository. On the basis of the literature review performed as part of Phase 1, it appears that additional phenomenological data are needed to bring the understanding of this subject to the level that would allow modeling waste package corrosion in the unsaturated zone.

8. Obtain field and laboratory data and perform analyses to investigate the issue of nonvertical flow at Yucca Mountain.

   An assumption used in the Phase 1 demonstration transport calculations was that flow was vertically downward in four columns underlying the repository. An auxiliary analysis, performed in Phase 1, to evaluate the potential for nonvertical flow indicated that nonvertical flow might occur given certain conditions. Nonvertical flow could affect transport of radionuclides. Therefore, it appears that additional field and laboratory data and additional analyses regarding the potential for nonvertical flow would be useful.

9. Obtain field and laboratory data on the transport of gaseous radionuclides, especially C-14, at Yucca Mountain.

   In the Phase 1 demonstration release of C-14 and other gaseous radionuclide through the gas pathway was not explicitly incorporated in the estimate of performance. An auxiliary analysis executed in Phase 1 indicates that the release of C-14 and possibly other radionuclides in the gas phase may be important. An obstacle to the realistic modeling of such releases is the lack of general and site specific data on gaseous radionuclide transport. It would be useful to have more data of this type.

APPENDIX A - SYSTEM CODE REVIEW

The following are summaries of several programs evaluated by the staff to determine their suitability as a whole or in part for use as a system code for this demonstration. Not all the programs presented are system codes per se, but each contained elements considered necessary to the approach used in this effort.

A.1 System Program Summaries

AREST

The AREST code (Engel, et al, 1989) was developed by Pacific Northwest Laboratory for DOE. The program takes a modular approach to the problem of making preliminary, quantitative performance assessments of the engineered barrier and near-field systems. Input variables to the code include values assigned to the spent fuel waste package, as well as to variables describing the physical and chemical environments of the repository/near-field system and the waste package.

AREST models the performance of the assemblage of individual waste packages from repository closure to the failure of the cannister, the release of radionuclides from the failed packages, and the subsequent movement of the radionuclides away from the waste packages. Average release rates and cumulative releases over time can be calculated from successive waste package simulations .

The code cannot be considered as a total system code as it treats only various failure mechanisms for the waste packages and not the possible scenario classes creating the conditions for failure.

SPARTAN

SPARTAN is a simple model developed by Sandia National Laboratories to support DOE's Environmental Assessment of a potential repository at Yucca Mountain, Nevada (Lin, 1985). Input, consisting of repository, hydrogeologic, waste package, and spent fuel characteristics, is used to simulate the one-dimensional, dispersionless transport of radionuclides in both a porous matrix and a fractured media.

Radionuclide release rates and cumulative curies released are calculated. From this, the performance of the repository can be measured relative to NRC performance objectives and to the EPA standard. The code does not take into account various scenarios.

TOSPAC

Sandia National Laboratories developed TOSPAC (Dudley, et al, 1988) for the Department of Energy specifically for the Yucca Mountain, Nevada site. It considers the one-dimensional transient unsaturated flow and transport of soluble waste materials with coupling between the matrix and fractures.

The code is a FORTRAN 77 program which uses various modules to manage the input and output tasks and to model the differential equations governing water flow, radionuclide transport, and liquid-phase mass transport. A management driver oversees the interactions between these modules. Input to the code covers the material properties of the geologic strata, the radionuclide properties, and different boundary conditions. Output consists of release over time, nuclide concentrations in the matrix and fractures versus time, and three-dimensional plots of concentration vs. time vs. distance.

REPRISK

REPRISK (EPA, 1983) is an EPA program which models the long-term radionuclide release and population health effects associated with the disposal of high-level radioactive wastes in mined geologic repositories. It was originally developed for a repository located in a saturated, porous salt media and can address variations in geologic setting, radionuclide inventories, radionuclide release mechanisms and pathways, time frames, and dose uptake pathways.

The code handles four designated "release mechanisms": 1) direct impact of a waste package with release to air and land, 2) direct impact of a waste package with release to an aquifer, 3) disruption of the repository with release to land, and 4) disruption of the repository with release to an aquifer. REPRISK does not treat radionuclide decay chains and does not incorporate a random sampling program (like Latin Hypercube Sampling) or any sensitivity and uncertainty analyses.

Consequences of a release to the accessible environment can be expressed as somatic or genetic health effects, a ratio of release amount to limits set in 40 CFR Part 191, and or total curies released per radionuclide.

SUNS

The Sensitivity and Uncertainty Analysis Shell (SUNS) (Campbell and Longsine, 1989) is a Sandia National Laboratories generic software shell created to perform Monte Carlo and LHS analyses. It is a modular menu driven code with a flexible input editor which can incorporate a variety of application models suitable for such analyses. The user provides replacement statements to equate model variable names to locations in the various SUNS arrays. The program is designed for parametric analyses and correlation studies.

SUNS performs all file management operations. Output is available in both statistical and graphical formats.

Code Coupler

Sandia National Laboratories developed the Code Coupler programs (Bonano, et al, 1989) to provide linkage between a suite of Sandia codes for a total system performance assessment. This linkage is given on two scales: 1) regional to local flow models, and 2) the local flow model and the radionuclide transport model.

Latin Hypercube sampling is used to create a common database for input in order to maintain a consistent description of the system for each of the models. Programs are available to plot estimated flow paths, discharge rates (Ci/day) vs. time (years), and complementary cumulative distribution functions (CCDFs).

A.2 References

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APPENDIX B - SOURCE TERM CODE REVIEW

B.1 Introduction

This appendix reviews models used in previous DOE analyses of the Yucca Mountain repository, and other models related to source term considerations in general. It covers both dedicated source term codes such as AREST and source term routines in systems codes. This is not a comprehensive list, but represents a sampling of codes whose reference were available to the staff.

B.1 Review of Available Source Term Models Used for assessing the Yucca Mountain Project site

B.1.1 Early DOE Assessment Models for Yucca Mountain

There are several preliminary, simplified assessments that were performed by DOE for the purposes of scoping the performance of YMP:

a. Environmental Assessment Model

The Environmental Assessment (DOE, 1986) model considered that there were three components of the repository; waste package, engineered barrier and geological barrier. The waste package would last 3000 to 30,000 years, during which time there would be no liquid releases of radionuclides. Their analysis adopted a 3000 year lifetime to achieve "some degree of conservatism". The source term model assumes that there would be congruent dissolution of the matrix, and the release rate is proportional to the water flow past the fuel and the solubility of the matrix. They estimate that for an infiltration rate of 0.5 mm per year, a fuel matrix solubility of 0.05 kilograms per cubic meter, and an infiltration area per canister of 0.33 square meters, there would be a fractional release rate by congruent solution of 2.5E-9 per year. The model does not take into account solubility limits for released radionuclides but assumes that with the exception of carbon, cesium, technetium and iodine, all solubility values would be less than or comparable to the value of the uranium dioxide matrix. The authors recognize that there are other sources of radionuclides in the pellet-cladding gap, hardware and clad, but except for C-14, they argue that the radionuclide inventories would not significantly affect their results for cumulative release. All C-14 releases are assumed to be from the matrix also, neglecting contributions from the cladding and gap compartments. Interestingly, a screening analysis they perform later indicates that most of the radionuclides would never reach the accessible environment except for carbon, technetium and iodine. Since these are the very elements that tend to collect outside of the matrix, neglecting the other compartments may be a weakness in this approach. This model appears to be virtually identical to that presented in Lin and Tierney (1986).

b. The TOSPAC Model

TOSPAC--Total System Performance Assessment Code--is a more sophisticated one-dimensional model by Sandia (Dudley, 1985) and considers transient unsaturated flow in one dimension with coupling between the matrix and fractures. The source term model considers either complete dissolution of the matrix with release of all radionuclides (extremely conservative) or a more-realistic congruent release model. The congruent release model assumes 1) the fractional release rate of radionuclides from the spent fuel inventory is equal to the fractional leach rate of the uranium dioxide matrix; 2) the rate of waste matrix dissolution is a function of the solubility limit of uranium dioxide and the availability of water and 3) transport of dissolved species to the source boundary is instantaneous and the transport behavior in the near field region of the waste package where the rock is thermally and mechanically disturbed is similar in the adjacent undisturbed rock. They neglect any releases from other compartments than the uranium matrix, but acknowledge their potential importance. They limit the amount of release of radionuclide to less than or equal to its solubility in the water contacting the waste. This model would not appear to treat daughter products for chain decay unless all daughters had the same solubility. They claim in most cases that the solubility limit would be greater than the concentration, so the release is truly congruent.

The authors recognize that the assumptions about how liquid water contacts the waste to begin the release process is not well understood. They assume that all of the water intercepted by a container (the product of the infiltration rate and the cross-sectional area of the canister) becomes saturated with waste. They also recognize that additional mechanisms may limit the dissolution of the matrix such as diffusion out of the waste container, and that the advection-only model may be pessimistic.

Waste canisters are assumed to fail at a uniform rate, for lack of any data on actual failures.

B.1.2 More Recent Modeling of YMP Performance

a. Yucca Mountain candidate site preliminary postclosure risk assessment, Doctor et.al., 1988.

Included in this preliminary risk assessment for the Yucca Mountain site was a source term code. Releases from the engineered barrier are evaluated using the AREST code (Liebetrau et al. 1987). The AREST model consists of three major components: The engineered system release (ESR) model, the Waste Package Containment (WPC) model and the Waste Package Release (WPR) model. The code treats waste packages individually with no interactions between adjacent waste packages. The WPC model simulates corrosion and degradation leading to package failure. The WPR model simulates release of radionuclides and their migration outward through the waste package barriers. The ESR model integrates the simulated releases from individual waste packages with respect to their failure time distribution. There is also a geochemical model to provide inputs to the three major component models. The authors used the concept of support models external to the AREST code to perform site-specific calculations that are too time consuming or difficult to include in the overall simulation.

The AREST code uses detailed site specific information about the physical and chemical environment of the waste package and the repository. The code describes the thermal, geochemical and hydrological environments of the simulated waste package. The geochemical model determines the chemical environment of the waste package. The hydrologic model for the unsaturated case determines the time that the waste packages might be rewetted after they cool, although it appears that they only consider porous media and not the possibility of fracture flow near the waste package. For saturated conditions, the hydrologic model calculates the time to achieve resaturation following repository closure. For unsaturated media, the thermal model calculates the time for the waste package to cool to a point where liquid water can come into contact with it.

The containment model assumes several mechanistic models of uniform and pitting corrosion, as well as empirical models derived from site-specific testing. The model does not differentiate between canister and cladding containment. For the present calculation of the Yucca Mountain case however, they did not use a mechanistic code for waste package containment. Instead, they chose arbitrarily a normal distribution of failure times with mean of 1000 years and standard deviation 200 years, with the lower tail truncated at 300 years.

The WPR model takes two approaches, one for saturated and one for unsaturated cases. The saturated model assumes low oxygen levels (leading to low dissolution rate for the uranium dioxide matrix), low radionuclide solubilities and low groundwater flow rates, so that releases are based on diffusive mass transfer. For unsaturated media, the model assumes that the environment is oxidizing and that transport is likely to be convective rather than diffusive. Radionuclides are released from the waste matrix congruently at a rate given by the forward matrix dissolution and the fractional inventory of the nuclide in the matrix. The model chooses the larger of the diffusive/solubility release rate or the convective release rate. The release rate may be solubility limited if the rate of congruent release is high and the solubility of the released species is low. The model also looks at the non-matrix components of the source term, and treats those radionuclides accumulated in the interstices and cladding gap as solubility/transport limited until the inventory is depleted. The modelers recognize that the uranium dioxide matrix dissolution may not be truly controlled by solubility but rather instability in an oxidizing environment, so that the rate could remain non-zero even when the solution becomes saturated with respect to the matrix. The modelers limited the release of the matrix radionuclides on the basis of an oxidized and more-soluble uranium silicate mineral.

Even if release rate is not controlled by the solubility of the matrix and the radionuclide in question is not solubility controlled, the rate of release might still be controlled by diffusion away from the waste form rather than convection if the latter is very small. The models allows for certain of the radionuclides to form colloidal species. Diffusion of colloids might also limit their release for very low flow rates. Since colloids have much smaller diffusion coefficients than molecular species, this rate must be very small when diffusion limited. It is not likely that both diffusion and convection need to be considered simultaneously for the Yucca Mountain case for any single species.

The WPR model makes no special provision for release of gaseous radionuclides such as C-14 dioxide. It assumes that all of this inventory is released upon failure of the canister. The non-volatile radionuclides that are not contained in the matrix generally have high solubilities and do not form colloids in oxidizing environments.

The geochemical model is used to determine the chemical environment of the waste packages. The model calculates the steady state equilibrium concentration of J-13 water in equilibrium with the tuff at different temperatures and in a saturated condition. It does not treat radiolysis reaction between the water and the corroding canister material, sorption of radionuclides, and water vaporization or rewetting. These may be serious omissions that should be tested with support models. In particular, the consequences of corrosion products of the canister and other materials on the rate of corrosion and dissolution of radionuclides, and the effects of concentration of minerals in the near field resulting from the effects of heat and drying should be tested.

B.1.3 Other Models not developed Specifically for YMP

1. NEFTRAN

NEFTRAN implements a Network Flow and Transport Model developed by Sandia National Laboratories, primarily for modeling of repository performance at saturated sites (Longsine, 1987). NEFTRAN contains models for solubility limited or leach limited cases. If so desired, the program will determine whether a particular release is limited by leaching or solubility. A third model, mixing cell, assumes that the radionuclides are released into a well-mixed cell. The concentrations of the radionuclides in the cell is governed by flowrate through the cell, volume of the cell and solubility of the radionuclide species.

The source term model follows three radionuclide inventories. The first tracks the total mass of radionuclides remaining in the waste and is called the "unleached inventory". The second inventory is "undissolved"; that which has been released from the matrix by leaching, but whose release to the geosphere is limited by solubility. The third inventory represents dissolved radionuclides. Releases of radionuclides from the matrix depend on the leach rate of the matrix, i.e., congruent dissolution. Releases become part of the soluble compartment if their solubility is greater than the concentration, or part of the undissolved compartment if vice versa. Concentrations of different isotopes of the same element are taken into consideration for solubility limits by specifying the fraction of the inventories for each isotope.

2. Exact and Asymptotic Solutions from University of California

The University of California, Berkeley, Earth Sciences Division has published a number of computer codes dealing mainly with the closed-form solution of flow and diffusive transport from waste packages and through the geosphere (Lee, 1989). Some of these solutions have been incorporated into the AREST code and the PNL assessment of Doctor et al. (1988). Some of the codes that may prove to be useful for defining the source term releases are:

UCBNE-101 - This code calculates the concentration of solubility-limited species as a function of space and time and its mass flux rate from a waste sphere buried in a nuclear waste repository in water saturated rock.

UCBNE-107 - This code calculates the fractional release rate of soluble radionuclides that are released from nuclear waste emplaced in water saturated porous media.

UCBNE-106 - This is a time-dependent version of UCBNE-107.

UCBNE-106D calculates the time history of the diffusion coefficient.

UCBNE-106N calculates the species concentration in the void water as a function of time.

UCBNE-106F calculates the fractional release rate of the species at the void/rock interface as a function of time.

UCBNE-108 calculates the mass flux rate and the fractional release rate at the interface between the first layer of porous material and the next layer of porous material of soluble species released in water-saturated porous media.

UCBNE-102 calculates the mass flux of the non-decaying contaminant outward from a spherical waste form when there is a stationary precipitation at a prescribed distance from the waste separating an inner region of higher solubility and an outer region of lower solubility.

In addition to these codes that are specifically for near field phenomena, there are a set of UCB codes that integrate the source term and the transport models. In order to get analytical solutions, the source term part of these models must be simple, either an impulse (i.e., instantaneous release), a step function in concentration or flux (band release), or a concentration boundary. None of these models can handle solubility limits, because these are inherently non-linear and cannot usually be solved in closed-form. The models can treat the releases of chain-decaying radionuclides in the source, providing their concentrations can be expressed by the Bateman equations and are not distorted by preferential removal of daughters.

3. CONVO

CONVO is a code developed for NRC to model the performance of the waste canisters and engineered barrier (Boyars et al, 1985). The code was primarily developed for demonstrating compliance with the NRC annual release criteria in 10CFR60.113, rather than the cumulative release criteria of EPA as embodied in 10CFR60.112. CONVO has three models for release of radionuclides:

1. A one dimensional, 2-media model;
2. A 3-dimensional, 1-medium model;
3. A 2-dimensional cylindrical 2-medium model.

These models assume that the radionuclides are released at the surface of the waste package through a porous packing material, and that release is limited by diffusion alone, and are limited by solubility. There is no consideration given to radioactive decay and the rate at which the radionuclides are released from the UO_2 matrix, or other compartments in the fuel. Release events are considered by two approaches:

1. The convolution approach, in which the time of peak releases is considered to be independent of time of canister failures.

2. The cascade approach, in which the sequential failures of the canister packing are considered.

The code was targeted mostly to a saturated, zero-velocity, low solubility groundwater system in which diffusion rather than advection was assumed to be the dominant transport mechanism for the release of radionuclides from the waste packages. It appears that in its present form that CONVO would be of little use as a source term model at YMP.

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APPENDIX C - FLOW AND TRANSPORT CODE SUMMARIES

C.1 Regional Flow Program Summaries

SUTRA

SUTRA (Voss, 1984) solves the equations for fluid density-dependent saturated or unsaturated ground-water flow and either transport of a solute in the ground water or transport of thermal energy in the ground water and solid matrix. Solute transport in ground water includes equilibrium adsorption on the solid matrix, production, and decay. Additionally, SUTRA may be used to examine variable density leachate movement and salt water intrusion. While energy transport simulations can be performed with SUTRA, the program only simulates the liquid phase without any consideration for phase changes.

The program uses an integrated-finite-difference method to approximate the governing equations. The finite element mesh can accommodate arbitrary geometries employing quadrilateral finite elements in Cartesian (one or two dimensions) or radial-cylindrical (quasi three dimensions) coordinate dimensions.

Explicit treatment of fractures is not accounted for in the model. However, a dual porosity type of treatment for simulating fracture matrix interactions would be possible through the use of a composite characteristic curves.

VAM2D

VAM2D (Huyakorn, 1989) is a two-dimensional, finite element program developed to simulate moisture movement and solute transport in variably saturated porous media. In solving the governing equations for ground-water flow the program can take into account hysteretic moisture characteristics and variable (due to moisture content) anisotropy in the hydraulic conductivity of the unsaturated media. The program is capable of simulating the transport of chains of radionuclides that accounts for retardation phenomena via a linear equilibrium isotherm.

VAM2D uses a finite element method to solve the flow and transport equations. Time integration is performed using implicit finite difference approximations with non-linearities being handled with either Picard or Newton-Raphson iteration schemes. Additionally, the iterative methods employs the Preconditioned Conjugate Gradient, PCG, for solving the matrix equations (the PCG method has recently emerged as very promising technique for handling the numerical difficulties of ground-water modeling).

The current version of VAM2D has no capability to handle fracture-matrix problems. Future (1990) development of the program will include a capability to account for fractures via a composite characteristic curve.

TRACER3D

The TRACER3D program (Travis, 1984) simulates two phase mass flow and transport in a three-dimensional, deformable, heterogeneous, reactive porous medium. The program solves the equations for mass conservation of the liquid and gas and a reduced form of the momentum equation. The program has the flexibility to solve a one-dimensional, single phase flow problems or include feature such as additional dimensions (up to three-dimensions), the gas phase, and solute transport.

The partial differential equations are approximated using an integrated-finite difference scheme. The iteration procedure is implemented using a Gauss-Seidel or SOR method.

TRACER3D does not explicitely account for fractures, although, the geometric flexibility integrated finite-difference approach would allow for discretizing very small elements which would tend to simulate fractures. However, the program represents the relative conductivity with the Brooks and Corey expression which is reasonable for porous media but may be unacceptable for fractures.

C.2 Two-Phase Flow and Heat Transport Program Summaries

TOUGH

TOUGH (Pruess, 1987) solves the equations for two-phase flow of air and water in the vapor and liquid phases, and heat transport in a fully coupled way. The formulation used in TOUGH is analogues to that used in multiphase, multicomponent geothermal or steam-flooded hydorcarbon reservoir problems. The governing fluid flow equations account for gaseous diffusion, Darcy flow, capillary pressure, vaporization and condensation with latent heat effects, and conduction and convention of heat are included in the energy equation. Water, air, and rock are assumed to be in thermodynamic equilibrium at all times. The flow domain can include liquid, gas, and two-phase regions, indicating that the code handles both saturated and unsaturated flow problems either individually or simultaneously. The thermophysical properties of liquid and vaporized water are represented by the International Formulation Committee's (1967) steam tables. Air is approximated as an ideal gas and additivity of partial pressures is assumed for air-vapor mixtures.

TOUGH solves three nonlinear partial differential equations simultaneously. These are the conservation equations for air, water, and heat. Air and water can be transported in either the liquid phase, the gas phase, or both. The dissolution of air in water is represented by Henry's law and flow (gas and liquid) by Darcy's law.

The code can simulate flow in one, two, or three dimensions because the method of solution is based on a general integrated finite-difference method. Time stepping is accomplished by a fully implicit procedure. The resulting non-linear difference equations are linearized by the Newton-Raphson technique.

The linearized equations are solved by the Harwell matrix solver that stores only the nonzero elements of a matrix thus reducing core storage requirements for the code.

NORIA

NORIA (Bixler, 1985) is designed to simulate liquid, vapor, air, and energy transport in partially saturated and saturated porous media. The following mechanisms are included in NORIA: (1) transport of water, vapor, and air due to pressure gradients; (2) transport of water, vapor and air due to density gradients; (3) binary diffusion of vapor and air; (4) Knudsen diffusion of vaport and air; (5) thermo-diffusion of vapor and air; (6) conduction of sensible heat; (7) convection of sensible heat; (8) evaporation and condensation; (9) nonequilibrium and equilibrium vapor pressure model; and (10) capillary pressure. Nearly all the thermodynamic and constitutive properties in the code can be defined nonlinearly in terms of the remaining dependent or independent variables by the user.

NORIA solves four nonlinear partial differential equations governing the flow of water, vapor, air, and energy. These equations consist of a water-pressure equation, a vapor partial-pressure equation, an air partial-pressure equation, and a heat equation. The equations are solved by the Galerkin finite-element method. Time stepping is accomplished by a two-step time integrator with automatic time step selection. The nonlinear difference equations formed by application of the finite-element method are solved simultaneously by Newton-Raphson iteration. Normally, a one-step iteration is used; however, a multistep iteration is used if the correction on the first iteration is larger than a specified amount.

PETROS

PETROS (Hadley, 1985) is designed to simulate problems similar to those simulated by NORIA. PETROS solves the same number and types of nonlinear equations and handles the same physical processes as NORIA, but in a slightly different manner. The main difference between the two codes is that PETROS solves only one-dimensional problems, either in linear, radial, or spherical coordinates, and solves the equations with the finite difference method. There are also some difference between the codes in the way the time integrations are performed. PETROS uses a modified version of the time integrator in NORIA.

PETROS solves three mass conservation equations and a heat conservation equation just as NORIA. However, the liquid conservation equation is PETROS is formulated with respect to saturation rather than pressure as in NORIA. The characteristic curves and the thermal conductivity as a function of saturation and temperature are supplied to PETROS through user-written function subprograms. Other parameters such as diffusion coefficients, water viscosity, saturation vapor pressure of water, and default values of the characteristic curves and thermal conductivity are supplied internally in the code as function subprograms. Constants such as gas viscosity, specific heats, and water density can either be set at default values or supplied by the user. The user can also choose between equilibrium and nonequilibrium vapor-pressure models.

The above equations are solved numerically by a finite-difference method. The equations are differentiated in both space and time. Differentiating in time results in fully implicit equations. The saturation and temperature equations are solved with a tridiagonal algorithm. Because the vapor and air pressure equations are stongly coupled, they are solved with a block tridiagonal algorithm.

C.3 Geochemical Program Summaries

PHREEQE

PHREEQE (Parkhurst, 1980) was developed to model geochemical reactions between water and rock material. Based on an ion-pairing aqueous model, the program calculates pH, redox potential and mass transfer as a function of reaction progress. The program performs a mass balance of elements in terms of their concentrations in the aqueous phase and uses electrical neutrality and electron balance relations to complete the set of equations needed to solve a given problem.

The program solves a set of nonlinear algebraic equations using a combination of a continued-fraction approach for mass balance and a Newton-Raphson iteration technique.

EQ3/6

EQ3/6 (Wolery, 1979) was developed to compute equilibrium models of aqueous geochemical systems. EQ3 performs distribution-of-species calculations for natural water compositions. EQ6 uses the results of EQ3 to predict the consequences of heating and cooling aqueous solutions and of irreversible reaction in rock water systems. Reaction path modeling is useful in analysing complex systems wherein analytical data do not permit the definition of reactions by mass balance alone.

The program uses a Newton-Raphson method to solve the algebraic governing equations of chemical equilibrium.

WATEQF

WATEQF (Plummer, 1976) simulates the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis. The program provides a general capability to calculate chemical equilibria in natural waters at low temperatures.

WATEQF uses a successive approximation method to solve the mass action and mass balance equations.

CHEMTRN

CHEMTRN (Miller, 1983) was developed to simulate one-dimensional transport of chemical species in ground water. Equilibrium is assumed in all chemical reactions and thermodynamic activities of all reacting species are related by mass-action expressions. The program includes the effects of dispersion and diffusion, advection, sorption via ion exchange or surface complexation, aqueous complexation, precipitation and dissolution of solids, and the dissociation of water.

The governing equations are approximated using a finite difference approach. A Newton-Raphson iteration technique is used to to solve the system of equations.

C.4 Transport Program Summaries

SPARTAN

The SPARTAN code is a simple performance assessment code developed by Y.T. Lin at Sandia National Laboratories. The model employs a simplistic hydraulic model for flow of water infiltrating the surface and reaching the water table. This model has little in the way of a mechanistic explanation for the way water would flow at YMP. The rate of infiltration in the matrix is assumed to follow Darcy's law, with a gradient of unity, a fixed permeability and fixed effective porosity. For infiltration rates less than 1 mm/year. the speed of groundwater movement is proportional strictly to the infiltration rate and does not take into account the change of hydraulic conductivity with moisture content. For infiltration rates greater than 1 mm/yr the model assumes that a fraction of the water infiltrating will move through the fracture zone faster than through the matrix and with transport properties typical of fractures. The transport model takes radioactive decay and a linear sorption (Kd) into account. It allows different retardation factors for daughters and parents.

The SPARTAN code was used for some very preliminary assessments of a proposed repository at Yucca Mountain. The test cases the authors demonstrated considered that there were 2 or 3 pathways for transport which was supposed to represent the different lengths from the repository to the water table. There were two pathways for matrix flow for the case of 0.5 mm/yr infiltration. For 5 mm/yr infiltration, they assumed that the water in excess of what the matrix could carry would travel through a third pathway as fracture flow. For the former case, only I-129, C-14 and Tc-99 would reach the accessible environment within 100,000 years. For the latter case, many more of the radionuclides would be released to the accessible environment.

TOSPAC Model

TOSPAC (Dudley, 1987), the Total System Performance Assessment Code, is a computer program designed to simulate water flow and transport of soluble waste in fractured porous unsaturated rock. The groundwater flow module solves either the transient or steady state partial differential equations for an equivalent porous-fractured medium in which the properties of the matrix and fractures are combined into one constitutive relationship for saturation versus hydraulic conductivity (or matrix potential versus hydraulic conductivity). The site is represented as a series of one-dimensional flow tubes with no lateral interchange. Within any one flow tube they solve either the steady state or transient flow equation for the equivalent matrix-fracture relationship. For steady state, the solution is iterative to allow the self-adjustment of the hydraulic conductivity and saturation values to correspond to the constitutive relationships for each layer. Once the solution reaches steady state, the hydraulic conductivity is known, and consequently so is the net downward flux and groundwater velocity that can then be used in the transport calculations. The transient solution solve for pressure head with a numerical solution of Richard's equation using Pickard iteration.

The module for radionuclide transport uses the velocities calculated from the flow module. First, the code estimates the fraction of flow in the matrix and fracture flow paths. Concentrations of each radionuclide are calculated for the matrix and fracture compartments with a dynamic coupling between them.

NEFTRAN

NEFTRAN (Longsine, 1987) is a network flow and transport code developed primarily for the NRC program in salt and other saturated rock repositories. The flow model in NEFTRAN consists of an arbitrary network of one-dimensional pipes, connected at nodes. Boundary conditions of pressure are set on some of these nodes, and the hydraulic properties of transmissivity and porosity are set within the pipes. The network model then solves for the steady state velocity and flux within the network. Radionuclides are transported in the network by the calculated flux. The model uses retardation factors to express the speed at which a particular species is transported. It also allows for transport between the actively flowing legs and immobile water adjacent to the leg in order to simulate matrix diffusion. Chain radionuclides can be transported also. There are two models for chain transport; the first model assumes equal retardation coefficients and up to a three component chain. The other model allows arbitrary retardation coefficients for chains up to 6 daughters. The former model is however much less time-consuming. NEFTRAN simulates dispersion along the legs using the Distributed Velocity Method (DVM) which assumes that dispersion is caused by the distribution of velocities in the flow field.

In its present form, NEFTRAN is not ideally suited for performance assessment of a repository located in unsaturated fractured tuff for the following reasons:

1. The model is set up for boundary conditions which are appropriate for a saturated site.

2. The flow model is for steady state coditions. (Transient recharge may be an important consideration in unsaturated fractured tuff)

3. The model assumes that the source term is concentrated in one leg only, and cannot represent source terms highly distributed in time and space. This limitation did not seem to be as important for saturated sites where the flow was more horizontal than vertical, but could be a limitation where multiple travel paths were needed to adequately account for system performance.

NEFTRAN is being modified now under Research contract A-1266 specifically for the Yucca Mountain case, and some of these limitations should be overcome. Sandia is developing a multidimensional finite difference model to calculate steady state and transient unsaturated flow in porous media. The output of this code will be fed directly into a modified NEFTRAN that can accept flux boundaries and transient flow conditions. If the flow model shows unusual flow patterns, the network in NEFTRAN can be modified to accommodate this, but cannot be modified within a single run for transient conditions. The source term still will not be represented by more than one leg, and therefore cannot truly simulate a highly distributed case. The limitation of a distributed source might be partially overcome by clever sampling of the path length, flow and release times in the systems analysis. (This would hold true for any of the one- dimensional approaches.)

The modified version of NEFTRAN was not available in time for the present study.

UCB Codes

There are a large number of an@lytical codes (i.e., closed form solutions) available that could serve to calculate flow and transport, particularly for one-dimensional steady flow in which there are really few considerations as to whether the flow is saturated or unsaturated. The University of California Berkeley (UCB) codes combine simple source term models with analytical solutions for one-dimensional, steady state flow, and radionuclide transport. The UCB codes have been used in a number of important US studies (e.g., WISP report and AREST code development). These codes are unique analytic solutions due to the fact that they have explicit solutions for chain decay with differing retardation coefficients for each daughter. However, the incorporation of more than one hydrologic layer may not be possible with the solution technique. This would make application to the Yucca Mountain site, where there are several distinct layers with different material properties, difficult.

Laplace Transform Solutions

Another class of analytical codes is Laplace Transform domain solutions (Robinson, Hodgkinson, et al.). The source term, transport model and even stochastic solution can be set up using this method, solving the linear differential equations in the Laplace domain and getting the time domain solution by numerical evaluation of the contour integral in the complex plane. This solution technique should be relatively easy to apply to the problem of transport through multiple layers. The recent development and progress of this solution technique in the United Kingdom needs to be followed for latter use in performance assessment.

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Appendix D
Auxiliary Analysis - Gaseous Releases of C-14

D1. Introduction

C-14 is produced in nuclear reactors by the activation of nitrogen impurities in the fuel cladding, and by the activation of O-17, particularly in the uranium oxide fuel and in the circulating water of light water reactors. The release of Carbon-14 from the waste packages may be of concern because there is at least the possibility of a fast gas pathway to the accessible environment through the unsaturated fractured rock, excavations and tunnels. Although we treat C-14 in the liquid pathway analysis by including the total release into the liquid phase, this would not be conservative from the standpoint of the gas pathway. In this Appendix we present models for the release of C-14 from the engineered barrier and its transport through the gas pathway to the accessible environment.

D2. Source Term

Carbon-14 is found in quantities an order of magnitude greater than would be allowed under 40CFR191 if all were released. The estimated inventory of C-14 in the 70,000 metric tons heavy metal assumed for this exercise is 98,000 curies (Doctor, 1988). The allowed release under 40CFR191 is 7,000 Curies. It has a half life of 5720 years. The majority of environmental C-14 comes from interaction of cosmic ray neutrons and nitrogen, although it is also created by activation of the rare O-17 isotope in the atmosphere (van Konynenberg, 1987). It is produced in great quantities in atmospheric nuclear explosions through neutron activation. Once in the atmosphere, C-14 is removed from the environment mainly by absorption in the bicarbonate ions in seawater with an apparent relaxation time (i.e., time for half to disappear from the biosphere) of approximately 9 to 15 years (Till, 1983). A portion of the C-14 recycles through the food chain and is very biologically active. The combination of biological activity and long half life lead to relatively large population doses per curie released.

In reactor fuel, C-14 is produced by the same mechanisms as in the atmosphere. The main routes to production are 1) activation of nitrogen impurities in the metallic structure of the reactor and the cladding of the fuel and 2) activation of O-17 in the uranium dioxide fuel and in the circulating water of the reactor, with subsequent deposition onto the cladding and other structural material.

Measurements indicate that about 1/3 of the total C-14 inventory resides in or on the cladding of PWR fuel, but similar measurements for BWR fuel are not available (van Konynenberg, 1987). The remainder is dispersed in the fuel, cladding gap and the intergrain boundaries. The staff expects that BWR fuel will be different because of the different oxidation potential present in the reactors. There is little or no information on inventories for other non-fuel parts of the reactor.

The two mechanisms for producing C-14 in the reactor are important to understanding its availability. Presumably, C-14 created by activation of nitrogen would be dispersed in the cladding because the nitrogen may also be dispersed. Much of the C-14 appears to be from the oxygen activation mechanism, and is adsorbed onto the cladding, fairly close to the surface. This fact may be important because it allows the C-14 to be more readily accessible to the environment than if it were uniformly dispersed in the cladding (SCP, Sections 8.3.5.9, 8.3.5.10).

D2.1 <u>Possible release modes from Spent Fuel</u>

Upon failure of the canister, gaseous C-14 could be released to the geologic setting. Most of the C-14 in the canister is apparently in the form of elemental carbon, metal carbides or oxycarbides (van Konynenberg, 1987). In inert nitrogen and helium atmospheres, spent fuel does not readily release its C-14. Upon exposure to air, however, some of the C-14 oxidizes and is usually released to the immediate atmosphere as C-14 dioxide. About 1 to 2 percent of the available C-14 inventory could be released quickly by this mechanism, but it is mainly the C-14 that is deposited on the surface as crud, or collected on the intergrain boundaries of the fuel (van Konynenberg, 1987). For elemental carbon, release could depend upon oxidation to carbon dioxide and carbon monoxide, the rate of which is extremely slow at low temperatures. Elemental carbon is known to be extremely stable under normal conditions, as is evidenced by the presence of graphite in schists exposed for thousands of years at the earth's surface. There is some experimental evidence to suggest however that carbon will oxidize to carbon dioxide at a temperature of 275°C within a radiation field of 10,000 rads per hour (van Konynenberg, 1987). Temperatures of the fuel may be in this range for the first few decades after storage, but are likely to be considerably cooler near the time required for minimum canister life. Radiation levels of 10,000 rad/hr are likely to be present for up to about 100 years. While the radiation field diminishes with time, we do not have any experimental evidence to indicate that there is a threshold below which no oxidation would occur. For the sake of conservatism, we assume that there is a mechanism available to oxidize available carbon to gaseous carbon dioxide for the lifetime of the repository.

The more likely C-14 release mechanisms from spent fuel are:

- Dissolution of the cladding and oxidation of the C-14 attached to the cladding, e.g., crud.
- Quick release of a small percentage of carbon dioxide gas from the cladding-pellet gap upon failure of the cladding.
- Diffusion of oxygen into the waste form, particularly the matrix, reaction of the carbon with the oxygen and the subsequent diffusion of carbon dioxide out of the matrix.

Other possible mechanisms might also release C-14 but we have little or no direct evidence that they apply:

- Galvanic reaction between elemental carbon in the cladding or metal carbides and the surrounding metal in the waste form.
- Reaction of metal carbides on the zirconium or uranium with water to form acetylene gas (Katz and Rabinowitz, 1951).
- Microbial action on carbon or carbon compounds in the waste.
- Release of methyl iodide created from the reaction of carbon and iodine present in the fuel. This could be a potential release mechanism for I-129. Methyl iodide would be volatile at temperatures of about 200°C expected in the repository during the first few decades after site closure.

The authors have little direct evidence to support a model for C-14 gaseous release, but have chosen what we consider to be a reasonable set of mechanisms based on limited information, and cover them below in their order of expected importance. We apply these mechanisms to our C-14 release model and have in all cases chosen conservative ranges of parameter values to apply to these models. We must stop short of stating that the overall models are conservative, however.

D2.1.1 Releases due to Oxidation of Uranium Dioxide

We assume that the C-14 trapped within the uranium dioxide fuel will be released at a rate coupled to the rate of oxidation of the fuel. Uranium dioxide is unstable in an oxidizing environment, and oxidizes to other forms, with corresponding increases in volume, porosity and fracturing in many cases. If the reaction proceeds fast enough, the UO_2 will spall, becoming more porous and less dense. The increase in volume could promote continued cracking of the cladding, allowing more pellets to be exposed.

Spallation is an indication that significant oxidation has occurred and may also provide for increased exposure of the C-14 to oxidants. Both UO_2 and C will be competing for the oxidants. From thermodynamic considerations alone, carbon would be oxidized first at low oxygen activities, followed by oxidation of UO_2 at higher oxygen activities. However, the relative rates of the competing reactions probably govern how the components of the spent fuel will be oxidized. Einsiger and Woodley (1985a) state that for irradiated fuel the uranium dioxide crystalline structure is damaged and pellets are fragmented, thereby opening more surface area to oxidation. In addition, gas bubbles and fission products may migrate to the grain boundaries where the interconnected paths can form, making grain boundaries preferential sites for oxidation. The radiation field can ionize or excite atmospheric oxygen or water, possibly enhancing the oxidation rate.

Einsiger and Strain (1984) present two curves bounding the time to spallation t_s as a function of temperature T:

$$\log t_s = (0.78 \times 10^{-4}/T) - 13.01 \qquad (D1)$$

$$\log t_s = (1.03 \times 10^{-4}/T) - 15.9 \qquad (D2)$$

where t_s is in given in hours, T in degrees Kelvin, and log denotes the base 10 logaritñm. Equations D1 and D2 are not directly useable to determine the rate of release of C-14 because they are formulated with steady temperatures in mind. Since the fuel temperature changes with time, it is more convenient to convert spallation time to an oxidation rate. If we assume that the rate of oxidation λ_s is the reciprocal of the spallation time t_s, we can then define a time-dependênt rate of C-14 release:

$$\lambda_s = 1/t_s \qquad (D3)$$

This model may be conservative from the standpoint that the time for the onset of spallation does not signal the total oxidation of the fuel pellets. On the other hand, the rate of release of C-14 may not be as low as indicated for long spallation times that occur at lower temperatures.

D2.1.2 Oxidation of Zirconium

A large fraction of the C-14 inventory may be in or on the cladding, caused by neutron activation of O-17 picked up from the circulating water particularly in BWR's, or nitrogen impurities in the metal itself. Corrosion of the zirconium may be the first step in releasing the C-14 to the atmosphere, although it is possible that this corrosion may not be necessary to initiate release. In addition, cladding corrosion leading to perforation could expose the UO_2 to oxidation.

Oxidation of the cladding has been studied for the case of dry cask storage of spent fuel. Einziger and Kohli (1984) present a rate equation for zirconium cladding in terms of temperature:

$$L = 3.68E8 \times t \times \exp(-15810/T) \qquad (D4)$$

where L is the oxide thickness in millimeters, t is the time in years, and T is the absolute temperature, degrees K. To find the growth of zirconium oxide layer with time, we first convert Eq.D4 to a rate, and integrate from the time of failure t_f, using the expected temperature of the waste:

$$L = \int_{t_f}^{t} 3.68E8 \ \exp(-15810/T(t))\, dt \qquad (D5)$$

The calculated oxide thicknesses are presented in Table D1 for a typical fuel temperature ranging from a high of 320 to 110 degrees C over 10,000 years, and an assumed failure time of $t_f = 0$.

Table D1 - Calculated zirconium oxide thickness

Temperature	t-yrs	L-mm
320	5	4.9E-3
300	25	1.25E-2
275	50	1.52E-2
250	75	1.59E-2
230	100	1.61E-2
200-110	10000	1.62E-2

A typical cladding thickness is 0.61 mm, so the maximum oxide growth is only about 3% of the total thickness. Most of the oxidation takes place when temperatures are highest, with virtually none after about 100 years.

Einsiger and Woodley (1985a) also describe a possible condition that might affect the rate of cladding failure in the absence of oxygen. Canisters might contain a few tens of milliliters of water from rods stored in cooling pools. The radiolysis of the water could provide oxidants that could oxidize the cladding (Reed, 1987).

The ramifications of zirconium oxidation are not entirely clear. It appears that there would be relatively little oxidation of the zirconium in the repository. If the fuel is kept cool; e.g., in wet storage casks prior to being placed in the canisters, the reaction would not proceed very far. It would be more oxidized in dry storage, but might be inhibited by the presence of inert atmosphere in the canisters. Although the percent oxidation may be small, most of the C-14 might be close to the surface as crud, or attached to an existing oxide coating since it might have been picked up externally from the circulating water. The fact that little if any oxidation of the zirconium alloy occurs at temperatures lower than about 230 C leads to a tentative conclusion for the purposes of this study that there will be little additional zirconium oxidation after canister failure. We will assume therefore that only the readily available portion of the C-14, about one percent, will be driven off during the pre-canister-failure period, and that there will be no additional releases from the zirconium compartment. Corrosion of the cladding might be relatively more important if it causes perforation, allowing oxygen to reach and oxidize the spent fuel matrix.

D2.2 Proposed Source Term Model

We have chosen for the Phase 1 study to employ the following model for the release of gaseous carbon from the engineered barrier incorporating the mechanisms discussed above:

- Canisters fail at a rate predicted by a normal probability distribution. We chose two different distributions to demonstrate the sensitivity of the C-14 release to the waste package lifetime.

- At the time of canister failure, oxygen will enter the canister and become available immediately to react with the uranium dioxide in the fuel rods. The model assumes that release rate is tied closely to the spallation rate of the fuel, and that there is sufficient oxygen available upon canister failure for the fuel oxidation to proceed. Although most fuel rods will have additional protection from oxidation based on resistance to corrosion of the zirconium alloy cladding, we will assume for the purpose of conservatism that all fuel rods are available for release of their C-14 inventories.

- On failure of the canisters, a small fraction of the C-14 inventory is released rapidly. This fraction represents the C-14 inventory of the cladding-pellet gap and the C-14 close to the outside surface of the cladding or crud that would be readily oxidized.

The average fractional release rate of C-14, $f(t)$, is calculated based on the random failures and oxidations of a large number of canisters to which is added the fractional prompt release f_p from the canisters at the time of failure t_f:

$$f(t) = \frac{1}{N} \sum_{i=1}^{N} [H(t-t_{fi})f_p + \int_{t_{fi}}^{t} \lambda_{si}(t)\, dt] \qquad \text{(D6)}$$

where N is the number of canisters, and $H(t-t_{fi})$ is the Heaviside unit step function at time $t = t_{fi}$.

D2.4 Results of Source Term predictions

Figure D1 illustrates the fraction of the total C-14 inventory released up to 10,000 years for two different assumed canister failure models. The higher release curve (solid) corresponds to canister failure with a mean failure time of 550 years, a standard deviation of 150 years and an upper and lower limit of 100 and 1000 years respectively. The lower (broken) curve corresponds to a mean failure time of 1000 years, a standard deviation of 300 years and an upper and lower limit of 200 and 1800 years respectively. The maximum cumulative releases were about 13.2% and 2.5% respectively, illustrating the strong dependence of C-14 release on waste package lifetime.

D2.5 Limitation of the C-14 Source Term Model

The C-14 release model has been based on the following limiting assumptions:

- A non-mechanistic failure of all canisters in a time short relative to the half life of C-14 and the 10,000 year period of interest.

- An influx upon canister failure of sufficient oxygen to cause unimpeded fuel oxidation. Oxygen will not be consumed by other reducing agents such as the canister walls and metal components of the fuel assemblies.

- The highly corrosion-resistant cladding on the fuel is assumed to offer no protection from oxidation.

- A prompt release from the cladding and pellet-gap inventories for 100% of the fuel rods. Actually the prompt release might occur only from failed fuel rods.

- Rate of oxidation equal to the reciprocal of the spallation time. Actually spallation time may be more representative of the oxidation of only a fraction of the fuel. This might be conservative at high temperatures, and may not be a conservative assumption at low temperatures.

D3. Gaseous Transport Model

Once released from the fuel, the C-14 would probably be carbon dioxide or another gas such as methane or acetylene. Van Konynenberg (1987) estimates that there would be no more than 22 kilograms of C-14 in the repository, as contrasted to greater than 300,000 kilograms of dead carbon in the immediate vicinity of the repository as carbon dioxide and even more as carbonate and bicarbonate ions. Part of the dead carbon will be available to exchange with the C-14 along the transport pathway. The effect of this exchange will be to retard the speed at which the C-14 could be transported to the accessible environment. A potentially important reaction is the precipitation of calcite (calcium carbonate) by the reaction of calcium ions and carbon dioxide to form a low solubility precipitate (Ross, 1988). The significance of retardation of C-14 or its removal by precipitation will depend on the relative rates of exchange between CO_2 gas, bicarbonate and calcite, and the velocity of air flow through the rock.

Several reports propose C-14 transport models. Knapp (1987) describes a one-dimensional model for C-14 transport by advection with exchange between the gas phase and the bicarbonate in the groundwater. The results of this study show that for Yucca Mountain, C-14 released as a pulse from the repository horizon at 2000 years after repository closure would reach the surface within 6000 years.

Amter et al (1988) expand on the concept of a C-14 transport model with more computational detail. Their model accounts for two dimensional gas and liquid advection, diffusion and exchange between liquid and gas compartments. They assume that gas and water are in equilibrium for carbonate species because of the rapid diffusion of carbon dioxide. Dissolved bicarbonate ions in the rock are considered to be essentially immobile because of the relatively high velocity of gas flow to liquid flow. Liquid phase diffusion is also ignored because liquid phase diffusion constants are much smaller than gas phase diffusion constants. The presence of the C-14 components in the liquid will have the effect of reducing the speed of transport by a retardation factor.

D3.1 Chemical Modeling

The chemical retardation of C-14 depends on equilibrium between carbon dioxide, bicarbonate ion and solid carbonate. The equilibrium between C-14 as CO_2 and bicarbonate is tied to several possible chemical factors including the presence of calcite, CO_2 partial pressure and pH. Ross (1988) assumes that CO_2 dissolved in water is immobile, a conservative assumption for atmospheric releases since there is likely to be a net movement of groundwater to the water table from the ground surface. CO_2 is produced naturally in plant roots. The the decline in the concentration of CO_2 with depth seems to indicate that it is being removed by some mechanism, possibly calcite precipitation. Ross speculates that this would require a source of calcium ions infiltrating the site. Although the groundwater is not saturated with calcium carbonate and it does not appear to be precipitating naturally, an increase in repository temperature might cause precipitation by evaporation, thereby concentrating the calcite. Calcite solubility is retrograde, decreasing with increasing temperature. This trend leads to some interesting possibilities how the bicarbonate ions in the heated area would react and whether there would be an irreversible deposition of C-14 in precipitating calcite.

Differences in the atomic weights of C-14 and C-12 may lead to fractionation because of the slightly different rates of reaction, evaporation, condensation, crystallization, adsorption and diffusion. Fractionation was estimated by comparison to enrichment factors for stable C-13, and found to be negligible (Amter, 1988).

Amter et al (1988) present the results of geochemical modeling to determine the complicated equilibrium among the C-14 gas, liquid and solid phases. The conceptual model of the geochemical system had three principal assumptions:

"1. Sufficient calcium carbonate is present in the unsaturated zone to dominate the aqueous chemistry and buffer the pH of the water.

2. A relatively minor amount of calcium is derived from silicate weathering reactions. As a first approximation, it can be assumed that calcium concentrations are the result of equilibration with calcium carbonate.

3. Fractionation plays a negligible role in removing carbon-14 from the gas phase, and concentrations of carbon-14 are proportional to those of carbon-12."

The effect of isotopic equilibrium between phases is to reduce the speed of transport by a factor B, defined:

$$B = 1 + \frac{\theta_T - \theta_D}{\theta_D} \frac{C_T^*}{C_T} \qquad (D7)$$

where θ_T = total porosity

θ_D = drained porosity

C_T^* = concentration of carbon ion in the liquid phase at equilibrium

C_T = concentration of carbon ion in the gas phase at equilibrium

Ampter et al (1988) determine the equilibrium concentrations needed for Equation D7 using the PHREEQE reaction path model. There are few data available on the chemistry of water in the unsaturated rocks of the repository, and therefore the data used in the analyses are somewhat subjective.

The results of the PHREEQE calculations were functions expressing the dependence of retardation on temperature for the hydrogeologic units. The expected retardation coefficients ranged from about 20 to 90 over the expected temperatures and concentrations of carbonate in the rock.

D3.2 Gas Phase Transport Modeling

Several mechanisms potentially drive the gas flow, but Amter et al (1988) consider two mechanisms to be dominant:

- Temperature-driven circulation caused by repository heat and the geothermal gradient;

- The difference in density between the moist, warm air in the rock and the cool dry air in the atmosphere.

The authors considered and eliminated the following potential mechanisms for transport of C-14:

- Liquid phase advection - The downward flux of liquid water is likely to be about one tenth the gas flux during the period of repository heating that is most important to HLW performance assessment.

- Diffusion - Using a travel distance of 350 meters and a retardation factor for C-14 of 70 gives a travel time for diffusion of 43,000 yrs, which is much larger than either the ambient of heat-driven travel times for the repository.

- Binary diffusion - A mass flow of air from higher to lower temperatures in the rock will be driven by diffusion, but this flow was shown to be much smaller than the temperature-driven flow.

- o Mixing by seasonally alternating flow - Under ambient conditions, gas within Yucca Mountain will move upward in winter and to a lesser extent downward in summer, but would move C-14 molecules only a few centimeters per season, much smaller than even the molecular diffusion effect.

The C-14 transport model relied on a temperature field developed by Tsang and Preuss (1987) that showed a gas phase velocity of meters to thousands of meters per year resulting from the repository heat, as shown in Figure D.2. The model of Amter et al (1988) predicted travel times for C-14 of several hundred years to several tens of thousands of years, depending on the location in the repository and the depth of the overburden, as shown in Figure D.3.

D3.3 C-14 Transport Model

The staff used the estimated travel times calculated by Amter (1988), as shown in Figure D.3 to develop a scoping model which accounts for transport of carbon dioxide from the repository to the surface of the earth. The model considers radioactive decay using the average travel time for C-14 from the repository to the surface. Amter calculated the travel times along a transect of the repository at zero, 2000 years, 10,000 years and 50,000 years. The fractional release f_i at the earth's surface for a parcel of C-14 released at time t_0 was determined by integrating along the path from the repository to the surface assuming that the velocity of the parcel would be everywhere equal, but varying with time (This is not necessarily a good assumption, because the velocity is known to vary in space within the complicated convection currents predicted by Tsang and Preuss, 1987):

$$L(t) = \int_{t_0}^{t} v(t)\, dt \qquad (D8)$$

Where L(t) is the normalized distance that the parcel has traveled relative to the distance to the surface, v(t) is the normalized velocity, defined here as the reciprocal of the travel time at time t, and t_0 is the time of release. The integral was evaluated graphically to find the time t when L(t) = 1. The object of the integration was to find the travel time of the parcel and determine if it could reach the surface within the stated time limit, i.e., 10,000 years. Once the travel time t_i was determined for each parcel with release time t_{0i}, the fraction f_i released at the earth's surface was determined by radioactive decay:

$$f_i = \exp(-\lambda t_i) \qquad (D9)$$

Where $\lambda = \ln 2/t_{1/2}$. The results of these calculations are summarized in Table D2 for releases at 500 to 6500 years. The fractional release ranges from a maximum of 0.91 to a minimum of 0.65. Releases after about 6500 years do not arrive at the surface of the earth before 10,000 years.

Table D2 - Release Fraction as function of release time

Time of release, years	Fraction Reaching Surface
500	0.86
1500	0.91
2500	0.86
3500	0.82
4500	0.74
5500	0.71
6500	0.65
beyond 6500	none in 10,000 yrs

D.3.3.1 Limitations of C-14 Gas Transport Model

Some of the limitations of the transport model are given below:

- There is the possibility that gaseous releases from the repository level may follow the shortest path and that there may be ample ground transport between one part of the repository and another because of the network of drifts, shafts and fractures. The effective travel time for C-14 released anywhere in the repository may therefore be more characteristic of the shortest travel time calculated.

- There is evidence that in natural waters, CO_2 is not in equilibrium with the atmosphere, partially because of unfavorable mixing conditions and the slowness of the gas transfer reaction (Stumm and Morgan, 1970). The chemical model for C-14 behavior is based on the assumption of equilibrium. Failure to attain equilibrium would have the effect of reducing the retardation of C-14.

- In their transport and chemical models, Ampter et al (1988) assume intimate contact between the gas and water phases. Such contact is unlikely at Yucca Mountain because under unsaturated conditions water would be present primarily in the smallest rock pores, and the flow of air would be most prevalent in the largest rock pores and fractures. Therefore, the potential for close air-water contact would be diminished, having the effect of reducing the retardation of C-14.

D4. Conclusions and Recommendations

The results of Amter et al (1988) and Knapp (1987) for transport of C-14 from the Yucca Mountain repository to the surface of the earth predict travel times ranging from a few hundred to a few thousand years, and are shortest during the period where there is significant heating from the radioactive decay. This period of short travel times coincides roughly with the period when the present model predicts most of the C-14 releases to occur, but any release depends on the failure of the waste canisters. The release of C-14 is very sensitive to the lifetime of the waste package in the present modeling approach, particularly because early failure times lead to faster and more complete oxidation of the uranium dioxide. Considering the 5720 year halflife of C-14, there would be relatively little attenuation of the cumulative release of C-14 at the earth's surface because of holdup in the geologic barrier.

The present release and transport models have been formulated using assumptions that we believe to be conservative, but there is little direct evidence to support these assumptions. We have identified the following areas where the collection of additional data would be most fruitful:

- Investigate the mechanisms for C-14 release, including the available information on dry cask storage, and the investigations to be performed as part of site characterization. There is considerable scatter in the data on spallation of the uranium dioxide fuel, and this could be a potential source of uncertainty. Direct measurements of C-14 releases from the various compartments of the fuel would be more reliable than models based indirectly on effects such as fuel spallation.

- Investigate geochemistry of calcite precipitation at the Yucca Mountain site under repository conditions to determine whether the released C-14 is removed effectively before reaching the accessible environment. There are several counteracting factors involved in the effectiveness of this mechanism for removing C-14. Knapp (1987) states that "Water-rock interaction is probably insignificant due to the low abundance of calcite at the Nevada site and due to the prediction that calcite will not precipitate". However calcite solubility diminishes with increasing temperature, leading to the possibility that repository-induced heating would cause calcite precipitation.

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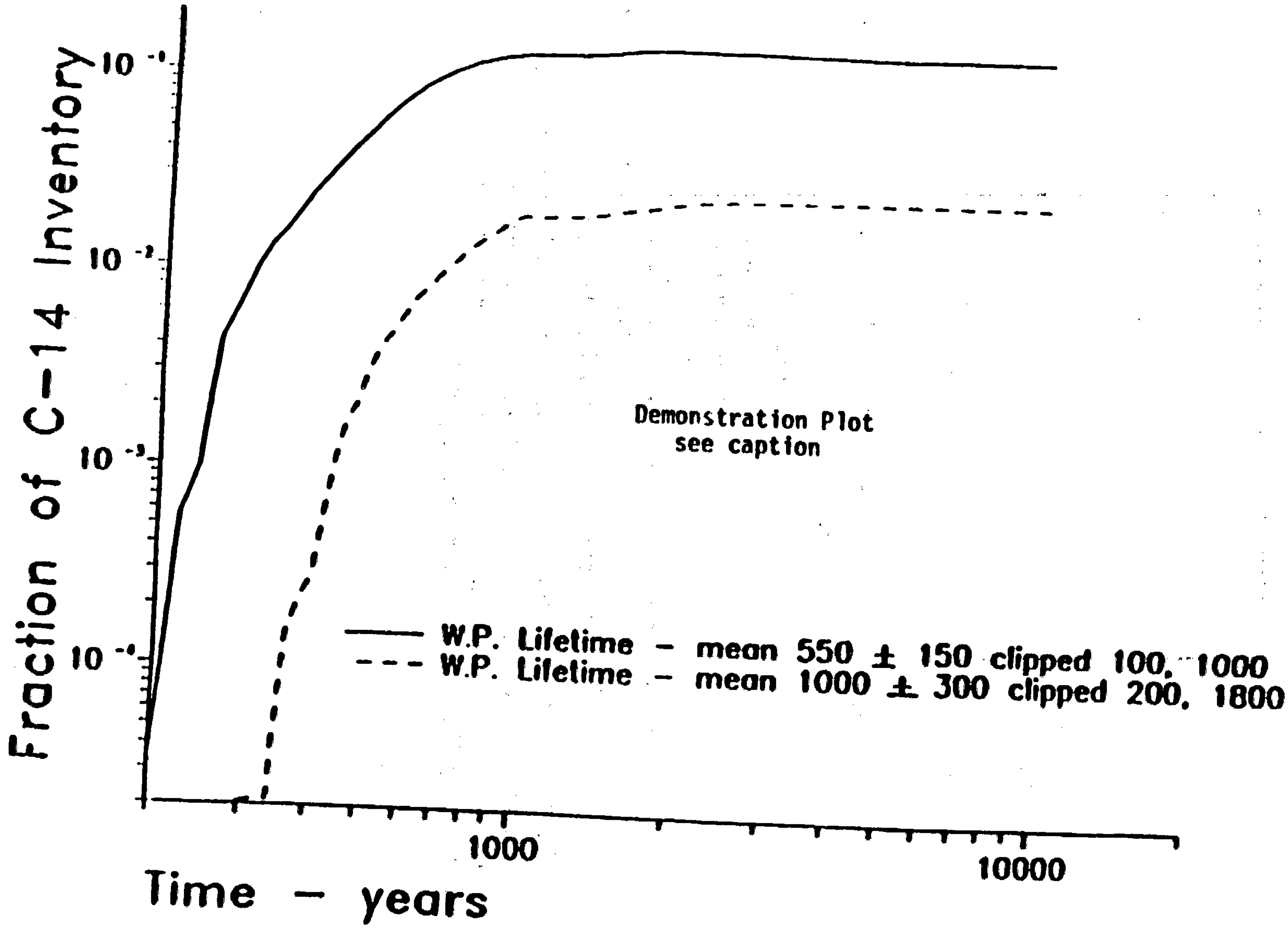

Figure D.1 Release of C-14 Inventory. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

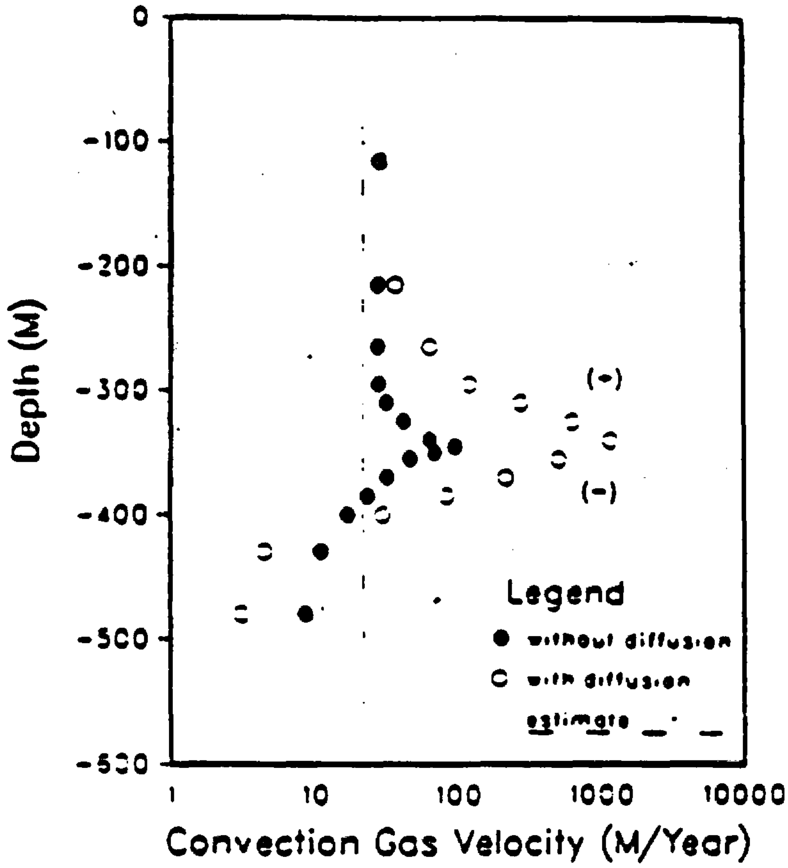

Fig. 02 Gas convection velocities along the repository center line at 100 years after waste emplacement. Plus and Minus signs refer to upward and downward fluxes at the repository depth for the case with binary diffusion. (after Preuss, 1987)

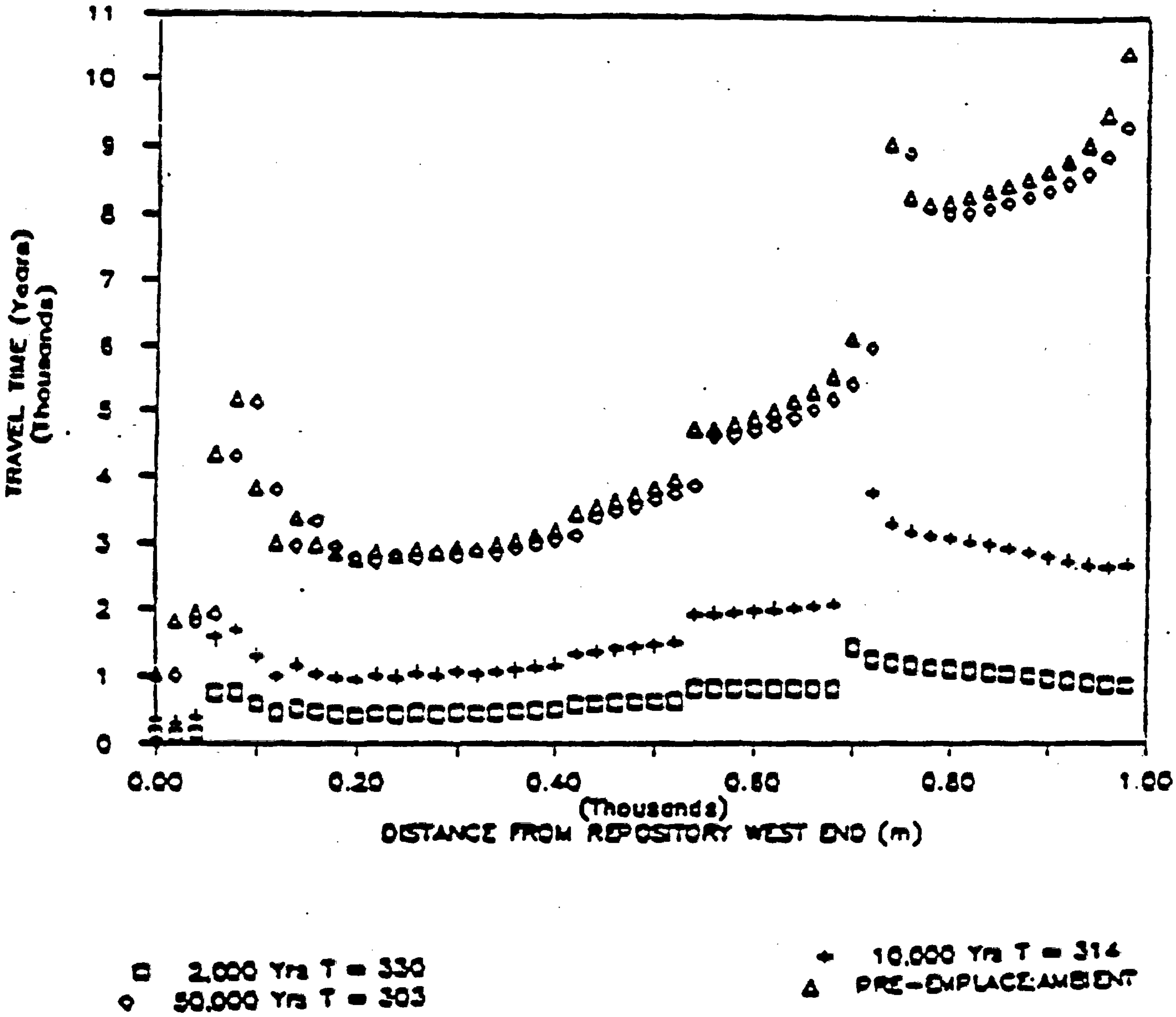

Figure D3 Carbon-14 travel time from the repository to the surface for ambient conditions, 2,000, 10,0000, and 50,000 years. (After Ampter, 1988)

APPENDIX E - TESTING STATISTICAL CONVERGENCE

The Latin Hypercube Sampling method is an efficient method for performing Monte Carlo analyses (Iman, 1980a). As with all Monte Carlo analyses, increasing the number of samples increases the convergence of the statistical results. We are usually interested in minimizing the number of repetitions, particularly for complicated, time-consuming calculations. A rough "rule of thumb" for LHS analysis is that the minimum number of samples should be 4/3 the number of independent variables for good statistical convergence (Bonano, et. al., 1989). It is not clear however whether the rule of thumb is meant to apply both to the generation of the CCDF curve and the sensitivity analysis or just the latter. The following example was designed to test whether or not this "rule of thumb" applies to highly nonlinear problems like the present calculation.

There are 47 independent variables sampled in the present analysis. The rule would therefore predict that about 63 samples would be sufficient to generate an acceptable output distribution; i.e., the CCDF of EPA release fraction. To test this hypothesis, we generated the 10,000 year CCDF for the base-case scenario from 500 LHS samples in order to have a smooth benchmark curve representing a statistically converged distribution. We then generated 5 CCDF curves for the same distribution, but using only 100 LHS samples each, with each case employing a new random seed. The results are shown in Figure E1. Only one of the five CCDF curves generated with the 100 point samples was close to the 500 point CCDF curve. Convergence was best in the low-release region, and generally poor in the high-release region. The 100-point case leads to a spread in the release in the high-consequence portion of the curve of about two orders of magnitude. This result indicates that the "rule of thumb" in this case is inadequate, and many more samples would be required (We should note however that this analysis used only a single scenario, and the statistical convergence treating all scenarios along with their respective scenario probabilities might behave differently).

The probable explanation for the inadequacy of the "rule of thumb" in this case is that there were relatively few samples giving high release, and many cases where there was no release at all within 10,000 years. The low-release samples were far more prevalent, as demonstrate by the generally good agreement in that portion of the curve. The result of this exercise points to the need for care in using the LHS method to assure that enough samples are generated for statistical convergence. Iman in fact warns that the sample size is highly problem-specific (Iman, 1980b) We should also pursue some of the more sophisticated sampling methods such as Fast Probabilistic methods and Importance Sampling (e.g. CNWRA, 1988).

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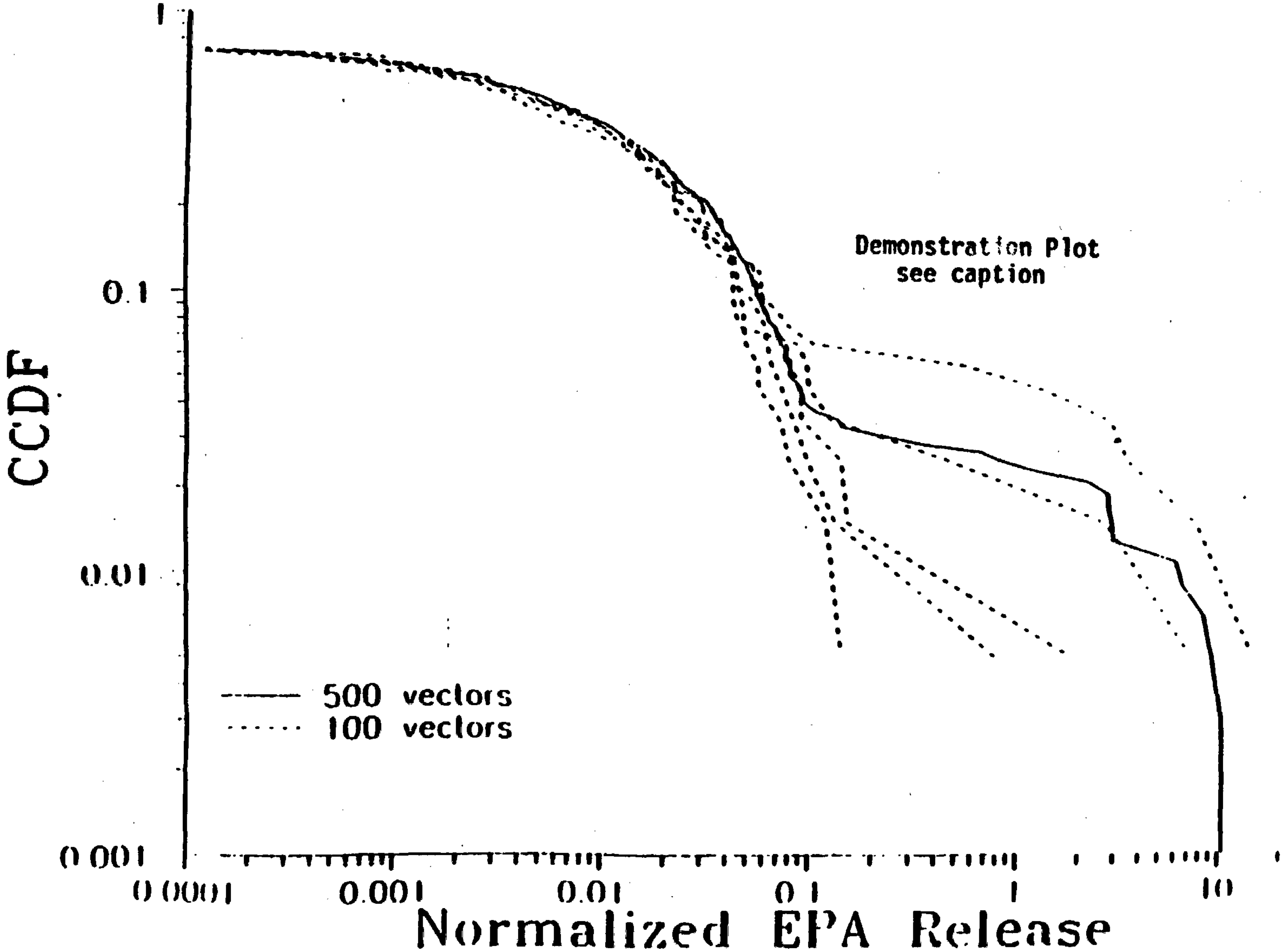

Figure E.1 Statistical Convergence; 100 vs. 500 Vectors, 10,000 Years, Base Case. This graph presents results from an initial demonstration of staff capability to conduct a performance assessment. The graph, like the demonstration, is limited by the use of many simplifying assumptions and sparse data.

APPENDIX F - AUXILIARY ANALYSIS OF HYDROLOGIC DATA

An auxiliary analysis of hydrologic data was conducted to determine if spatial correlations could be identified for porosity and hydraulic conductivity parameters. This analysis did not identify any spatial correlation with depth for saturated hydraulic conductivity data or for Calico Hills unit porosity data. A large scale trend of decreasing porosity with increasing depth was identified for the Topopah Springs unit and a small scale correlation length of less than 40 meters was identified in data from two holes in the Topopah Springs unit.

The identification of spatial correlation is important to performance assessment modeling, because longer correlation lengths increase the probability that contaminated ground water pathways will be encountered which might provide quicker transport of radionuclides to the water table. To look for correlation lengths the program GEO-EAS (Geostatistical Environmental Assessment Software)(Englund, 1988) was used to generate scatter plots, histogram plots, cumulative distribution plots (probability plots) and variograms of depth, porosity, and saturated hydraulic conductivity data for the Calico Hills and Topopah Springs units. A variogram is a means of quantifying the commonly observed relationship that samples close together will tend to have more similar values than samples far apart. In this analysis the scatter plots were used to look for trends with depth, while the variograms were used to look for spatial correlation in the vertical distance between pairs of measurements.

Since unsaturated zone hydrology parameters were of interest, this study only used core data. The data input files from DOE data (Anderson, 1981, 1981a, Hayden, 1985, Lahoud, 1984, Peters, 1984, Sinnock, 1986, Weeks, 1984). In all runs depth is in meters, porosity is unitless, and saturated hydraulic conductivity is in meters/second.

Histogram plots of Topopah Springs and Calico Hills porosity data were prepared using all the porosity data from these units in the data base. The histogram plot of the Topopah Springs porosity values was made from 6 wells and 200 samples. The histogram plot of the Calico Hills porosity values was made from 6 wells and 174 samples. From the histograms it was concluded that (1) the Topopah Springs unit tends to have lower porosity values than the Calico Hills unit, (2) the distribution of Topopah Spring porosity data are skewed to the lower porosity values, (3) the Calico Hills porosity data are skewed to higher porosity values and are bimodal (Figures F-1 and F-2). These results may reflect the difference in matrix porosity values between the nonwelded Calico Hills unit and the welded Topopah Springs unit.

Scatter and variogram plots where made only for holes which had enough data to conduct this type of analysis. Data from 5 holes (holes: USW GU-3, USW G-1, USW G-4, USW H-1, UE25a-1) were used in the analysis (Figure F-3). Separate plots of saturated hydraulic conductivity, porosity, and distance were made for each hole for the Calico Hills and Topopah Springs units.

No correlations with depth could be identified in scatter plots and variogram plots of saturated hydraulic conductivity from either the Topopah Springs or Calico Hills units. In addition no correlations with depth could be identified in plots of porosity data from the Calico Hills unit.

However, a trend of decreasing porosity with depth was identified in scatter plots of some of the holes in the Topopah Springs unit (UE25a-1, USW GU-3, and USW G-4) (Figures F-4, F-5, F-6). This trend may be the result of increasing welding with depth, resulting in decreased porosity with depth. Porosity variogram plots of the Topopah Springs unit for two holes (USW GU-3 and USW G-1) contained a pattern, which could be due to the trend noticed in the scatter plots. When the trend was removed, there appeared to be spatial correlation displayed in variograms for holes USW G-4 and UE25a-1 (Figures F-7 and F-8). In both cases the variogram has a sill of 40 meters or less, indicating that beyond a 40 meter separation distance there is no spatial correlation for porosity.

In summary, a large scale trend of decreasing porosity with increasing depth was identified in data from three holes drilled into the Topopah Springs unit and a small scale correlation length of less than 40 meters was identified in data from two holes drilled into the Topopah Springs unit. However, this analysis did not identify any spatial correlation with depth for Calico Hills porosity data or for saturated hydraulic conductivity in either the Calico Hills or the Topopah Springs units. This result was relevant to the flow and transport modeling, because long correlation lengths lead to a broad travel time distribution for each column (Section 9.3.1.4). Very short correlation lengths lead to the conclusion there is a single ground water travel time per column and little likelihood of long, fast ground water flow paths. In the flow and transport modeling, it was assumed that there was no apparent spatial correlation for saturated hydraulic conductivity beyond 10 meters separation (Section 9.3.1.5).

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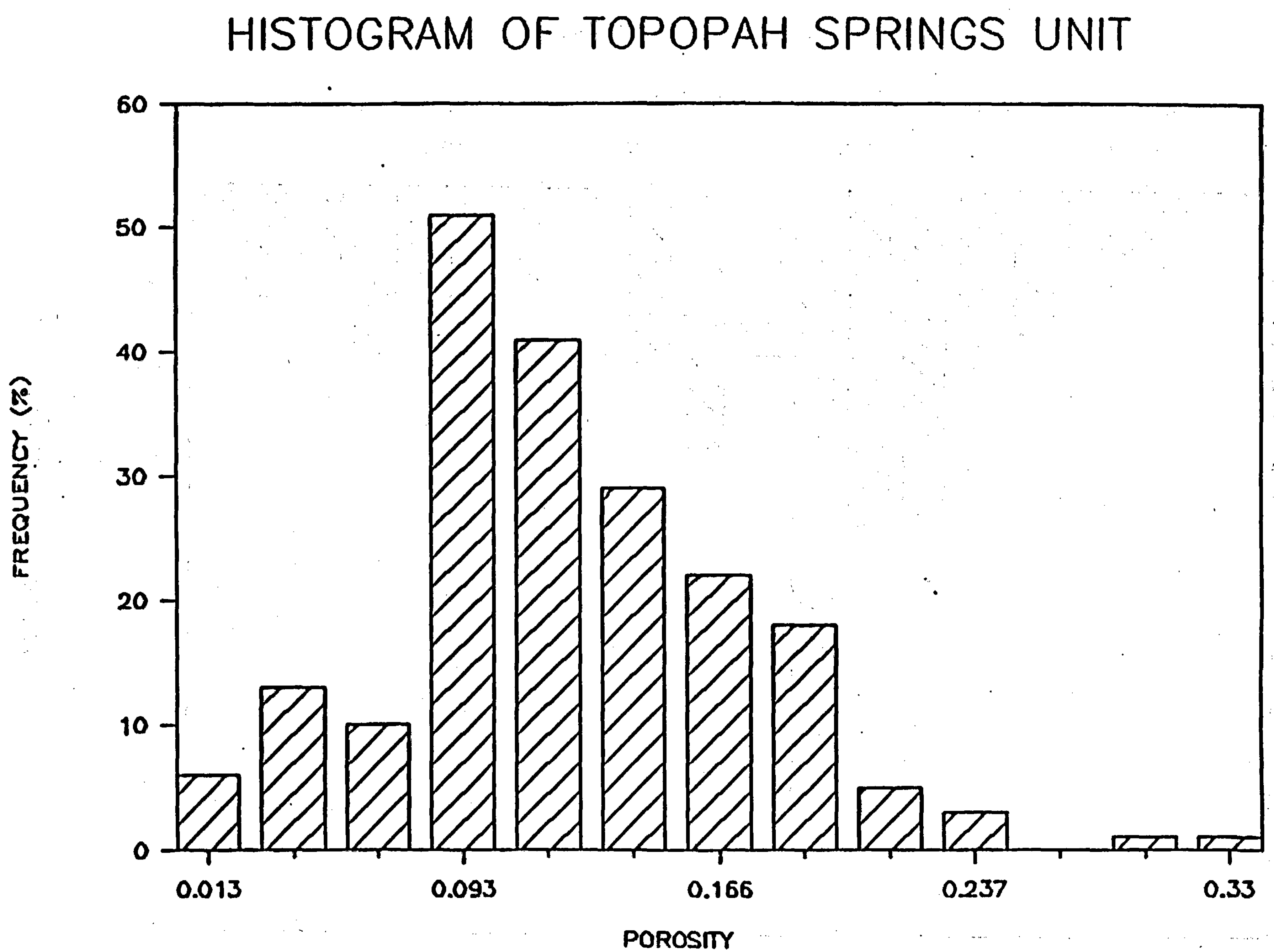

Figure F-1 Histogram of Topopah Springs Porosity Values

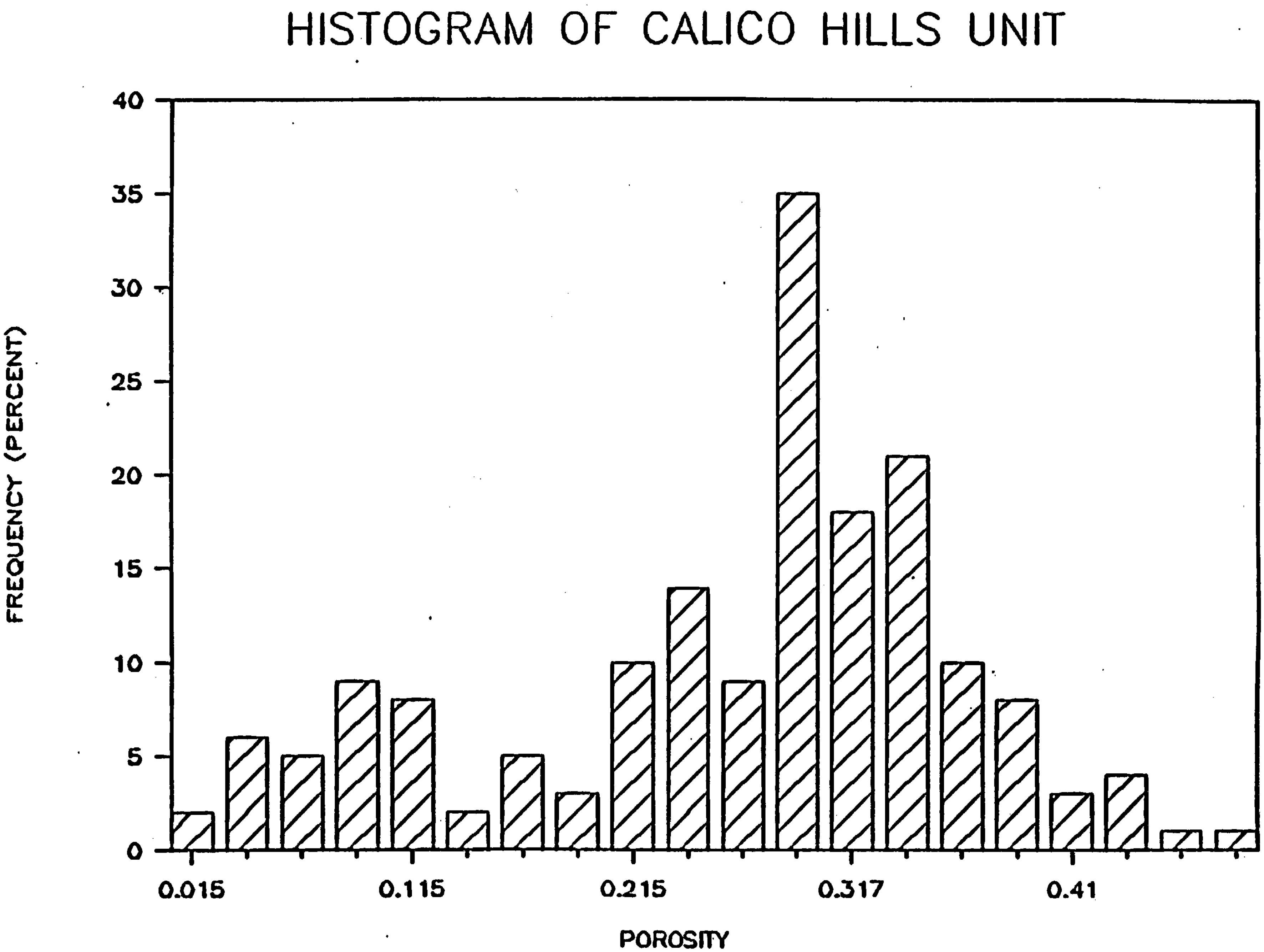

Figure F-2 Histogram of Calico Hills Porosity Values

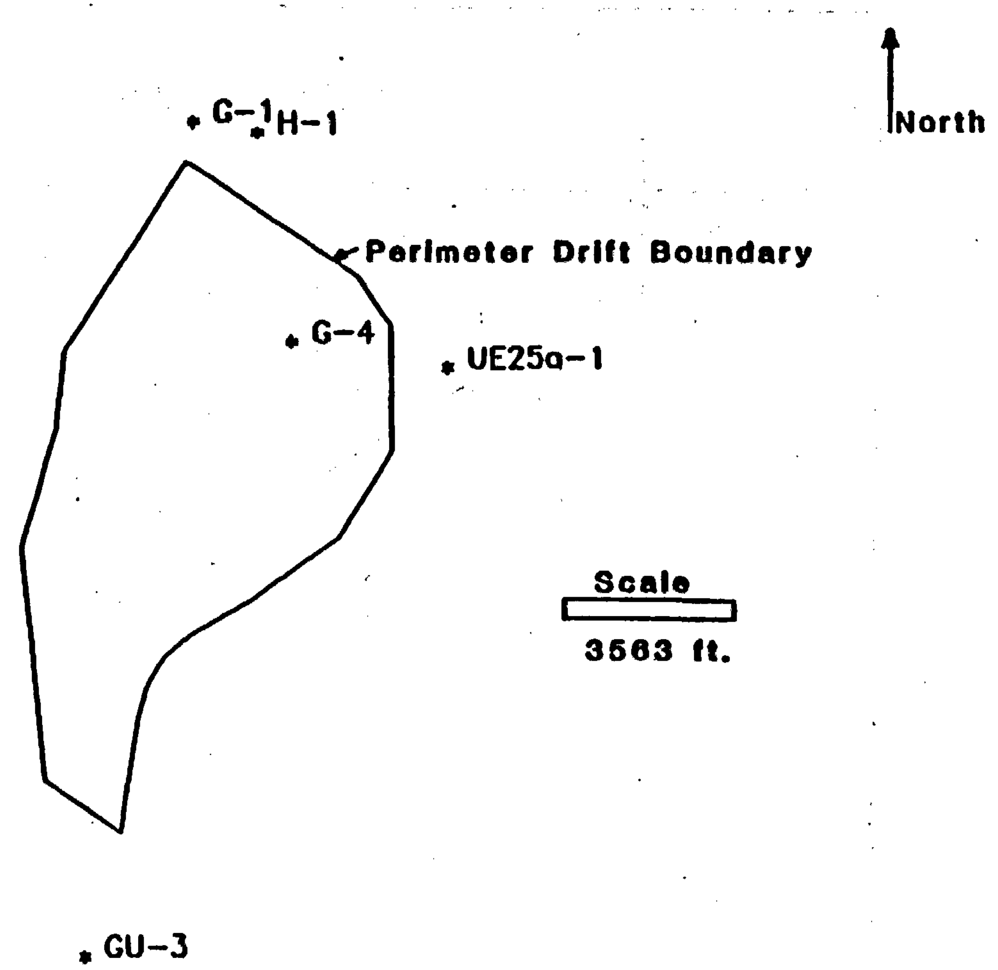

Figure F-3 Location Map of Holes Used in Scatter and Variogram Plots

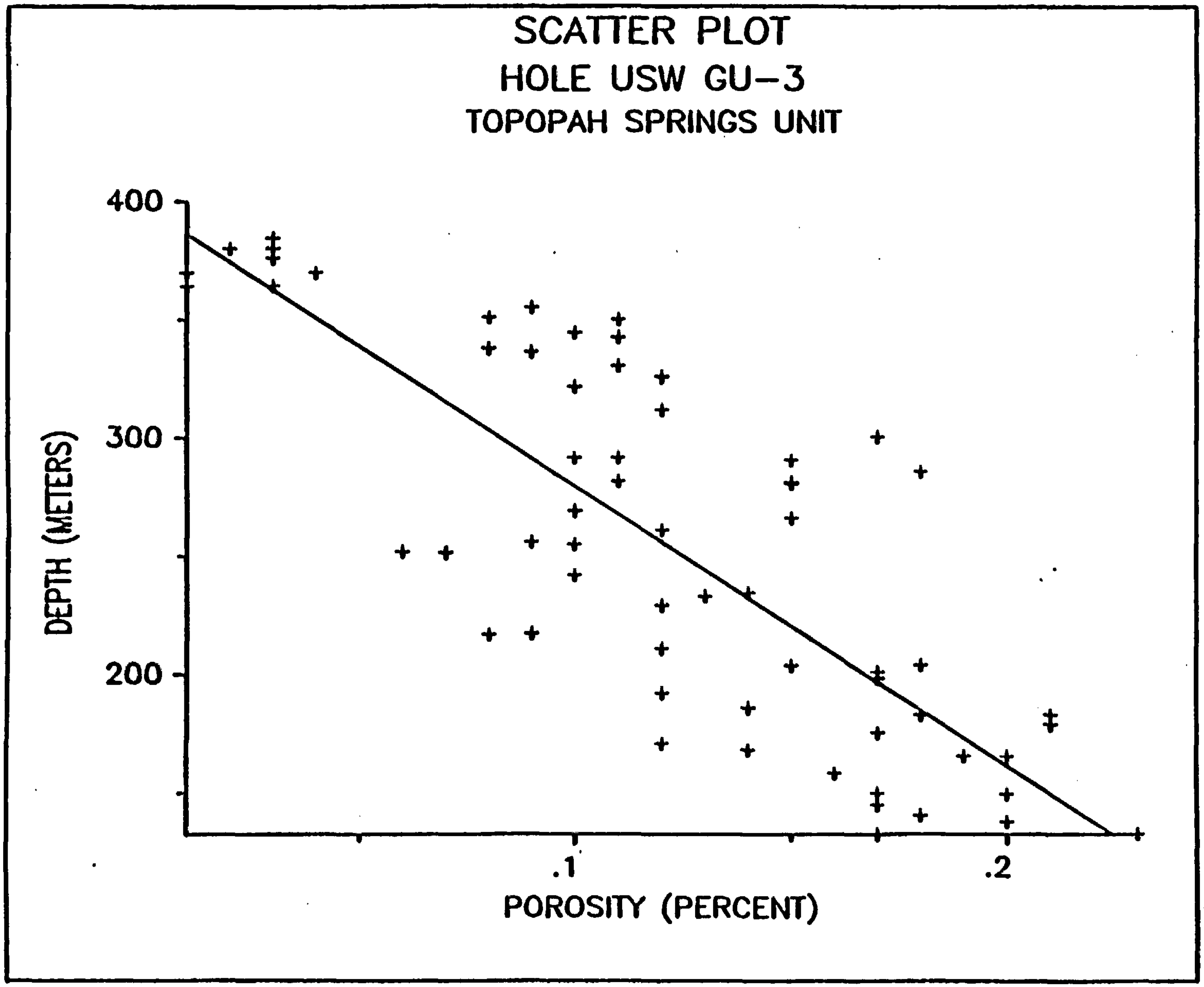

Figure F-4 Scatter Plot, Hole USW GU-3, Topopah Springs Unit

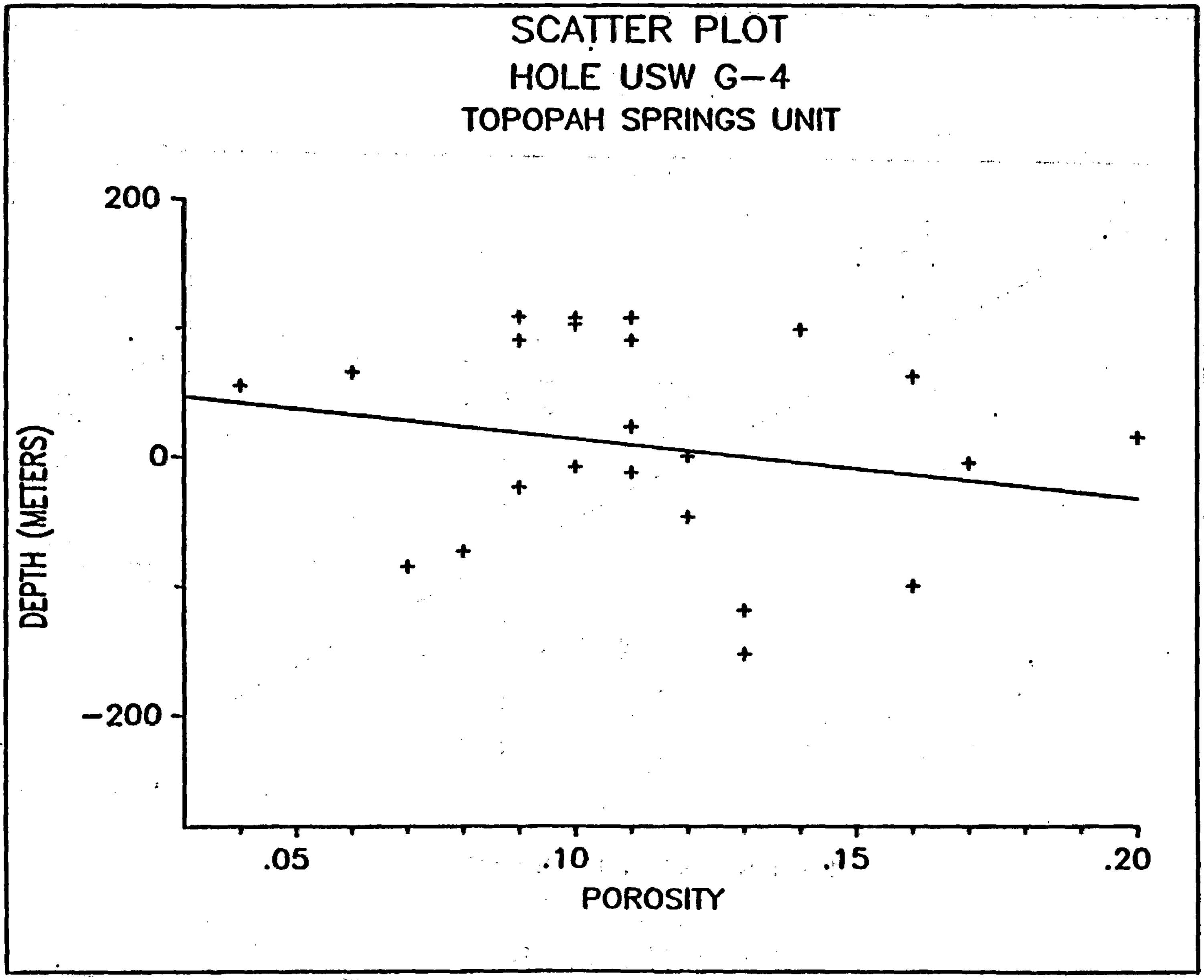

Figure F-5 Scatter Plot, Hole USW G-4, Topopah Springs Unit

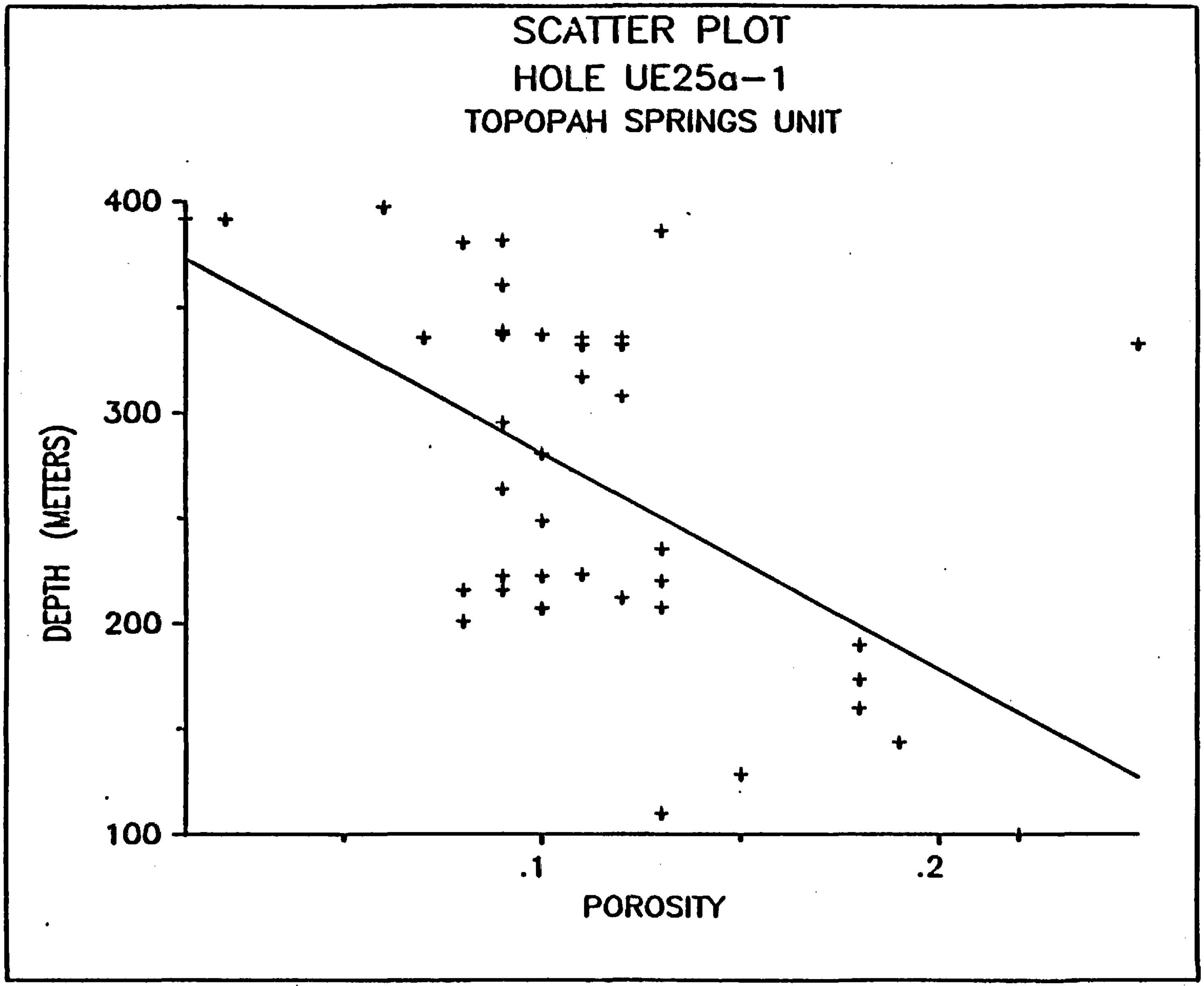

Figure F-6 Scatter Plot, Hole UE25a-1, Topopah Springs Unit

Variogram for POROSITY

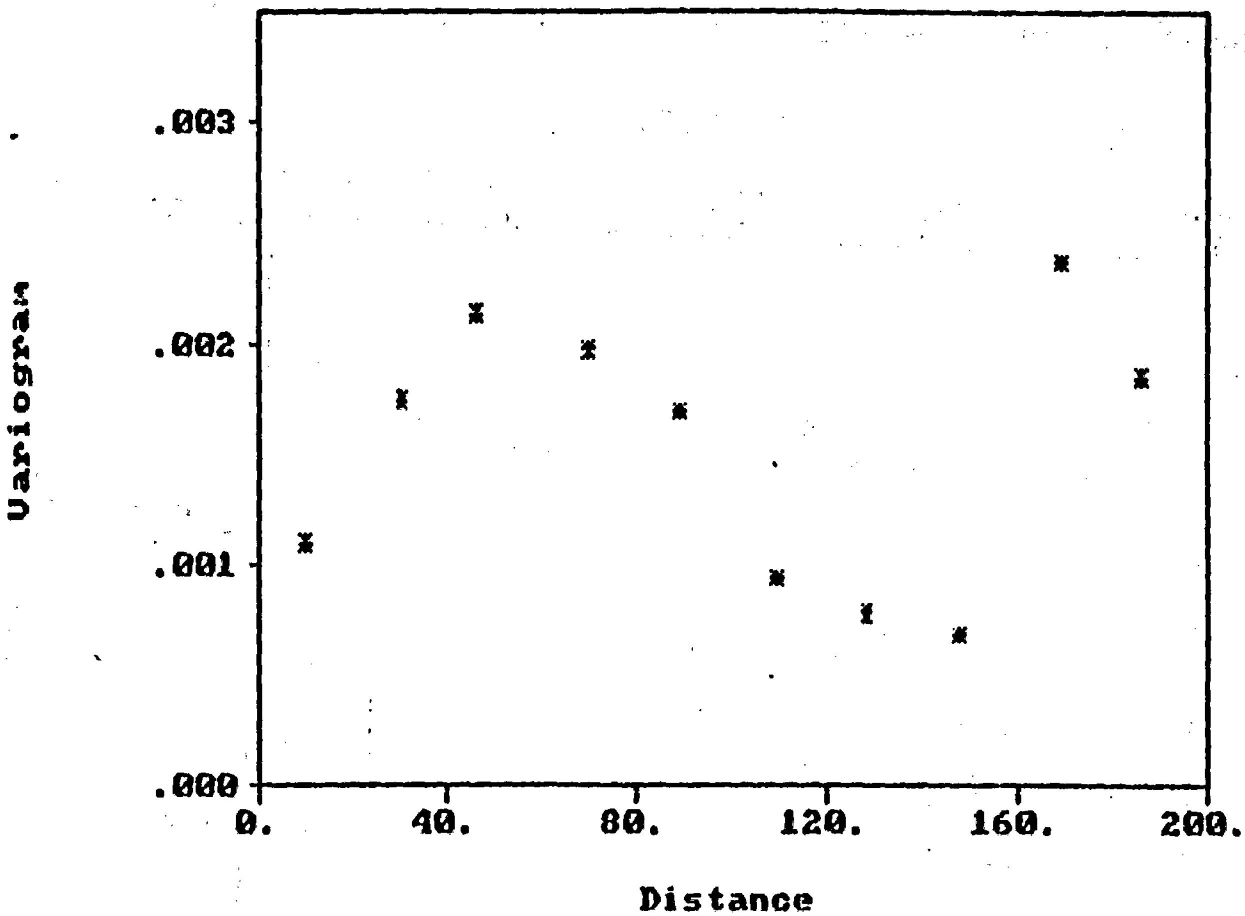

Figure F-7 Porosity Variogram, Hole USW G-4, Topopah Springs Unit

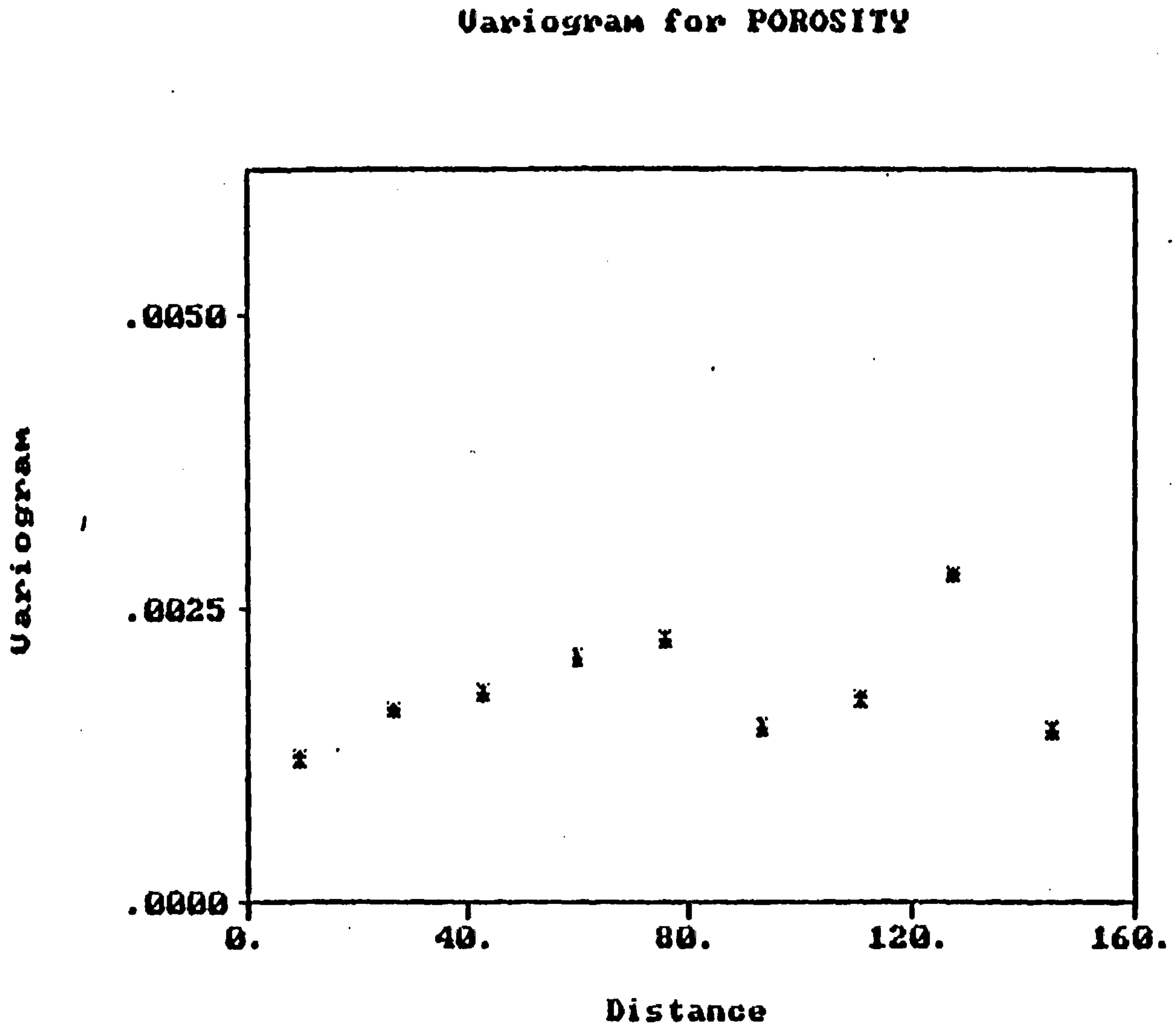

Figure F-8 Porosity Variogram, Hole UE25a-1, Topopah Springs Unit

APPENDIX G - TWO-DIMENSIONAL CROSS SECTIONAL FLOW MODEL

G.1 Introduction

The HYDROCOIN unsaturated fractured tuff test case described a hydrogeologic sysytem which was comprised of layers whose matrix properties varied over many orders of magnitude. Due to contrasts in properties at unit interfaces and a dip (average dip of 6 degrees) of the units it could be expected that water would perch or preferentially move down-gradient with a horizontal velocity component rather than move only vertically.

The degree of horizontal flow is an important consideration because: 1) above the repository flow diversion could lead to a reduction in flux through the repository, and 2) below the repository horizontal flow could lead to a shorter path to the water table. Hydrologic modeling can be useful in identifying the conditions (e.g., flux rate) that lead to horizontal flow and the influence these conditions have on flux through a repository and the geometry of travel paths.

G.2 Purpose

Hydrologic modeling of unsaturated fractured tuff currently is limited to a dual-porosity approach for the treatment of fracture-matrix interaction and is computationally intensive. However, some relatively simple modeling of layered systems can be done to: 1) gain insights into the flow diversion issue and how this affects the fluid flux through the repository and the validity of the vertical flow path assumption, 2) understand the numerical limitations better, and 3) provide simple initial simulations studies as the basis for understanding the effects of further modeling refinements.

G.3 Problem Set-up

This initial analysis assumed matrix flow only and used the description of the tuff site description defined by DOE in the HYDROCOIN Project (Prindle, 1987) and used the VAM2D computer program to simulate the matrix flow problem. The analysis involved a steady state simulation using the layering and parametric values presented in Figure G.1 and Table G.1, respectively. The boundary conditions were: a constant infiltration rate on the upper surface, a constant head at the lower (water table) boundary, and noflow conditions on the sides. Addtionally, all the layers were tilted six degrees.

G.4 Results and Conclusions

The diversion of flow at the interfaces was investigated by simulating the HYDROCOIN test case with different infiltration rates of .1, .2, and .5 mm/yr (for the .5 mm/yr simulation the low conductivity upper layer was not included due to the fact that the infiltration rate was greater than the saturated conductivity of the layer). The results of the simulations, presented as the ratio of horizontal to vertical flow immediately above an interface, are presented in Table G.2. Vertical flow dominated in all units when the infiltration was .1mm/yr. When infiltration was .2 mm/yr or more, horizontal flow was at least an order of magnitude higher than vertical flow above the low conductivity unit (Layer C). The horizontal gradient, a result of the tilted bedding of the layers, and the low hydraulic conductivity of the unit underlying Layer C are the primary reasons that a significant component of velocity was in the horizontal direction in the lower portion of Layer C. Although the nonwelded unit (Layer E) shows a large component of horizontal flow, this result was due to the imposed boundary condition and the tilt of the layers rather than increased infiltration.

These simulations indicate that infiltration rates greater than .2 mm/yr combined with the six degree slope in unit bedding could produce a significant amount of horizontal flow. If similar conditions existed at Yucca Mountain, these flows could result in perched zones or localized fracture flow (However a conclusion on what effect horizontal flow would have on overall performance cannot be made by this analysis). It is very important to note, that this analysis did not account for the presence of fractures, heterogeneities, or anisotropy in hydraulic parameters. Future modeling efforts should examine the influence of these additional complications.

G.5 References

Prindle, R.W., 1987, Specification of a Test Problem for HYDROCOIN Level 3 Case 2: Sensitivity Analysis for Deep Disposal in Partially Saturated, Fractured Tuff, Sandia National Laboratories, SAND86-1264, Albuquerque, New Mexico.

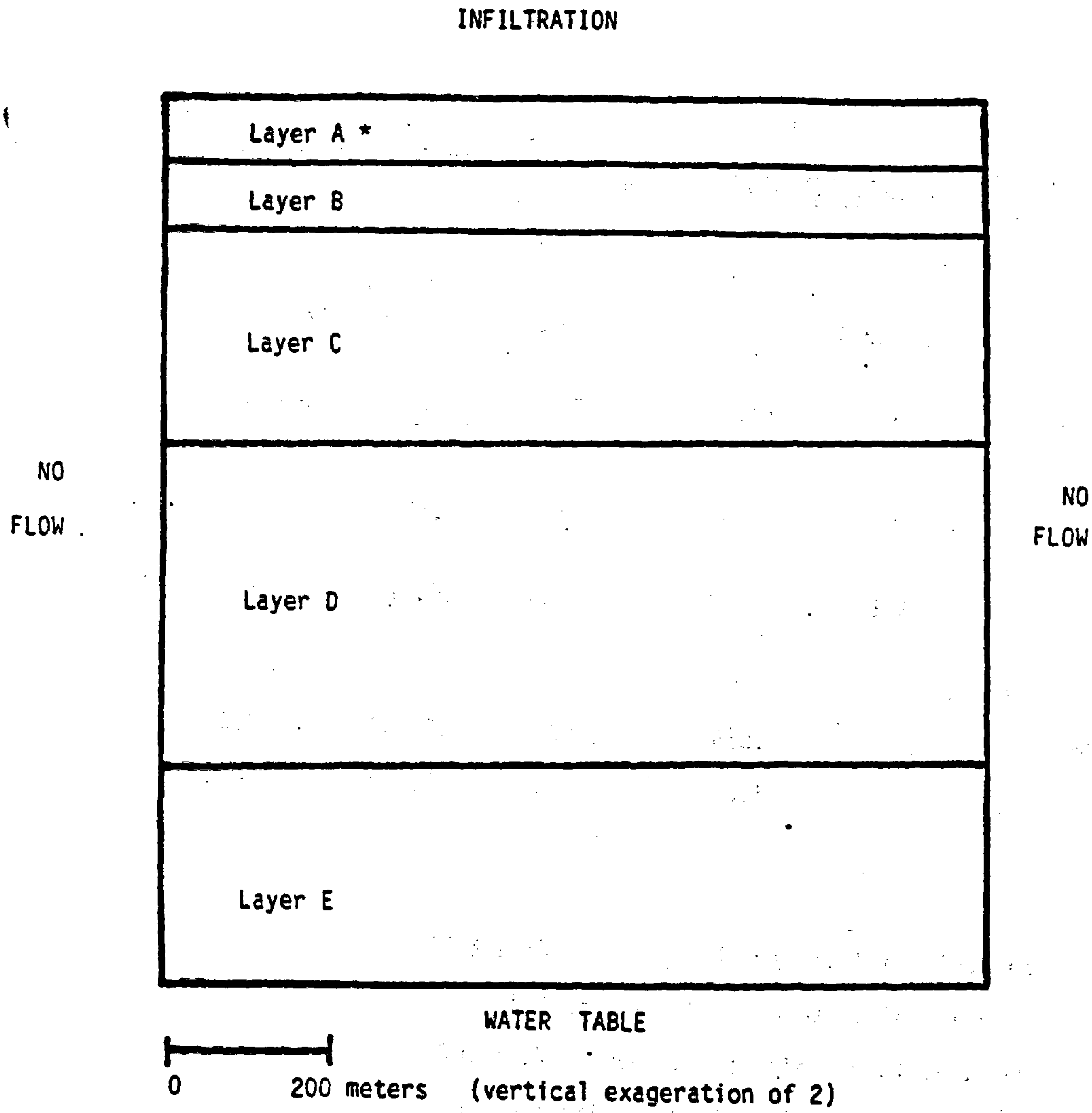

Figure G.1 Hydrogeologic units and boundary conditions used in the cross sectional simulation using the VAM2D computer program (note: the figure does not show the six degree incline that was included in the simulation).

* see Table G.1 for Layer descriptions

Table G.1 Hydraulic properties used in the two-dimensional simulation of a layered tuff site (Prindle, 1987).

PROPERTIES	Layer A	Layer B	Layer C	Layer D	Layer E
Saturated Conductivity (mm/yr)	.3	10,000.	.6	.6	8,000.
Porosity	.08	.40	.11	.11	.28
Thickness (m)	26.8	38.1	130.1	205.1	130.3
van Genuchten Parameters:					
Alpha (1/m)	.00821	.015	.00567	.00567	.016
Beta	1.558	6.872	1.798	1.798	3.872

layer A: moderately to densely welded, devitrified tuff

Layer B: partially welded to nonwelded vitric tuff

Layer C: moderately to densely welded, devitrified tuff

Layer D: moderately to densely welded, devitrified tuff

Layer E: nonwelded vitric and zeolitic tuffs

Table G.2 Ratio of horizontal to vertical flow at the interfaces between different hydrologic units over differing infiltration rates.

RATIO OF HORIZONTAL TO VERTICAL FLOW

Interface	Infiltration Rates .1 mm/yr	.2 mm/yr	.5 mm/yr
Layer A (Ksat = .3 mm/yr) Layer B (Ksat = 10,000. mm/yr)	.05	.07	--
Layer B (Ksat = 10,000. mm/yr) Layer C (Ksat = .6 mm/yr)	.07	15.	19.
Layer C (Ksat = .6 mm/yr) Layer D (Ksat = .6 mm/yr)	.005	.005	.005
Layer D (Ksat = .6 mm/yr) Layer E (Ksat = 8,000. mm/yr)	.010	.010	.010
Layer E (Ksat = 8,000. mm/yr) water table	.19	.19	.19

APPENDIX H - ANALYSIS FOR DRILLING SCENARIO

The analysis for the drilling scenario largely follows the concepts discussed in the DOE SCP, used to make an estimate of the EPPM; however the analysis in the SCP is expanded upon and modified is some significant ways. The drilling scenario is in some ways the archetypical direct release scenario and it is anticipated that many of the approaches to analyzing both the probabilities and the consequences of this scenario can be extended to similar scenarios, with appropriate modifications.

Scenario Probability

To analyze this scenario many of the concepts used in formulating Appendix B of 40 CFR 191 are used. Although this part of that regulation is offered as guidance and is not binding on either the DOE or the NRC, the concepts expressed are a useful starting pont for this initial analysis. Two fundamental ideas behind the drilling analysis are: (1) that the institutional memory and control preventing disturbance of the repository fail after some period of time, (2) that the permanent markers at the site fail in their function after some time. After the greater of these times, it is assumed that drilling for economic resources commences. It is assumed that this drilling occurs at the same rate of drilling as today for the type of rock involved. Because of these assumptions, a natural approach to the analysis is to assume that drilling occurs randomly in space and time and that it can be effectively described as a Poisson process. Although these are rather sweeping assumptions, viable competing hypotheses appear to be at least as speculative or arbitrary. Furthermore, the purpose of the analysis is to reveal any weaknesses in the design or siting of the repository, so if these assumptions preserve important relationships between the important variables affecting the performance of the repository, then their inherent verissimilitude may not be important.

To begin the analysis assume that exploratory drilling takes place at a constant rate, r [per year per square kilometer]; then the rate of drilling over the repository is:

$$R=rA_r \qquad (1)$$

where,

R is the rate of drilling into the repository,

A_r is the area of the repository.

If we assume that this drilling occurs in a random fashion, with no memory of previous drilling, then a Poisson distribution may be used to describe the probability of N boreholes being drilled into the repository over a period of time, δt:

$$P(N) = \frac{(R\delta t)^N \exp(-R\delta t)}{N!} \qquad (2)$$

where,

δt is the time period over which drilling occurs,
N is the number of boreholes.

In general, under this set of assumptions, there can be any number of boreholes over a particular period of time; however, the form of the distribution given in equation (2) assures that the expected value of number of boreholes, $\bar{N}$, is equal to $R\delta t$. Without too much difficulty at this stage of the analysis, a somewhat more general approach to drilling probability can be taken by assuming a Weibull distribution instead of the Poisson distribution. For the Weibull distribution we have,

$$F(t) = \begin{cases} \dfrac{\beta}{\delta} \{(t-\Gamma)/\delta\} \exp\{-[(t-\Gamma)/\delta]^{\beta}\} & t>\Gamma \\ 0 & t<\Gamma \end{cases}$$

For this analysis the location parameter, Γ, would be taken to be the time at which drilling is assumed to commence, T_d. The scale parameter, δ, would be taken to be $1/R\delta T$. The shape parameter, β, could be chosen to represent a gradual change from a zero rate of drilling to the constant value R used in the Poisson distribution, (2) above. Of course the distribution would need to be suitably modified to account for the finite number of boreholes, N. This refinement was not used in the present analysis.

For the purpose of this scenario the time period of interest is the time between the commencement of drilling, T_d, and the time duration of the simulation (the period of time over which the performance of the repository is to be estimated, e.g. 10,000 years), T_p. That is:

$$\delta t = T_p - T_d \qquad (3)$$

Then combining equations (2) and (3), the probability of N boreholes penetrating the site is given by,

$$P(N) = \frac{(R(T_p - T_d))^N \exp(-R(T_p - T_d))}{N!} \qquad (4)$$

and the probability that no boreholes penetrate the site is obtained from (4) by setting N = 0,

$$P(0) = \exp(-R(T_p - T_d)) \qquad (5)$$

Both of the above probabilities assume that $T_p > T_d$; that is that drilling starts sometime before the end of the period of consideration. If drilling starts at a later time, then equations (4) and (5) must be replaced by,

$$P(N) = 0 \qquad (4a)$$

and

$$P(0) = 1 \qquad (5a)$$

The probability of the drilling scenario, P_s, i.e. that some drilling into the repository occurs, is given by:

$$P_s = 1 - P(0)$$

or

$$P_s = 1 - \exp(-R(T_p - T_d)) \qquad (6)$$

For the assumptions used in the SCP (r = .0003 boreholes per square km per year, A_r = 5.1 square km, T_p = 10,000 years, and T_d = 0), P(0) = 2.27 E-07, P_s 1, and R = 15.3. This means that the likelihood of no drilling is very small and that, on average, at least 15 boreholes will be drilled at the site over the 10,000 year period of consideration.

The discussion above establishes the probability for the drilling scenario overall and the probability of N boreholes being drilled on the repository site. However, the analysis of this scenario is made more complex, because a borehole can either penetrate the emplaced waste or merely excavate some of the surrounding host rock. In effect, embedded in this scenario is a two-branch event tree:

```
                          |drill excavates
                          |     waste and host rock
                          |
drilling occurs ----------
on site                   |
                          |
                          |
                          |drill excavates only
                             host rock
```

In the event that only host rock, i.e. no waste, is excavated, some radiological consequences may occur, because in general the host rock will be contaminated to some level by the movement of contaminated groundwater from the repository. The probabilities and consequences of these two event-tree branches need to be considered in the analysis.

First consider the probability of excavation of waste given that drilling occurs on the repository site, P_e. Assuming that the interception area of drilling is small compared to the repository area, then:

$$P_e = \frac{\text{intercept area}}{\text{repository area}}$$

or

$$P_e = \frac{N_T A_p}{A_r} \qquad (7)$$

where A_p is the projected intercept area of a waste package on a horizontal plane

and N_T is the total number of waste packages.

For vertical emplacement the projected intercept area is a circle with a radius equal to the sum of the package radius and the drill radius (see figure 1a.). Thus for vertical emplacement:

$$A_p = \pi\ (\ r_p + r_d\ )^2 \qquad (8a)$$

where r_p is the radius of the waste package
and r_d is the radius of the drill.

For horizontal emplacement, the projected intercept area is a rectangle with height equal to the sum of the package diameter and the drill diameter and width equal to the sum of the package length and drill diameter (see figure 1b.). Thus for horizontal emplacement:

$$A_p = [2(r_p + r_d)]\ [L + 2r_d] \qquad (8b)$$

where L is the length of the waste package.

For the current repository and waste package design (r_p = .34 m, L = 4.3 m, N_T = 18,000, A_r = 5.1 square km, and assuming the drill diameter is 6 cm), we find for vertical emplacement:

$$P_e = .001518$$

and for horizontal emplacement:

$$Pe = .01139$$

Consequence Analysis

With such small target-strike probabilities, the usual outcome will be to excavate contaminated host rock rather than waste. Therefore, it is important to estimate the consequences of excavating contaminated host rock.

First consider the volume of waste that would be excavated if a borehole penetrated a waste package. Considering the manner in which the probability of excavation was calculated, a conservative assumption is being used here; i.e., if the waste package is touched by the drill, then the entire cylinder of material excavated from the horizon of the waste package top to the horizon of the waste package bottom is assumed to be solid waste. For boreholes just tangent to the perimeter of the waste package or only partially overlapping it, this is clearly a conservative assumption. For this assumption the volume of excavated waste, V_e, for vertical emplacement is given by:

$$V_e = \pi r_d^2 L \qquad (9a)$$

For horizontal emplacement the situation is somewhat more complicated because the length of the column of excavated waste depends on the location on the package at which the drill impinges (see figure 2.). If we let h be the height of the column of waste and x be the distance from the center of the drill to the midpoint of the waste package, then

$$h = 2 (r_p^2 - x^2)^{\frac{1}{2}}$$

where $x = \langle 0, r_p \rangle$

and x is considered to be uniformly distributed over the indicated range. The average value of height, h, is:

$$\hat{h} = \frac{\pi r_p}{2}$$

whereas the maximum value of h is $2r_p$. Since the ratio of the maximum value of height to the average value is $4/\pi$, a slightly conservative assumption is to assume that the maximum height should be used in calculating the waste volume. But since the values are so close, either choice is reasonable. For a very detailed analysis, in which a great many simulations would be run, the location parameter, x, could be treated as a random variable selected from a uniform distribution; however, this seems to be an excessive level of analysis for this aspect. Therefore, we take as the average volume of waste excavated for each borehole penetrating a horizontally emplaced waste package:

$$V_e = \frac{r_p (\pi r_d)^2}{2} \qquad (9b)$$

Now the concentration of waste in the waste package can be considered to be:

$$C_w = \frac{A_s\, Q_w}{N_T\, V_p} \qquad (10a)$$

where A_s is the specific activity of the emplaced waste (curies per MTHM)

Q_w is the total quantity of emplaced waste (MTHM)

N_T is the total number of waste packages

V_p is the volume of a single waste package.

The concentration of waste in the host rock depends upon a number of factors including the solubility of the waste, how long the waste has been dissolving, how rapidly the waste is being dispersed in the groundwater system, the porosity of the rock, and the degree of saturation of the rock. As an upper limit (closely following the assumptions for waste leaching used in the groundwater release scenario) on the concentration of waste in the rock, assume that the water is at the saturation limit for the uranium matrix and that the rock is fully saturated. Then, neglecting sorption on the rock and accounting for waste only dissolved in groundwater, the concentration of waste in the host rock is given by:

$$C_r = A_s\, C_s\, \varepsilon\, F \qquad (10b)$$

where C_r is the concentration of radionuclides in the host rock in curies per cubic meter

A_s is the specific activity of the emplaced waste (curies per MTHM)

C_s is the solubility limit for the uranium matrix in water (g UO_2 per g H_2O)

ε is the porosity of the rock

and F is a conversion factor of 1.E-06 MT/g * 1.E+06 cc/m^3 * 1. g/cc of H_2O

Then the ratio of concentration in the rock to concentration in the waste is:

$$C_r/C_w = \frac{C_s\, \varepsilon\, F}{(Q_w / N_T\, V_p)} \qquad (11)$$

For the values assumed here (ε = .36 - a high representative value, C_s = .001 - the upper limit of the range sampled) the ratio indicated in (11) becomes 3.6E-04 : 2.49. Thus for equivalent waste volumes the amount of radioactivity released by excavating host rock will be about .01 % of the amount released by excavating waste, given the assumptions used here which tend to overestimate the amount of contamination in the rock. However the rock could be contaminated in much of the space below the emplacement horizon. Given a single borehole, the length of a cylinder of contaminated rock could be as much as the distance from the emplacement horizon to the water table (assuming that the much larger quantities of water in the saturated zone will substantially reduce the concentration). According to the SCP Overview the static water table is 1300 to 2000 feet below ground surface and the repository is 1000 feet below ground surface. Therefore the length of a contaminated rock column could be from 100 to 330 meters. For vertical emplacement the length of the waste column is 4.3 m and for horizontal emplacement averages .53m. Thus the contaminated rock volume could be 77 or 630 times the volume of waste excavated for vertical and horizontal emplacement respecively. This corresponds to .011 and .091, for vertical and horizontal emplacement respectively, as the ratio of consequences between rock excavation and waste excavation. Since excavation of waste is approximately .0015 and .0114 times less likely than the excavation of contaminated rock, for vertical and horizontal emplacement respectively, excavation of contaminated rock could contribute in a significant way to the consequences of this scenario. That is, the incremental risk from excavation of rock could be 7.3 and 8.0 (vertical and horizontal empla cement respectively) times more than excavation of waste. If the sorption of radionuclides by the rock were accounted for, the significance of the excavation of rock could be greater than the above estimate; however, if radionuclides are sorbed, then the concentration of radionuclides in the groundwater would decrease. Of course for very long times and for radionuclides with long half lives, the entire rock column down to the water table could be at the concentration limit for that radionuclide and the rock itself could be contaminated by sorption to several times that concentration limit. Such considerations, which were omitted from the above estimates, could more than compensate for other assumptions which may have overestimated the consequences of excavating host rock. For example, if a saturation condition of 0.2, on average, is assumed instead of a value of 1 (complete saturation), the consequences estimated above would be reduced by a factor of 0.2. Regardless, the result of this evaluation appears to be clear; consequences from the excavation of host rock should be included in the model.

To begin a more precise consideration of the consequences from this scenario, consider first the consequences of excavating waste. The consequence of excavating waste by a single borehole at some time, t, is just the release of radionuclides at that time:

$$C_i(t) = \frac{V_e}{V_T} I_i(t) \qquad (12)$$

where,

$C_i(t)$ = is the incremental release of nuclide i at time t

V_e is given by equations (9)

V_T is the total volume of waste emplaced and as used in equation (10a) is given by the product, $N_T V_p$.

$I_i(t)$ is the inventory present in the repository as a function of time.

Now the inventory in the repository at any time depends on two factors: (1)how the inventory changes due to radioactive decay and, in some cases, production and (2)how the inventory changes due to dissolutions and migration by groundwater. Factor (1) is relatively easy to handle and is conventionally treated in considering the release of radionuclides to the environment by groundwater migration. Factor (2) is very important to treat in this case because it provides the coupling between this scenario and the groundwater transport scenarios. That is, we would expect that a "tight" repository would be more vulnerable to releases by drilling, because more of the waste remains in place. Alternatively, a "loose" repository that releases a lot of radioactive material to the geosphere, beginning at an early time, would be less vulnerable to drilling because less waste remains in place. The coupling is not precisely this clear, because, as discussed above, substantial consequences could result from excavating contaminated rock.

The two factors discussed above may be explicitly considered by writing:

$$I_i(t) = D_i(t)L(t) \qquad (13)$$

where,

$D_i(t)$ is the function of time describing radionuclide decay and production, which is radionuclide dependent

and

$L(t)$ is the function of time describing removal of inventory from the repository by dissolution and migration, which can be nuclide dependent, but was assumed to be the same for all nuclides in the groundwater migration scenario and is also assumed here.

Now for decay only,

$$D_i(t) = I_i(0)\exp(-\alpha_i t) \qquad (14)$$

where,

$I_i(0)$ is the emplaced inventory of nuclide i for the entire repository

and

α_i is the decay constant for the ith radionuclide

To consider decay and production the Bateman equations must be used instead of equation (14); however, for this stage of the analysis only decay is considered.

For the treatment of the source term used in the analysis of the groundwater release scenarios it has been assumed that releases begin from the engineered barrier system at some time after closure, T_s, and release of the uranium matrix occurs at a constant rate, until all the matrix is gone, after passage of the time period, T_L. This means that the function, L(t), in equation (13) is given by:

$$L(t) = \begin{cases} 1 & t<T_s \\ 1 - \dfrac{(t - T_s)}{T_L} & T_s \le t < (T_s+T_L) \\ 0 & t \ge (T_s+T_L) \end{cases} \qquad (15)$$

where,

T_s is the time at which releases from the EBS start

and

T_L is the time for the waste to move completely from the EBS to the geosphere.

The above equation assumes, implicitly, that the amount of waste excavated by drilling is small compared to the total amount of waste in the repository, since the inventory is reduced in time only by the amount of radionuclides removed by groundwater and not by the amount removed by drilling.

It is clear from equations (12) through (15) that the consequences of excavating waste by a single borehole depend significantly on the time at which such excavation occurs. One approach to treating this issue is to simulate a number of realizations in which the number and drilling times of the boreholes are random variables. Another approach would be to divide the time interval of interest into subintervals and to use a representative consequence for each interval. The approach chosen here is to calculate the expected value of consequences over the entire interval of interest. Since equation (12) represents the consequence (incremental increase in radionuclide i released to the environment) from a single borehole excavated at time, t, the consequence of N boreholes excavated at time, t, is just:

$$C_i^N(t) = N\, C_i(t) \qquad (16)$$

Let us take this value of the consequence of N boreholes as representative of the consequences that occur over some time increment, δt, where t is some time in the interval δt. Then the expected value of consequences, averaged over all possible values of number of boreholes, is:

$$\bar{C}_i(t) = \sum_{N=1}^{\infty} P(N)\, C_i^N(t)$$

$$= \sum_{N=1}^{\infty} P(N)\, N\, C_i(t)$$

Where P(N) is the probability of N boreholes over the time interval, δt. but since P(N) is given by equation (2), we find:

$$\bar{C}_i(t) = \sum_{N=1}^{\infty} \frac{(R\delta t)^N \exp(-R\delta t)}{N!}\, N\, C_i(t)$$

Since $C_i(t)$ and $\exp(-R\delta t)$ do not depend on the number of boreholes, N, these terms can be taken from under the summation to give:

$$\bar{C}_i(t) = C_i(t) \exp(-R\delta t) \sum_{N=1}^{\infty} \frac{(R\delta t)^N}{(N-1)!}$$

or

$$\bar{C}_i(t) = C_i(t) \exp(-R\delta t)\, (R\delta t) \sum_{N=1}^{\infty} \frac{(R\delta t)^{N-1}}{(N-1)!}$$

or

$$\bar{C}_i(t) = C_i(t) \exp(-R\delta t)\, (R\delta t) \sum_{N=0}^{\infty} \frac{(R\delta t)^N}{(N)!}$$

or

$$\bar{C}_i(t) = C_i(t) \exp(-R\delta t)\, (R\delta t) \exp(+R\delta t)$$

or

$$\bar{C}_i(t) = C_i(t)\, (R\delta t) \qquad (17)$$

Taking the limit of equation (17) as δt approaches zero, we have:

$$d\bar{C}_i(t) = C_i(t)\ (Rdt) \qquad (18)$$

Then integrating this result over the time period of interest gives:

$$\bar{C}_i(t) = R \int_{T_d}^{T_p} C_i(t)\ dt \qquad (19)$$

Combining equations (12) and (13) with the above gives:

$$\bar{C}_i(t) = R\ \frac{V_e}{V_T} \int_{T_d}^{T_p} D_i(t)\ L(t)\ dt \qquad (20)$$

where $D_i(t)$ can be obtained from equation (14) and $L(t)$ can be obtained from equation (15).

To perform the integration indicated in equation (20), it is useful to note the following: (1)if $T_d \leq T_p$ then the integral in (20) is zero (no drilling during the time period of interest); (2)if $T_d > T_s + T_L$ then the integral in (20) is zero (drilling commences after all the waste has migrated from the EBS). Assuming that $T_d > T_p$ and that $T_d < T_s + T_L$, then we may write:

$$\bar{C}_i(t) = R\ \frac{V_e}{V_T}\ (I_\alpha + I_\beta) \qquad (21)$$

where,

$$I_\alpha = \begin{cases} 0 & \text{if } T_d > T_s \\ \dfrac{I_i(0)}{\alpha_i}\ [\exp(-\alpha_i T_d) - \exp(-\alpha_i T_s)] & \text{if } T_d < T_s \end{cases} \qquad (22)$$

and

$$I_\beta = \frac{I_i(0)}{T_L \alpha_i^2}\ [(1+\alpha_i\{T_b - T_s - T_L\})\exp(-\alpha_i T_b) - (1+\alpha_i\{T_a - T_s - T_L\})\exp(-\alpha_i T_a)] \qquad (23)$$

where,

$$T_a = \begin{cases} T_s & \text{if } T_d < T_s \\ T_d & \text{if } T_d > T_s \end{cases} \qquad (24a)$$

and

$$T_a = \begin{cases} T_s+T_L & \text{if } T_p > T_s+T_L \\ T_p & \text{if } T_p < T_s+T_L \end{cases} \qquad (24b)$$

The above formulas provide an estimate of the consequences of excavating waste. Since the previous analysis also shows that excavation of contaminated rock could be significant and that the probability of excavating rock is much higher than excavating waste, the following analysis is developed to estimate the consequences of excavating contaminated rock.

We proceed in a manner very similar to that used for estimating the consequences of excavating waste. We rewrite equation (12) for the excavation of rock:

$$C_i'(t) = \frac{V_e'}{V_T'} I'_i(t) \qquad (25)$$

where,

$C_i'(t)$ is the incremental release from excavated rock of nuclide i at time t

V_e' is the volume of rock excavated by a single borehole

V_T' is the total volume of rock that is potentially contaminated by waste from the repository

$I_i'(t)$ is the inventory present in the contaminated rock as a function of time.

As an approximation to the total volume of contaminated rock we use:

$$V_T' = A_r \, d_r \qquad (26)$$

where,

A_r has been defined previously as the area of the repository

and

d_r is the depth of rock underlying the repository subject to contamination

As discussed above, a reasonable assumption is that the concentration of waste in the rock is reduced substantially below the water table, because more flow is available to dilute and disperse the contamination entering from the unsaturated zone. For the Yucca Mountain repository, the water table is at different depths below the repository horizon depending on the lateral location in the repository. This variation in depth is shown in Table 1 of Chapter 3. Based on the information in this Table and taking the weighted average of these depths one obtains an average depth of 249.1 m.

A consistent approximation to the volume of rock excavated is then given by:

$$V'_e = \pi \, r_d^2 \, d_r \tag{27}$$

Then

$$V'_e/V'_T = \pi \, r_d^2/A_r \tag{28}$$

As in the analysis for the excavation of waste we can express the time dependence of inventory as the product of a term related to radioactive decay, D'(t), and a term related to migration of radionuclides from the repository into the geosphere, L'(t). In an analogue to equation (13) we have:

$$I'_i(t) = D'_i(t)L'(t) \tag{29}$$

where,

$D'_i(t)$ is the function of time describing radionuclide decay and production, which is radionuclide dependent

and

$L'(t)$ is the function of time describing movement of inventory from the repository to the host rock by dissolution and migration, which can be nuclide dependent, but was assumed to be the same for all nuclides in the groundwater migration scenario and is also assumed here.

To be consistent with the analysis for excavation of waste we assume that the decay function for waste in the geosphere is the same as for waste in the repository and that the removal function for the geosphere, L'(t), is the complement of the removal function for the repository. That is:

$$D'_i(t) = D_i(t) \tag{30a}$$

and

$$L'(t) = 1 - L(t) \tag{30b}$$

where $D_i(t)$ is given by equation (14) and L(t) is given by equation (15). These assumptions comprise a compartmental analysis for the waste. Whatever waste does not decay must be either in the repository or in the geosphere. Further undecayed waste moving out of the repository must be in the geosphere. This estimate of waste excavated is conservative, because the waste transported by other means such as groundwater or gas movement to the accessible environment is not assumed to be removed from the compartments subject to excavation.

Combining (15) and (30b) we obtain:

$$L'(t) = \begin{cases} 0 & t<T_s \\ \dfrac{(t-T_s)}{T_L} & T_s< t <(T_s+T_L) \\ 1 & t >(T_s+T_L) \end{cases} \tag{31}$$

In a manner similar to the derivation of equations (16) through (20) we obtain the analogous result for excavation of contaminated rock:

$$\bar{C}_i'(t) = R \frac{V_e'}{V_T'} \int_{Td}^{T_p} D_i(t)\, L'(t)\, dt \tag{32}$$

As in the previous analysis, to perform the integration indicated in equation (32), it is useful to note the following: (1)if $T_d \geq T_p$ then the integral in (20) is zero (no drilling during the time period of interest); (2)if $T_p < T_s$ then the integral in (20) is zero (leaching commences after the time period of interest, so all the waste is in the EBS). Assuming that $T_d < T_p$ and that $T_p > T_s$, then we may write:

$$\bar{C}_i'(t) = R \frac{V_e'}{V_T'} (I_\alpha' + I_\beta') \tag{33}$$

If $T_s+T_L > T_p$ then $T_d < T_s+T_L$ and:

$$I_\beta = 0$$

and

$$I_\alpha = \frac{I_i(0)}{T_L\alpha_i^2} [(1+\alpha_i\{T_a-T_s\})\exp(-\alpha_i T_a) - (1+\alpha_i\{T_p-T_s\})\exp(-\alpha_i T_p)] \tag{34a}$$

where

$$T_a = \begin{cases} T_s & \text{if } T_d < T_s \\ T_d & \text{if } T_d > T_s \end{cases} \tag{34b}$$

If $T_s+T_L < T_p$ then:

$$I_\beta = \frac{I_i(0)}{\alpha_i} [\exp(-\alpha_i T_p) - \exp(-\alpha_i T_c)] \tag{35a}$$

where,

$$T_c = \begin{cases} T_s + T_L & \text{if } T_d < T_s + T_L \\ T_d & \text{if } T_d > T_s + T_L \end{cases} \qquad (35b)$$

and

$$I_\alpha = \begin{cases} 0 & \text{if } T_d > T_s + T_L \\ \dfrac{I_i(0)}{T_L \alpha_i^2} [(1+\alpha_i\{T_a - T_s\})\exp(-\alpha_i T_a) - (1+\alpha_i T_L)\exp(-\alpha_i\{T_s+T_L\})] & \text{if } T_d < T_s + T_L \end{cases} \qquad (35c)$$

$$T_a = \begin{cases} T_s & \text{if } Td < T_s \\ T_d & \text{if } T_d > T_s \end{cases} \qquad (35d)$$

If the events of excavating rock and waste were mutually exclusive, then one could just multiply each consequence by its probability of occurence and sum to find the average consequence. However, since every time waste is excavated there is nothing to prevent the column of host rock from also being excavated (unless we assume that drilling would stop if waste were brought to the surface). Therefore here we will assume that the consequences given by equations (33 to 35) occur with conditional probability 1.0 (i.e. if drilling occurs with probability given by equation (6)). To find the average consequences, the consequences of excavating waste, as given by equations (21 to 24), must be multiplied by the conditional probability of such excavation, P_e, as given by equation (7), and summed with the average consequence of excavating host rock. That is,

$$\bar{C}_i(t) = P_e \, \bar{C}_i(t) + \bar{C}_i'(t) \qquad (36)$$

where,

$\bar{C}_i(t)$ is the overall average consequence

and the other terms have been defined previously.

APPENDIX I - SYSTEM CODE STEPS

The following is a more detailed step-by-step outline of the system code operation than that provided in Section 4.4.4.

1. Set parameters and dimension the neccessary arrays

2. Open input and output files
   - A. EPALIM.DAT : file of EPA limits for 28 radionuclides based on an initial inventory of 10,000 Metric Tons Heavy Metal (MTHM)
   - B. SYS.INP : analyst-supplied input for a particular run, consisting of input/output flags, manner of execution, what scenarios and which release pathways to treat
   - C. SYS.DAT : file for more detailed output; amount placed here dependent on system code input values
   - D. SCENPROB.DAT : file of scenario probabilities
   - E. CCDF.DAT : file containing only that data needed to graph a CCDF

3. Read in input/output flags, simulation time, and fundamental events from SYS.INP

4. Write date and time of run to output file SYS.DAT

5. Read in EPA limits from EPALIM.DAT and calculate weighting factor for each radionuclide

6. Sequence thru scenarios
   - A Read in from SYS.INP scenario names, number of pathways, and pathway designators for the first scenario identified
   - B. Generate consequence model input vectors through LHS routine if run is internal
   - C. Check if groundwater pathway is accessed for radionuclide release if so, continue with 1) below if not, go to step 6D
     - 1a) run groundwater flow and transport model if run is internal
     - 1b) ask for name of groundwater model output file to access if run is external; read in file name from SYS.INP
     - 2) Open groundwater model output file
     - 3) Read in radionuclides and cumulative releases for each input vector until all data are input to the program
     - 4) Call ORDER subroutine
       - a. compare radionuclide names against names for which EPA limits are given
       - b. calculate normalized releases using EPA weighting factor corrected for initial inventory of 70,000 MTHM
       - c. places releases into four dimensional CUMREL array according to scenario, radionuclide, vector, and pathway

D. Check if groundgas pathway is accessed for radionuclide release
   if so, repeat steps C1 to C4 above
   if not, go to step 6E
   Note: no consequence model is installed at the present time for the groundgas pathway

E. Check if direct release pathway is accessed for radionuclide release
   if so, repeat steps C1 to C4 above
   if not, go to step 6F
   Note: only release via drilling is installed at this time

F. Go to step 6A and check if more scenarios are to be modeled
   if so, continue at step 6A
   if not, continue with step 7 below

Summing Calculations

7. Sum normalized releases in CUMREL over release pathway into three dimensional PEPASUM array

8. Sum normalized releases in CUMREL by radionuclide into three dimensional REPASUM array

9. Sum REPASUM over release pathway into two dimensional SEPASUM array

10. Sum PEPASUM by radionuclide into two dimensional FEPASUM array

11. Compare SEPASUM against FEPASUM for errors

Calculations for CCDF

12. For each scenario treated, sort summed normalized releases in SEPASUM in ascending order top to bottom using the ASORT subroutine

13. Place ordered releases into EPASUM by scenario and vector, along with the probability of each consequence given that each vector in a scenario is equally probable, i.e., $P(R) = (\text{number of vectors})^{-1}$

14. Compress EPASUM by comparing each release with all other releases within the same scenario; if a match is found, the probabilities are combined and duplicate release values are deleted

15. Read in scenario probabilities

16. Calculate the total CCDF
    A. Place releases and their associated likelihoods for all scenarios from EPASUM into TSDF, a three dimensional array
    B. Sort TSDF from top to bottom in ascending order
    C. Compress TSDF array and recalculate probabilities as in step 14
    D. Create a running cumulative probability in the third dimension of TSDF

17. Generate system code output files
    A. SYS.DAT filled according to flags set in SYS.INP
    B. Place TSDF array into CCDF.DAT file

APPENDIX J - DOCUMENTATION OF FILES AND PROGRAMS ON INEL CRAY XMP/24 FOR REPOSITORY PERFROMANCE CALCULATIONS

J.1 Introduction

This appendix documents briefly the more significant computer programs, data files and output files used to generate and manipulate the results on source term and transport presented in this report.

J.2 FORTRAN Programs

J.2.1 NEFTRAN6

This is the modified version of NEFTRAN for the Yucca Mountain demonstration. It has the following modifications from the standard version in NUREG/CR-4766:

a. All calculations having to do with the determination of the flow through saturated flow tubes using Darcy's law are removed. Flux is now an input variable based on infiltration and fracture flow as determined by saturated hydraulic conductivity.

b. Most input variables needed for unsaturated flow and transport are contained in subroutine GETRV. This subroutine reads the random input vectors on TAPE10 generated by program LHSVAX, and generates an output vector file of radionuclide releases cumulated over time (either 10,000 or 100,000 years) and written to TAPE20.

c. There are minor changes to the output format of TAPE20 to include the scenario number on each record.

J.2.2 CCDFLIM

This program takes the TAPE20 output files generated by NEFTRAN6 for the 4 columns and generates a CCDF for each scenario. It multiplies the output cumulative releases for each radionuclide by their respective EPA release limit factors to get an EPA ratio for each vector. The vectors are then combined for the four columns, sorted and written to a file for transmission to NRC and plotted with the commercial program GRAPHER on a PC. The CCDFLIM program also calculates the average contribution to the EPA ratios by radionuclides and sorts them in descending order. CCDFLIM allows the compiled output results to include or reject output vectors on the basis of limits on the input parameters or combinations of parameters read into NEFTRAN. For example, the program can screen out all vectors for which the groundwater travel time exceeds 1000 years, with the groundwater travel time determined from a combination of input parameters.

J.2.3 COMBINE

This program combines the four TAPE20 output files from NEFTRAN for the four columns into a single combined TAPE20 output file. The main reason for this is to avoid having to send four lengthy files from the Cray system to the NIH system on BITNET, and to avoid a problem on BITNET which was causing some of the long lines of output to get clipped at 79 columns. The new output file is identical to the old TAPE20 output, except that the long lines are no longer written in list-directed form, but in formatted form with a line length of 68 characters. If the output for a particular chain is all zeros, then list-directed output is still used in order to take advantage of the compact structure.

J.2.4 LHSVAX

This program generates the Latin Hypercube sample for input to NEFTRAN6. The staff has modified it in the following way:

a. It now contains its own random number generator, RAN1 from Numerical Recipes.

b. It reads the names of the inputs and output files.

J.2.5 STEP

This program performs the stepwise linear regression and rank regression on the outputs of NEFTRAN6 for each scenario in order to determine sensitivities and uncertainties. The main modification to this program was to take the TAPE20 output from the four columns generated by NEFTRAN6 and combine them into EPA ratios for each vector using the EPA release limit factors. The combined EPA ratios are written to a temporary file and read into the STEP program to generate the regressions.

J.2.6 C14B

This program calculates the carbon-14 release from the waste packages as a function of time. The program assumes that the canisters fail with a normal probability distribution. Once failed, oxygen attacks the fuel matrix and releases its inventory according to a rate based on the spallation time, randomly picked from a uniform probability distribution bounded by two lines that are functions of temperature. To the release rate is added the prompt release at the time of canister failure.

J.3. Batch Script Files

The following batch files execute programs in the batch mode on the Cray using the batch queue function QSUB:

J.3.1 STATCON.SUB

This batch file executes in sequence the program LHSVAX and NEFTRAN6 for all four columns and then the program CCDFLIM, to generate a CCDF. The main purpose of this script file is to simplify the multistep operation for generating the CCDF, particularly for the statistical convergence exercise that demonstrated the sensitivity of the CCDF to the number of Latin Hypercube vectors samples chosen (either 100 or 500). We chose a new seed for each of the runs with 100 vectors.

J.4 Data Files

J4.1 ympyuc2.dat - This file was used in every case to generate the Latin Hypercube samples for NEFTRAN6 based on the distribution and ranges specified for 47 variables. When used in the statistical convergence test, we chose a new random input seed specified in this file, for each CCDF run.

J4.2 epalim.dat - the EPA release limits by radionuclide in terms of permissible releases per 10,000 metric tons heavy metal.

J4.3 t51nl - This is the NEFTRAN6 card image input file for the basic parameters in column A, 10,000 year base case scenario, 500 vectors

J4.4 t52nl - same as above, but column B.

J4.5 t53nl - same as above, but column C.

J4.6 t54nl - same as above, but column D.

J4.7 t51100 - same as t51nl, but 100,000 years

J4.8 t52100 - same as t52nl, but 100,000 years

J4.9 t53100 - same as t53nl, but 100,000 years

J4.10 t54100 - same as t54nl, but 100,000 years

J4.11 TAPE10 - The random vectors produced by LHSVAX for the input file ympyuc2.dat

J.5 Output files

J5.1 tape2051.10, tape2052.10, tape2053.10, tape2054.10 - These are the TAPE20 output files from NEFTRAN6 for the base case, 10,000 year cumulative releases for the four columns referred to in the text as columns A, B, C and D, respectively.

J5.2 tape201.500, tape202.500, tape203.500, tape204.500 - These are the TAPE20 output files from NEFTRAN6 for the base case, 100,000 year cumulative releases for the four columns refereed to in the text as columns A, B, C and D, respectively.

J5.3 tape20cmb.10 - This is the combined output for tape2051.10, tape2052.10, tape2053.10 and tape2054.10 produced by program COMBINE.

J5.4 ccdf10.out - This is the output file for plotting the CCDF for the 10,000 year base case scenario.

J5.5 ccdf100.out - This is the output file for plotting the CCDF for the 100,000 year base case scenario.

J5.6 TAPE6 - The normal printed output file for each NEFTRAN run.

HLW
VOL. 16 149 JC JG JK KD file

UNITED STATES
NUCLEAR REGULATORY COMMISSION
ADVISORY COMMITTEE ON NUCLEAR WASTE
WASHINGTON, D.C. 20555

December 2, 1991

'91 DEC -3 PM 4:12

The Honorable Kenneth C. Rogers
Commissioner
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555

Dear Commissioner Rogers:

SUBJECT: NRC CAPABILITIES IN PERFORMANCE ASSESSMENT AND COMPUTER MODELING OF HIGH-LEVEL WASTE DISPOSAL FACILITIES

The purpose of this letter is to respond to the first two questions in your memorandum of April 29, 1991, requesting ACNW comments on the adequacy of the performance assessment and computer modeling capabilities of the Office of Nuclear Regulatory Research (RES) and the Division of High Level Waste Management (HLWM), including the Center for Nuclear Waste Regulatory Analyses (CNWRA). Our comments are based on deliberations and discussions with the NRC staff and members of the CNWRA during an Advisory Committee on Nuclear Waste (ACNW) Working Group meeting on October 16, 1991, and during the 36th and 37th ACNW meetings on October 18 and November 20-21, 1991, respectively. During the Working Group meeting, we had the support of a team of invited experts.

General Observations

It is our general conclusion that the NRC HLW staff is a highly qualified and professional group and is developing a suitable program for performance assessments of an HLW disposal facility. If supported by careful and appropriate experimental confirmation studies and selectively focused assessments, this program should be sufficient for the NRC to demonstrate to a licensing board whether a repository meets the requirements of 10 CFR 60.112 and 60.113. Although we consider the NRC program to be adequate, we recognize that its assessments cannot be totally independent, due to the necessary reliance by the NRC staff on models, data, and computer codes developed by other organizations. Additional points that should be considered, include:

1. The staff intends to conduct a selectively focused review of the performance assessments conducted by the U.S. Department of Energy (DOE), supported by in-depth analyses in only certain key areas. This approach is historically consistent with reviews conducted by the NRC in the evaluation of other types of license applications. It represents a realistic method for handling such reviews. A relatively simple bounding performance analysis -- supported by experience with more detailed, independently evaluated process codes -- provides an independent product that can be understood and defended within the licensing arena.

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2. As stated above, the assessments by the NRC staff must, of necessity, involve to a considerable extent the use of data, codes, and methodologies developed by the DOE. This approach is acceptable as long as the NRC staff has the capability to independently evaluate the quality and applicability of such information and techniques.

3. To ensure the continuation of a successful performance assessment and computer modeling program, the NRC staff would benefit from an endorsement and affirmation from the Commission and upper NRC management. Such an affirmation would include a clear delineation of what the NRC staff's role and responsibilities are in using these techniques in the licensing process. There is also a need to provide funds for additional staff and facilities.

Specific Comments

In the way of specific comments, we offer the following:

1. There is a need for the development of a strategy document that specifies the goals of the NRC HLW performance assessment program. This document should provide details on what the program is designed to accomplish, how it is to be executed, and a timetable for its implementation. While the Implementation Plan, the Program Plan, and the License Application Review Plan will address parts of this concern, the staff needs to address the scientific and technical problems and other facets of performance assessment in greater detail and sophistication. This document should provide the fundamental transition from Phase 1 into the longer range Iterative Performance Assessment Program.

2. The NRC staff continues to have difficulties in obtaining data and software that have been developed by DOE and its contractors. We believe that formal generic arrangements should be developed that permit ready access by the NRC staff to DOE data and codes. The staff should be mindful of the quality assurance and quality control status of these codes and data. It is essential that the software used for modeling repository performance be compatible with the data and information. Furthermore, codes that are used sequentially should have compatible assumptions and limitations; otherwise, the results would be inconsistent and unreliable.

3. The NRC staff is expanding its performance assessment capabilities beyond the ability to estimate radionuclide releases; namely, it is expanding the codes to provide estimates of the doses to individuals and population groups. To increase the effectiveness of this effort, the NRC staff should also expand its interactions with appropriate groups in foreign countries

so as to benefit from the codes that have already been developed for making such estimates. The Commission and upper NRC management should encourage and cultivate NRC staff participation and interaction with international efforts such as the modeling of source-term parameters (near-field and far-field).

4. The insights and products gained through the application of the Iterative Performance Assessment Program can have important benefits, both in helping the NRC staff to develop needed capabilities for licensing a repository and in establishing research priorities. The role that performance assessment methodologies can play should be formally incorporated into the protocol for assigning priorities to research. Areas in which such methodologies would be helpful include the selection of specific research projects in the geosciences (such as geochemistry), and the determination of which of these should be assigned to the CNWRA. Furthermore, all members of the NRC staff who are involved in the HLW program should be required to become familiar with the methodologies of performance assessment.

5. The initiation of the Phase 2 performance assessment of the proposed Yucca Mountain repository offers the NRC staff an opportunity to explore several key difficult analyses in depth. Several challenging and complex, yet realistic, analyses involving natural phenomena (e.g., climate change, tectonic, and other processes) should be performed. These analyses should be chosen to illustrate the mechanisms for the solicitation and use of expert judgment, for the identification and quantification of uncertainties, and to gain a better understanding of the difficulties in determining compliance with the standards of the Environmental Protection Agency.

6. The NRC HLW staff must accept and provide for the role of expert judgment. Although hard data, validated complex computer codes, and large-capacity computational equipment are available, the staff should devote an intensive effort to developing a strategy for the use of expert judgment in performance assessments and computer modeling, both in conducting NRC's analyses and in reviewing how DOE uses expert judgment in its assessments.

<u>Computer Modeling Capabilities</u>

Our comments on the adequacy of the NRC computer modeling capabilities are addressed to the related hardware and software and personnel training needs.

1. The computer hardware currently used by the NRC staff is outdated and inadequate. Moreover, electronic communication between the computers at NRC headquarters and those at other facilities, including the CNWRA, is almost nonexistent, primarily because of a lack of equipment at the NRC headquarters end of the link. In contrast, the CNWRA appears to have adequate hardware to meet its present needs and responsibilities, and has plans to acquire additional capability as needed. Having said this, it is important to note that the NRC staff is fully aware of these problems and has been granted funds under a pilot program that should enable it to correct its hardware deficiencies within the next year. Continuing upgrades will be needed.

2. In sharp contrast to its hardware, the NRC staff has generally good capabilities for developing conceptual, mathematical, and computer models. These capabilities reside within the agency staff, as contrasted to existing solely or primarily within the staffs of its contractors. Although the CNWRA has had difficulty in recruiting the needed expertise, the current performance assessment program element manager has excellent modeling and performance assessment skills.

3. We are pleased to note that training for the NRC staff in the field of performance assessment and computer modeling is being implemented. We endorse plans for providing training opportunities to the staff both through the capabilities of the NRC itself and through outside groups. The CNWRA appears to have a similar, but perhaps less formal, program. The Commission and NRC management should encourage this continuing education process.

In summary, it is our conclusion that HLWM and RES have capable staffs, that they are developing a suitable performance assessment program, and that they have sound computer modeling capabilities. Primary needs in HLW performance assessment are to develop a strategy document detailing the goals of the program and the specific means to achieve these goals, to upgrade the NRC staff's computer hardware, to resolve current limitations on the availability of key software and data, and to ensure that adequate resources are provided to meet future personnel and equipment needs as the performance assessment program evolves.

Sincerely,

Dade W. Moeller

Dade W. Moeller
Chairman

Vol. 16 150

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UNITED STATES
NUCLEAR REGULATORY COMMISSION
WASHINGTON, D.C. 20555

FEB 21 1992

MEMORANDUM FOR: Commissioner Rogers

FROM: James M. Taylor
Executive Director
for Operations

SUBJECT: U.S. NUCLEAR REGULATORY COMMISSION STAFF CAPABILITIES IN PERFORMANCE ASSESSMENT FOR HIGH-LEVEL WASTE FACILITIES

Your memorandum of April 29, 1991, requested an Advisory Committee on Nuclear Waste (ACNW) review of the adequacy of the U.S. Nuclear Regulatory Commission (NRC) staff's and the Center for Nuclear Waste Regulatory Analyses' performance assessment and computer-modeling capabilities regarding a geologic repository for high-level radioactive waste. The ACNW provided its comments to you in a letter dated December 2, 1991. In the enclosure to this memorandum, the NRC staff presents its views and, particularly, its responses to the ACNW comments.

I appreciate the ACNW's generally favorable critique of our program, and I have found the ACNW's recommendations helpful.

James M. Taylor
Executive Director
for Operations

Enclosure:
Staff Response to 12/02/91
ACNW Letter

cc: The Chairman
~~Commissioner~~ Commissioner Curtiss
Commissioner Remick
Commissioner de Planque
SECY
OGC
ACNW

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ENCLOSURE

STAFF RESPONSE TO DECEMBER 2, 1991, ADVISORY COMMITTEE ON NUCLEAR WASTE (ACNW) LETTER

PERFORMANCE ASSESSMENT
General Observations

1. The ACNW endorses our plans to conduct selectively focused, rather than comprehensive, reviews of the performance assessments submitted by the U.S. Department of Energy (DOE) in support of a license application. As noted by the ACNW, we intend to support our relatively simple bounding performance analyses with in-depth analyses in key areas. We appreciate the ACNW's endorsement of our plans. We agree that such a review provides a product that can be understood and defended in the licensing process and is historically consistent with the U.S Nuclear Regulatory Commission's (NRC's) approach in other types of license reviews.

2. The ACNW notes that the NRC staff must make considerable use of the data, codes, and methodologies developed by DOE. We have spent, and will continue to spend, considerable resources to develop and maintain the expertise necessary to independently evaluate the quality and applicability of DOE's information and techniques.

3. The ACNW recommends that the Commission endorse and affirm the staff's approach to the use of performance assessment in support of licensing. When considering whether such endorsement and affirmation are warranted, the Commission may wish to consider the enclosed document, which gives a general overview of the Division of High-Level Waste Management's (HLWM's) performance assessment strategy. The staff plans to revise the enclosed strategy, in about a year, to incorporate "lessons learned" from the staff's current "Phase 2" iterative performance assessment (IPA) activities. The "audit-type" review approach outlined in this strategy is consistent with that previously described in HLWM's August 1991 white paper entitled "Development and Implementation of the Division of High-Level Waste Management Proactive Program," which was the subject of an August 28, 1991, briefing to the ACNW. Moreover, the staff has made the Commission aware of its audit-type review philosophy during the past several years through the Commission review of the Five-Year Plan and the budget. In the Five-Year Plan and the budget, for example, the staff has noted that it intends to perform detailed reviews on approximately 20 percent of DOE's Study Plans.

The ACNW also recommends additional funding for performance assessment staff and facilities. We agree with the ACNW that adequate resources are essential to ensure the continuation of a successful performance assessment program, in light of the need to continue development of staff capability, as well as to review increased DOE initiatives in this area. The need for additional staff and resources will be considered in future budget requests.

Specific Comments

1. The ACNW agrees with the need, previously identified by the staff, to develop a strategy specifying the goals of the NRC high-level waste (HLW) performance assessment program and the details of the staff's plans for accomplishing those goals. The enclosed strategy, which was previously reviewed by the ACNW, is a first step toward development of the recommended strategy. As just noted, the staff plans to revise and update the enclosed document after completion of the current "Phase 2" IPA activities, as the program transitions, from an emphasis on developmental activities, to implementation to support review of DOE activities, which will culminate with the license application review.

2. The ACNW notes staff difficulties in obtaining data and software developed by DOE and its contractors. The ACNW believes that formal generic arrangements should be developed that permit ready NRC staff access to DOE data and codes. The staff is completing negotiations, with DOE, to revise the NRC/DOE "Morgan-Davis Procedural Agreement," identifying the interface protocol between the two agencies during the site characterization phase. Revisions to this agreement (currently being agreed to by both staffs) will facilitate NRC's timely access to DOE data and analyses. The staff will seek additional revisions to this agreement, to address NRC access to software.

Also, the staff is mindful of the need for quality assurance (QA) in software and data as pointed out by the ACNW. For IPA "Phases 1 and 2," guidance for software and data QA was promulgated. For IPA "Phase 2," software and data QA have been enhanced by adoption and implementation of a configuration management and control system, at the Center for Nuclear Waste Regulatory Analyses (CNWRA), for all IPA-related work. Moreover, the NRC and CNWRA staff will evaluate the QA pedigree of any IPA codes or data acquired from DOE, as appropriate, and use these codes or data in a manner that is consistent with that pedigree.

3. The ACNW recommends, in its letter, that the NRC staff expand its interactions with appropriate groups, in foreign countries, so as to benefit from their efforts in developing codes for estimating the radiation doses that might result from radionuclide releases. Although the staff actively participates in a variety of HLW international activities, including meetings of the Performance Assessment Advisory Group of the Nuclear Energy Agency, specific participation in activities for establishing doses has been marginal, because of limited staff availability and resources. Given that the U.S. Environmental Protection Agency's HLW standards emphasize limits on releases of radionuclides to the environment rather than radiation dose limits, the staff continues to believe that development of a capability to project releases should have a higher priority than translation of those releases to radiation doses. Future resource needs will be evaluated for additional international interactions specifically focused on dose modeling.

4. The ACNW agrees with the staff's use of performance assessment as one of the ways to establish research priorities in the HLW repository program. Performance assessment will provide insights for this identification and prioritization. It can do this not only through uncertainty and sensitivity analyses, but also, more importantly, through the identification of gaps, in the knowledge, that affect the validity of the performance assessment models themselves.

The final report of the staff's current "Phase 2" performance assessment will document specific research needs. This information will be used to revise and prioritize Research Need Summaries, which communicate licensing office needs to NRC's Office of Nuclear Regulatory Research (RES). RES staff participation in the "Phase 2" work will also help to establish research priorities. RES will consider HLWM recommendations for HLW research based on IPA, its own insights gained from IPA, and other sources of technical information and programmatic considerations, in establishing research priorities. It should also be noted that RES is developing a research program plan for NRC's HLW repository program, in coordination with HLWM. Through this process, the two staffs will establish, and periodically revisit, a mutually agreed-on set of priorities regarding HLW research.

The ACNW also endorses the staff's plan to provide performance assessment training for all members of the staff in the HLW repository program. HLWM intends that all HLW staff will receive this training. Two week-long sessions have been offered through the Office of Personnel, and the staff is currently working with the Idaho National Engineering Laboratory (INEL) to continually improve this course. In addition, NRC staff participates in training related to specific performance assessment models and codes. The extent of training will be commensurate with each staff member's expected involvement in IPA activities.

5. The ACNW recommends that the staff use the ongoing "Phase 2" performance assessment activities as an opportunity to illustrate the mechanisms for formal use of expert judgment in a performance assessment. The staff agrees that such a demonstration would be useful. Since completion of "Phase 2" is planned in June, and incorporation of a formal elicitation process at this point would disrupt this analysis involving interdependent modules, we propose that "Phase 2" be completed as planned. After completion of "Phase 2," the staff then proposes a "Phase 2.5," in which formal elicitation methods will be used to produce expert judgments, for comparison with the "Phase 2" results. Completing "Phase 2" will provide a baseline for evaluating the advantages and disadvantages of the more formal elicitation methods recommended by the ACNW, and their consistency with the NRC licensing process.

6. The ACNW agrees with the staff's plans to develop a strategy for use of expert judgment in performance assessments and computer modeling, both in conducting NRC's analyses and in reviewing how DOE uses expert judgment in its assessments. The staff will study the feasibility of using formally elicited expert judgment in a licensing process, and will develop a strategy based on the following principles:

a. Formal elicitation of expert judgments must be carried out in a manner compatible with NRC's licensing procedures;

b. Judgment should be used to interpret data and analyses, but not as a substitute when data and/or analyses are reasonably available or obtainable; and

c. Expert judgment, even if formally elicited, is no better than the rationale on which it is based. If an expert (or group of experts) is unable to articulate a convincing basis to support a judgment, then that judgment may carry little weight in NRC's decision-making process.

COMPUTER MODELING CAPABILITIES

1. The ACNW notes that the computer hardware NRC staff currently uses is outdated and inadequate, and that there is inadequate electronic communication between NRC headquarters and the CNWRA, primarily because of a lack of equipment (e.g., hardware) at NRC headquarters. The staff agrees that hardware upgrades are needed and, as noted by the ACNW, has developed a plan for a pilot program to define these needs and to resolve any deficiencies. As part of the mid-year budget review, the availability of resources to support this plan will be determined. In the meantime, the CNWRA will initiate the first task in this plan, which is to update a 1990 NRC staff assessment of hardware and software functional needs in the area of HLW.

2. The ACNW believes that the NRC staff's capabilities for developing conceptual, mathematical, and computer models are good. The staff will endeavor to retain and expand on this strength, and will continue to encourage the CNWRA to expand its expertise in this area, also.

3. The ACNW endorses the staff's efforts to provide performance assessment training for itself and for the CNWRA. The staff will continue to pursue training opportunities, including those discussed in Item No. 4 above, both within and outside of NRC.

ATTACHMENT

NRC POST-CLOSURE PERFORMANCE ASSESSMENT STRATEGY FOR A HIGH-LEVEL NUCLEAR WASTE REPOSITORY

In its broadest sense, any qualitative or quantitative estimation of the isolation capability (pre- and post-closure) of the high-level nuclear waste repository constitutes a performance assessment (PA). In this paper, however, performance assessment is restricted to mean only quantitative post-closure estimates of the repository's isolation capability. Furthermore, the quantitative estimates are restricted to those that are called for in relevant regulations, primarily 10 CFR Part 60 and 40 CFR Part 191.

The U.S. Department of Energy (DOE) is required, by regulation, to provide a comprehensive performance assessment in its license application. The law requires the U.S. Nuclear Regulatory Commission (NRC) to review the license application prior to granting, or denying, a construction authorization. As a part of the review process, the NRC will form its own estimates of the potential performance of the repository described in the license application. If it determines that it is necessary and appropriate to do so, the NRC may use independent calculations in forming these estimates. It should be understood that performance assessment is only one input, albeit important, into NRC's decision process as will be made clear in the much broader License Application Review Strategy (LARS) that is currently under development. It is also worth noting that at no time during the life cycle of the repository is the NRC expected to carry out its own site investigations or perform any engineering design. It will, however, provide guidance to the DOE on both site characterization and engineering design.

The general question considered in this paper is how should the NRC use performance assessments in implementing its proactive and reactive regulatory program? This breaks down to the following issues: (1) where in its review of DOE's license application should the NRC perform independent performance assessments, and (2) how should performance assessment be used in the overall program? In essence, what should be the NRC's performance assessment strategy, taking into account its mission and resource availability?

REGULATORY BASIS FOR PERFORMANCE ASSESSMENT

The Regulatory requirements for the geologic repository are codified in 40 CFR Part 191 (EPA) and 10 CFR Part 60 (NRC) - two complementary, but independent regulations. Part 191, the "generally applicable standards for protection of the general environment from off-site releases from radioactive material in repositories" (NWPA, Sec. 121) is concerned with the acceptable level of performance of the overall repository system. It specifies three broad quantitative performance objectives: (1) limiting the cumulative release at the accessible environment boundary over 10,000 years; (2) individual protection objectives for the first 1,000 years; and (3) requirements for protection of special sources of ground water for the first 1,000 years. (For purposes of this document, it is assumed that 40 CFR Part 191, though vacated by Court Order, will be repromulgated without material change.)

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In contrast, Part 60, the "Disposal of High-Level Radioactive Wastes in Geologic Repositories" is more comprehensive in its scope. The generally applicable environmental standards of Part 191 are incorporated into Part 60 by reference. In addition, consistent with the mandate of the Nuclear Waste Policy Act as amended (NWPA), Part 60 makes it explicit that a repository include a system of multiple barriers. This concept of multiple barriers is enforced by establishing three minimum sub-system performance objectives, namely, the substantially complete containment performance objective for the waste package; the release rate performance objective for the engineered barriers; and the ground water travel time performance objective for the site. In addition to performance objectives, siting and design criteria (for waste package and engineered barriers) are also specified in Part 60. However, the subsystem performance objectives of 60.113(a) for the engineered barriers apply only with respect to the "anticipated processes and events." An additional flexibility with respect to the subsystem standards is included in 60.113(b). So long as the total system performance objective is met for anticipated processes and events, the NRC can approve or otherwise specify a radionuclide release rate, containment time, or groundwater travel time other than the nominal values stated in section 60.113(a).

With regard to judging compliance with these objectives (including the EPA Standard) and criteria, Part 60 states: "Proof of the future performance of engineered barrier systems and the geologic setting over time periods of many hundreds or many thousands of years is not to be had in the ordinary sense of the word. For such long-term objectives and criteria, what is required is reasonable assurance, making allowance for the time period, hazards, and uncertainties involved, that the outcome will be in conformance with those objectives and criteria."

In the Supplementary Information Statement, the Commission explained that the subsystem performance objectives of Part 60 are meant to provide confidence in meeting the overall system performance objective. Technical support is provided in NUREG-0804 Part C by evaluation of the extent to which compliance with the three subsystem performance objectives increases the likelihood of compliance with EPA's overall system performance criteria. Additional analyses of how the three subsystem performance objectives increase the likelihood of compliance with EPA's overall performance criteria are given in NUREG/CR-3111. This technical support was prepared prior to promulgation of Part 191. An early working draft of Part 191 was used to carry out the evaluation. EPA is currently in the process of reissuing Part 191, and changes from the earlier working draft and the remanded final version are uncertain. A performance assessment capability will allow the NRC not only to reevaluate the extent to which the subsystem performance objectives will provide additional confidence of compliance with the EPA's standards, but it also will identify refinements to the subsystem objectives that might be appropriate.

Because of the long period of regulatory concern (10,000 years set by EPA) and large spatial scales (tens of cubic kilometers), the future subsystem and total system performance of the repository are expected to be projected by way of mathematical models. Direct performance testing of either the total system or its subsystems over such scales is not possible. The DOE has the responsibility to develop, validate, and implement, to the degree appropriate, these models and to provide a complete description of the performance assessments in its license application. The NRC, on the other hand, has the responsibility of assuring that the licensed repository will adequately protect public health and safety. In performing its regulatory function, the approach to be taken will be one of reviewing DOE's entire performance assessment at a broad level of detail and doing more detailed reviews in the most significant areas. The NRC must, therefore, decide which selected parts should include independent verification through independent performance assessments. The NRC will adopt the strategy described below in applying performance assessments in its high-level waste work.

NEED FOR THE NRC'S PERFORMANCE ASSESSMENTS

Many relatively complex technical issues of a multi-disciplinary nature are involved in assessing the future performance of the geologic repository. To meet the NRC mission of protecting public health and safety, the NRC staff must, during the licensing process, take positions on the potential performance of the repository as it relates to the performance objectives. In addition, the NRC will comment on and provide guidance to the DOE on the completeness and adequacy of the site characterization program and engineering design, as well as on the DOE's plans to construct, operate and close the repository. Thus, the NRC has a definite role to play throughout the life cycle of the repository.

It is conceivable that the NRC staff can form an opinion about the performance of the repository without independent calculations. However, due to the complexity of the system and in the absence of accumulated historical experience, such an opinion will not be sufficiently well founded to support licensing decisions. Therefore, the NRC should conduct its own performance assessments. The NRC must devise a plan based on this strategy to select critical portions of DOE's license application for intensive review by independent performance assessments. This strategy should also help the NRC in meeting its obligations to provide guidance to the DOE during site characterization, construction, operation and closure. This strategy will be implemented by all of the NRC organizations involved in performance assessment aspects of the High Level Waste Program and their contractors.

STRATEGY FOR PERFORMANCE ASSESSMENT

The key features of NRC's performance assessment strategy are derived from a few basic considerations: The complex and interdisciplinary nature of PA; its potential use in both the reactive and proactive programs; a top-down approach to guide resource utilization by identifying components important to repository performance; the integration of technical work performed on how the subsystems work; and keeping the NRC staff knowledgeable in PA methodology. These features are discussed below.

General Program

Assessing performance of a geologic repository requires execution of a number of steps. These include conceptualizing the system in terms of its identifiable components, the formulation of mathematical models representing all important processes, the translation of the mathematical models into computer programs, the verification and to the extent possible validation of the models, the analyzing of field and laboratory data to extract model parameter values, the executing of computer programs, performing sensitivity and uncertainty analyses, and, finally, analyzing results to draw conclusions.

While all parts of the performance assessments presented by DOE will be reviewed at some level, critical parts will be selected for in-depth review (see License Application Review Strategy for definitions of various review levels). In reviewing DOE's performance assessments, the NRC staff will not need to duplicate the work done by the DOE. The DOE will perform these calculations under an auditable QA program. As part of its reactive HLW licensing program, the NRC will conduct audits as needed. The NRC staff will perform, at least at a rudimentary level, a calculation to check all of the DOE estimates of performance. In addition, the NRC staff will use independent calculations to evaluate the significance of key assumptions regarding conceptual models, process models, and parameter values included in DOE's performance assessments. This evaluation will draw heavily from the proactive work described below. Other applications of PA in the review of DOE's program will include determination of the adequacy of performance allocations and other facets of the DOE's site characterization program. Particular attention will be given to evaluating DOE's evolving iterative performance assessment program. Auxiliary analyses done as part of independent performance assessments will also provide a technical foundation for evaluating alternatives with respect to conceptual models, process models, parameter values, and sensitivity analyses presented by DOE, and to identify those that may not be considered adequately in the DOE's work. Such work will provide technical credibility to recommendations that the NRC will make to the DOE for its investigations. The NRC HLW research program will generate scientific information to support staff positions on whether alternatives have been adequately explored by the DOE.

Special attention will be paid to uncertainties involving the assumptions that form the basis of models, future states of nature, and estimation of parameter values that are fed into performance assessment computer programs. Again, one may assume that the DOE's raw data will be collected under an approved QA program. The interpretation of these data leading to model parameter values not only will be spot checked, but the NRC itself will interpret selected data sets for critical parameters. It is in the interpretation of these data that alternate hypotheses or inferences may be identified that were not adequately considered by the DOE. Special attention may be directed to issues identified by external reviewers as well as those identified by the NRC staff.

The primary aim of the NRC's proactive performance assessment program will be to evaluate its regulations, develop sound technical guidance, train and keep its staff current, and develop appropriate technical review procedures. The NRC will use the DOE developed computer codes, if available, provided that these codes have enough flexibility to also allow NRC evaluation of DOE assumptions about conditions that may have public health and safety implications and the sensitivity of DOE's conclusion to these assumptions. Otherwise, the NRC will develop its own codes or modify existing codes to suit its purpose. The proactive program will be also supported through NRC's HLW research program (see draft NUREG-1406). Performance assessment issues that are related directly to NRC's regulatory function of technical review will be addressed through NRC's HLW research program. Such issues will include (1) understanding processes that affect HLW repository performance, (2) understanding coupling among processes that affect HLW repository performance, (3) techniques for probability estimation, (4) assessing reliability of long-term mathematical predictions and (5) numerical methods (if needed).

Because performance assessment of nuclear waste repositories is a relatively new field and because it is interdisciplinary in nature, very few formal educational opportunities exist to train staff in this aspect. While the NRC has developed a course on performance assessment, learning through experience, by conducting limited performance assessments, is the best and most efficient method for training of the NRC and contractor staffs. Insights gained by NRC staff will allow development of meaningful regulatory guidance and review procedures. Together with the NRC's Systematic Regulatory Analysis (SRA) program, performance assessment modeling also will help in evaluating current regulations regarding their interrelationships, completeness, and sufficiency in providing assurance that public health and safety will be protected.

Integration of Subsystems

NRC's regulations require that the total repository system should include engineered and natural barriers. These regulations also require that each of several barriers attain a certain performance objective. Therefore, these subsystem performance objectives have an important role in assuring that the multiple barrier concept is maintained and thereby provide additional confidence that public health and safety goals are met. In view of this, the DOE is expected to develop a repository system that will be comprised of engineered and natural barriers. Due to potential complex interactions between these barriers under future environmental states, the net impact of individual barriers on the total system performance is not known a priori. Therefore, it is natural and necessary to account for all of these barriers in conducting performance assessments of the total system.

It has recently been suggested that there is a need to reevaluate the relationship between the subsystem performance requirements of 10 CFR Part 60 and the EPA HLW Standard. As discussed previously the staff will do this reevaluation in connection with repromulgation of the EPA standards. This reevaluation will examine the extent to which meeting subsystem requirements of 10 CFR 60.113 relates to compliance with the EPA standards. The data and analyses needed for compliance determination with requirements of Section 60.113 will also be examined.

The relative contribution of each barrier in meeting the total system performance objective can be determined only after an assessment of total system performance is conducted. Therefore, from the performance assessment view, there is no natural hierarchy to subsystems, that is, all subsystems will be considered during performance assessments of the total system. Depending on their relative technical importance, which will be determined during initial iterations, eventually and for certain purposes (e.g., sensitivity analyses) some subsystems may be treated in more detail than others.

Irrespective of the relative importance of any barrier in meeting the EPA standard for the total system performance, subsystem performance assessments will be conducted to judge whether the subsystem performance objectives of Part 60 are met. As stated before, the subsystems do not perform independently of each other; that is, the performance of the engineered barriers is determined by the site conditions and vice versa. Also, due to large time and space scales inherent in the subsystem performance objectives, like the total system, the subsystem performance assessments will also require mathematical modeling. In view of the above, it is possible that the assessments of the subsystems can become a part of the total system performance assessments. However, it is also possible to investigate the performance of these subsystems in greater detail by isolating them within properly selected boundaries. Initially, both options will be followed by the NRC staff. However, eventually the subsystem performance assessment efforts and the total system performance efforts will be thoroughly integrated. This will be done by implementing an "interdisciplinary team approach" in conducting the performance assessments. The members of the various teams will be drawn from various NRC branches involved with the HLW program's offices and subcontractors. Suitable management controls will be designed and implemented for the success of the team approach.

Timing and Iterative Nature of Assessments

There are two different approaches to decide upon the right time to carry out a performance assessment. In the first approach, one waits until the computational tools are fully developed and the collection of site-specific data is complete before attempting a performance assessment. In the second approach, iterative performance assessments are carried forward with the help of available data at a given time with computational tools available at that time. From a regulatory perspective, the second approach should receive the higher priority by the NRC staff. This approach should apply to both the subsystem and the total system performance assessments.

Performance assessment of geologic repositories, including engineering barriers, is inherently iterative in nature. Because different conceptual models must be explored, the effect of various simplifications must be assessed, and uneven and sparse data must be dealt with. The selection of iterative performance assessments as the primary NRC staff approach is based on the fact that NRC has responsibility to make a series of judgments during site characterization and the license review, for which performance assessment is needed. Additionally, in making these judgments, it is axiomatic that complete scientific understanding of processes, fully validated computational tools, and complete and unambiguous site-specific data are objects to be strived for, but are unable to be achieved. Therefore, NRC recognizes that judgments will be made under conditions of substantial uncertainty and that it is necessary to learn to use less than perfect computational tools and incomplete data sets.

There are several other reasons why the iterative performance assessment approach will be followed. Iterations will be invaluable in pointing out the shortcomings in existing models and data, and will also indicate topics in need of further investigations or research. Incremental improvements in understanding of processes, computational tools, and data will be strived for in each iteration. It is also imperative that the iterative performance assessments perform a technical integration function by being truly interdisciplinary. Thus, the concepts developed for the engineered subsystem and the natural subsystem must be brought together in each iteration of the performance assessment.

Top-Down Approach to Resource Allocation

Iterative performance assessment will provide an important input to deciding priorities on work in both NMSS and Research in order to best use limited resources. This input will be in the form of problems identified during iterative performance assessments that need a solution. In addition to identification of problems, iterative performance assessment, especially sensitivity and uncertainty analyses, will show which unresolved problems contribute most to uncertainties in performance. Obviously, priorities indicated by PA should be considered in conjunction with needs identified by other means.

Training of Staff

Iterative performance assessments combined with participation in international performance assessment programs such as INTRAVAL will keep the NRC staff current on pertinent methodologies. This is an essential step in providing assurance that the staff will have at its disposal the needed skills to review critically DOE's performance assessments at the time of license application review. Of equal importance, it will provide the staff with needed tools for developing regulatory guidance and additional reactive work, such as review of prelicense submittals including site characterization data and interactions with the DOE, State, and other affected parties.

PROGRAMMATIC PRIORITIES

Highest priority in the near term will be given to developing staff and contractor technical capabilities in the conduct of performance assessments. Progress has already been made as indicated by the recently released staff report entitled, "Phase I Demonstration of the Nuclear Regulatory Commission's Capability to Conduct a Performance Assessment for a HLW Repository" (April, 1990). The second phase of this effort has been initiated and is intended primarily to combine the knowledge of specialized technical disciplines (engineering and earth sciences) with those of the system modelers to produce integrated performance assessments. Special attention will be directed toward improvements in methodology for scenario identification and screening, retardation phenomena, mechanistic treatment of radionuclide release and near-field coupled effects, disruptive consequences, and alternative sensitivity and uncertainty analysis methods. Of equal importance in this effort is a planned evaluation of the effects of the NRC subsystem requirements on EPA Standard compliance.

Skills acquired in the Phase-I development exercise and the planned second phase will have immediate applicability to the other two principal areas of performance assessment work: support to the DOE program review and the development of regulatory guidance for use by the staff and DOE. The staff Phase I effort has already had substantial influence in dealings with DOE in its site characterization activities and led to the staff's first formal technical exchange with DOE on performance assessment (November 27-29, 1990). Immediate benefits also accrue to the regulatory guidance efforts under the Systematic Regulatory Analysis (SRA) program, which is investigating technical uncertainties related to model validation, scenario identification, data uncertainty, and use of expert judgment. Depending on SRA program results, rulemaking may also be warranted.

In the future iterations, high priority will be given to integration of the subsystem performance assessment work with the total system performance assessment. In the present organizational structure, important work on the subsystems, including compliance determination with respect to the siting and design criteria of 10 CFR Part 60, is being funded separately. Irrespective of the funding mechanisms, a plan to implement a team approach for integration of work with respect to each one of the subsystem performance assessments will be developed. To be successful, each team must be comprised of experts from different disciplines interested in a particular subsystem and the total system. The compositions of the teams, the responsibilities of the team leader, relation of the teams to line management, and funding of the work of the teams will be the subject of the "NRC Performance Assessment Implementation Plan."

UPDATING OF STRATEGY

The NRC performance assessment strategy will be reviewed periodically (once a year) and updated based on possible program redirection. This applies especially to the updating of programmatic priorities stated in the last section. The proportion of reactive and proactive performance assessment work may also change from year to year depending upon the extent and nature of DOE's pre-license submittals.