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Performance Assessment Plans and Methods
for the Salt Repository Project

May 1, 1984

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PREFACE

This Performance Assessment Plan (PAP) is a major revision of the previous version, dated 3/1/83. The major changes have resulted in the generation of the first seven chapters of this version, which give an overview of the methodology and rationale of SRP performance assessment. The previous "Validation and Verification Plan" has been incorporated into this Performance Assessment Plan. The next PAP version will be produced by the end of CY 84, and will be compatible with the Site Characterization Plan of the SRP.

The PAP is the product of contribution of many individuals. The bulk of the work needed for this version was done by Mrs. Vicki McCauley, at the general direction of Dr. Terry L. Steinborn. Significant portions of the text were provided by Dr. John F. Kircher and Mr. William V. Harper. Mr. Joseph Peters also contributed. The previous version of the PAP was produced by Dr. Sumant K. Gupta. Critical comments from Ms. Leslie A. Casey (DOE-SRPO) and Dr. Peter L. Hofmann were most useful. Critical reviews of the previous PAP version and the Validation and Verification Plan performed by members of the Argonne National Laboratory staff were also considered in preparation of the current version. The appendix of computer code status and summaries was adapted from an Argonne compilation.

Critical comment is solicited by the reader of this version. Please address review comments to Dr. John F. Kircher, ONWI-PAD.

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1 SALT REPOSITORY PROJECT PERFORMANCE ASSESSMENT PLAN

The U.S. Department of Energy (DOE) is responsible for the disposal of spent fuel, commercial and defense high-level nuclear waste, and commercial transuranic waste. The Civilian Radioactive Waste Management (CRWM) program was established to accomplish this task, in accordance with legislation and schedules provided in the Nuclear Waste Policy Act of 1982. The present proposed disposal method is the use of deep geologic repositories in media such as salt, basalt, tuff or granite. The system is referred to as a mined geologic disposal system (MGDS).

The Salt Repository Project (SRP) of the CRWM program was established to design a salt repository and to assess its ability to contain nuclear waste. To assess the performance of a salt repository, the SRP must first develop, verify, validate and document relevant technologies, then use these technologies to predict the performance of a salt repository system. This document presents postclosure performance assessment and preclosure radiological assessment plans and methods for the SRP. Nonradiological aspects of preclosure performance assessment are not addressed in this document.

1.1 NATURE OF PERFORMANCE ASSESSMENT

Performance assessment (PA) is the analysis of the response of a system to conditions that may prevail during the period over which that system is expected to operate. For the case of a nuclear waste repository, performance assessment is "a tool to predict the probable consequences of creating a waste repository, to compare the consequences with acceptability criteria, and to present the results for judgment by the appropriate bodies." (IAEA, 1981, p.1).

Performance assessment is primarily concerned with whether the repository can accomplish its task -- that is, to contain nuclear waste effectively. It is not concerned with site selection or repository design except as they affect repository performance. It does support these activities, however. If the results of performance analyses indicate that acceptability criteria are not being met, then this information is provided to those involved in site selection and repository design, with recommendations for appropriate action.

Performance analyses will be used to specify design requirements where necessary to assure compliance with acceptability criteria.
Effective performance assessment requires a considerable amount of data. System and subsystem models require not only input data dictated by the model structure, but also data which can be used to verify and validate model results. Sensitivity and uncertainty analyses will be used to identify data requirements efficiently, by determining which input variables control the uncertainty in the results and the degree of uncertainty in each variable that can be tolerated. As models change, data needs can be expected to change and, as new data become available, models may also change.

Although a performance assessment can be used to provide comparisons to acceptability criteria, it is not sufficient for determining that a site is acceptable. Models are developed to analyze and predict system behavior, computer codes that execute these models are verified and validated, and the codes, models, and data involved in the analyses are documented, all as part of a performance assessment. The performance assessment is then presented to the appropriate decision-making body, which makes the ultimate judgment.

The decision-making body responsible for licensing a repository is the Nuclear Regulatory Commission (NRC). The NRC is also responsible for developing the acceptability criteria upon which the decision to license will be based. Performance assessment is anticipated to be an important means by which a planned repository system may be justified to the NRC. It will be a primary focal point of any NRC review.

The success of the Salt Repository Project rests heavily on the results and credibility of its performance analyses. To assure that each analysis is of the high quality demanded by the NRC, this Performance Assessment Plan (PAP) has been developed. The methods by which the peformance assessments will be carried out and the quality of results which may be achieved are described in this document, which will be updated periodically as new information becomes available and understanding of the salt repository system improves.

1.2 ROLE AND SCOPE OF THE PERFORMANCE ASSESSMENT PLAN

The objectives of this Salt Repository Project Performance Assessment Plan are:

- To describe performance assessment and its application to the Salt Repository Project of the CRWM program
- To present the technical approach to be used for satisfying CRWM requirements
- To provide a schedule of milestones which are proposed for carrying out these tasks.

The PAP will also show how performance assessment analyses contribute to the Salt Repository Project in evaluating repository designs and in setting site characterization and other data requirements. All performance assessment work is performed with strict adherence to SRP quality assurance requirements and procedures.

1.3 DEFINITIONS

As presently conceived, a MGDS will be used for the containment of high-level radioactive wastes, such as those generated by commercial nuclear power plants. For the Salt Repository Project, the repository will be located in either bedded or domal salt, roughly one-half mile underground. It will consist of a series of long, narrow excavated tunnels. Individual waste packages will be placed in vertical boreholes located at regular intervals along the tunnel floors. When the waste packages are in place, the boreholes and tunnels will be backfilled, probably with the crushed salt originally excavated, and the holes leading to the repository will be sealed.

Analyses cover two fundamentally different periods. Preclosure or operational analysis deals with repository construction and waste emplacement; postclosure analysis is concerned with the repository after it has been closed and sealed, and for as long as the radioactivity remains a concern. The types of performance analyses required for the two phases are fundamentally different, and regulations applying to the two are different as well.

The geologic disposal system is defined to consist of three subsystems. Figure 1-1 illustrates the roles and interactions of the subsystems for postclosure performance assessment; Figure 1-2 shows the extent of each of the subsystems. Waste package analyses pertain to very near-field performance assessment. The very near field consists of a single waste package and the disturbed zone in the salt surrounding the package. Repository analyses pertain to near-field performance assessment. The near field consists of the

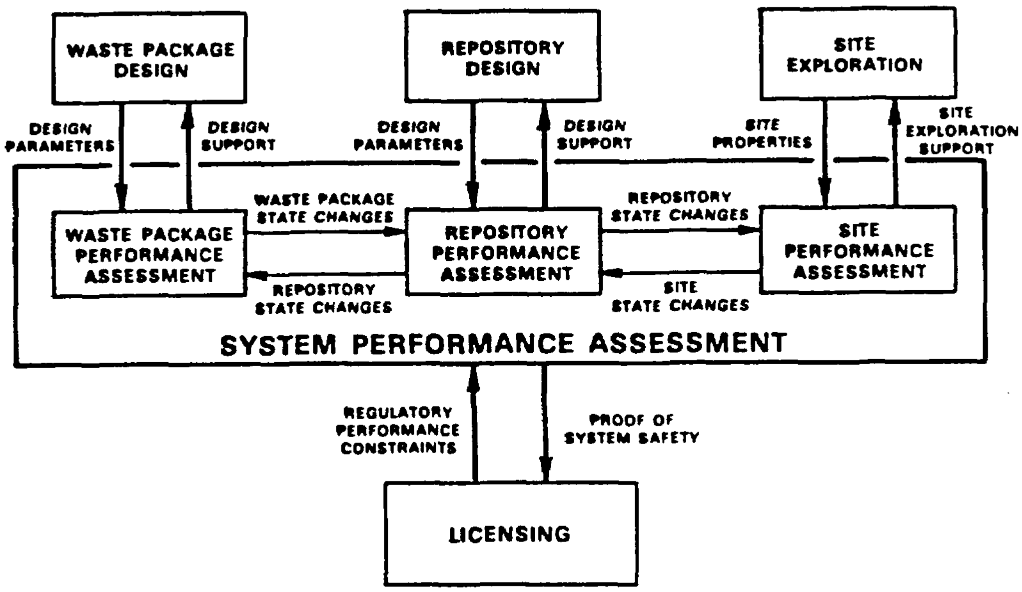


Figure 1-1. Objectives and Interfaces of Performance Assessments

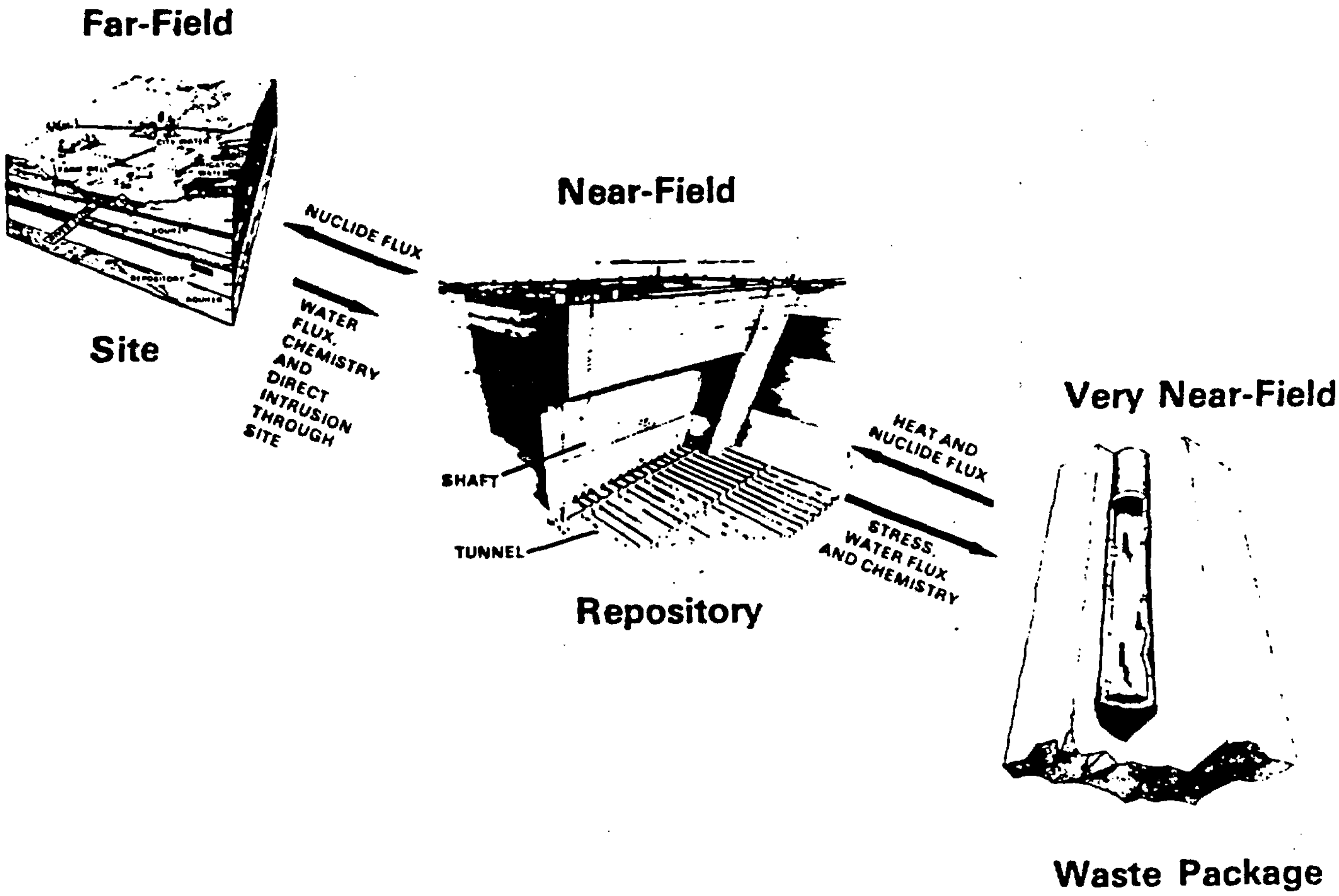


Figure 1-2. Broad Subgrouping for Detailed Performance Assessment

repository and surrounding salt. Site analyses pertain to far-field performance assessment. The far field is defined as the surface and subsurface region containing the repository and the natural barriers to radionuclide release; the regional ground-water basin is included.

The purpose of performance assessment is to assess system and subsystem performances. This is achieved by calculating performance measures, the quantitative results of performance analyses, and comparing them to performance targets, the numerical values set by a standard or regulation that must be met to assure acceptable system performance. Also to be considered are performance criteria, the descriptive conditions that must be met by a disposal system for licensing acceptability. System and subsystem performance criteria have been established by DOE (1981, 1982a, 1982b, 1982c). Specific performance targets are established by the EPA in 40 CFR 191 (EPA, 1982, 1984) and by the NRC in 10 CFR 60 (NRC, 1983).

Performance measures are not so much exact numbers as ranges of values. The range of values is a result of the many uncertainties which affect the results of modeling efforts. Uncertainty and sensitivity analyses are a means by which performance measure uncertainty may be quantified. Uncertainty analysis expresses the degree of uncertainty in code results based on uncertainties in the input parameters. Sensitivity analysis determines the sensitivity of the results to various input parameters.

Assessments must be performed for expected conditions and unexpected conditions. The expected condition is that the repository will remain isolated and undisturbed. An unexpected condition would be a natural or human-induced event or process which might jeopardize the integrity of the system. The various conditions which the system might experience are described by scenarios. Scenarios are descriptions of events or processes which could create pathways for groundwater flow. Such an intrusion of water into the repository is the only anticipated means by which radionuclides could be transported from the repository.

Computer codes are used extensively in performance assessment to model physical processes. Every code used in an assessment must undergo verification and validation to demonstrate the reliability of its results. Verification provides assurance that the code correctly performs the calculations specified in the mathematical model on which it is based. This assurance is provided by comparing code results to results from similar codes number at the upper right-hand corner of the block. The milestones are grouped by the type of endeavor, i.e., performance assessments of the major subsystems, site, repository, and waste package, or efforts such as verification and validation of codes and models. To indicate key interfaces and to simple analytical solutions. Validation is the means by which the model is shown to represent the physical process correctly. Validation usually entails a comparison of model results to available data.

Within the Salt Repository Project, a Performance Assessment Department (PAD) is responsible for the activities described in this plan. PAD interacts heavily with other components of the SRP. The Engineering Technology Department, the Repository Project Office, and the Site Function are responsible for waste package design, repository design, and site selection, respectively. PAD receives data and proposals (designs or sites) from these groups, and supplies them in turn with performance assessment results and revised data needs. PAD also provides data needs to the Exploratory Shaft Project Office, which is responsible for generating much of the site-specific data. The Site Characterization Plan Project Office (SCPPO) will coordinate efforts on the generation of required Site Characterization Plans (SCPs). PAD will play an important role in specifying data needs and performance assessment plans for the SCPs. The Environmental/Socioeconcmic Function will provide information needed by PAD to address preclosure radiological safety questions. PAD will have to provide data needs to this group, as well.

1.4 SCHEDULE AND MILESTONES

Performance assessment analyses are required for all major SRP milestones, most of which result in major programmatic documents. As will be discussed in the following chapters will show, these programmatic performance assessments require a great deal of supporting work. This work includes conceptual model development and modification, code development, documentation, validation and verification, and data compilation and statistical analysis. Such PA activities contribute to many other requirements of the SRP in addition to major licensing documents. These requirements include analysis of subsystems for specification of data needs and evaluation of designs. The major Performance Assessment Milestones are given chronologically in Table 1-1 and are based on the overall SRP strategy as shown in Figure 1-3.

Table 1-1. Performance Assessment Milestones

	Title	Schedule
1.	ONWI Submits PAP Rev. #1 in Support of Initial SCP to clearance	11/01/84
2.	ONWI Submits PA Report in Support of Waste Package Conceptual Design to Clearance and Engineering	12/01/84
3.	ONWI Submits Radiological Protection Criteria and Procedures Report in Support of Repository Site Specific CD to clearance	06/01/85
4.	ONWI Submits Benchmarking and Verification Reports of Preliminary Set of PA Codes in Support of SCP update to clearance	09/01/85
5.	ONWI Submits PAP Rev. #2 in Support of SCP Update to clearance	10/01/85
6.	ONWI Submits PA of Preliminary Design Analysis Report in Support of Repository Conceptual Design to Engineering	10/15/85
7.	ONWI Submits PA Status Report in Support of Site to clearance	12/15/85
8.	ONWI Submits Safety Analysis Report in Support of Repository Conceptual Design to clearance	04/01/86
9.	ONWI Submits Site Specific Validation of PA and Site Models Prediction Report in support of Hydro Testing to clearance	06/01/86
10.	ONWI Submits Preliminary Data Requirement in Support of Waste Package Preliminary Design to Engineering	06/01/86
11.	ONWI Submits PA Report in Support of Repository Conceptual Design to Engineering	07/15/86
12.	ONWI Submits Benchmarking and Verification Reports of Improved PA Codes in Support of SCP Update to clearance	09/01/86
13.	ONWI Submits PAP Rev. #3 in Support of SCP Update to clearance	10/01/86

(Continued)

14.	ONWI Submits PA Status Report Update in Support of Site to clearance	12/15/86
15.	ONWI Submits PA of Preliminary Salt Waste Package Report in Support of Waste Package Preliminary Design to clearance	02/01/87
16.	ONWI Submits Data Requirements Update in Support of Site to Geology and clearance	02/01/87
17.	ONWI Submits PA Requirements for Title I Repository Design Specification Report in Support of Title I Repository Design to clearance	08/04/87
18.	ONWI Submits Preclosure Safety Analysis Report in Support of Title I Repository Design to clearance	09/30/87
19.	ONWI Submits PAP Rev. #4 in Support of SCP Update to clearance	10/01/87
20.	ONWI Submits PA Requirements for Final Waste Package Specification Report in Support of Waste Package Demo Testing to clearance	11/04/87
21.	ONWI Submits PA Status Report Update #2 in Support of Site to Geology and clearance	12/15/87
22.	ONWI Submits PAP Rev. #5 in Support of SCP Update to clearance	11/01/88
23.	ONWI Submits Title I Interim PA Analysis Report in Support of Title I Repository Design to clearance	11/01/88
24.	ONWI Submits PA Status Report Update in Support of Site to Geology and clearance	12/01/88
25.	ONWI Submits PA & Site Model Validation Report in Support of DEIS to clearance	12/01/88
26.	ONWI Submits PA of Salt Waste Package Final Design Report in Support of Waste Package Final Design to clearance	02/01/89
27.	ONWI Submits PA of Repository Title I Design Report in Support of Title I Design to clearance	02/01/89
28.	ONWI Submits Safety Analysis Sections in Support of DEIS to Review	04/01/89
29.	ONWI Submits Sensitivity and Uncertainty Analysis Sections in Support of DEIS to Review	04/01/89

(Continued)

30.	ONWI Submits PA Report in Support of DEIS to clearance	06/01/89
31.	ONWI Submits PA Report in Support of SAR to clearance	01/04/90
32.	ONWI Submits PA Report in Support of FEIS to clearance	06/01/90

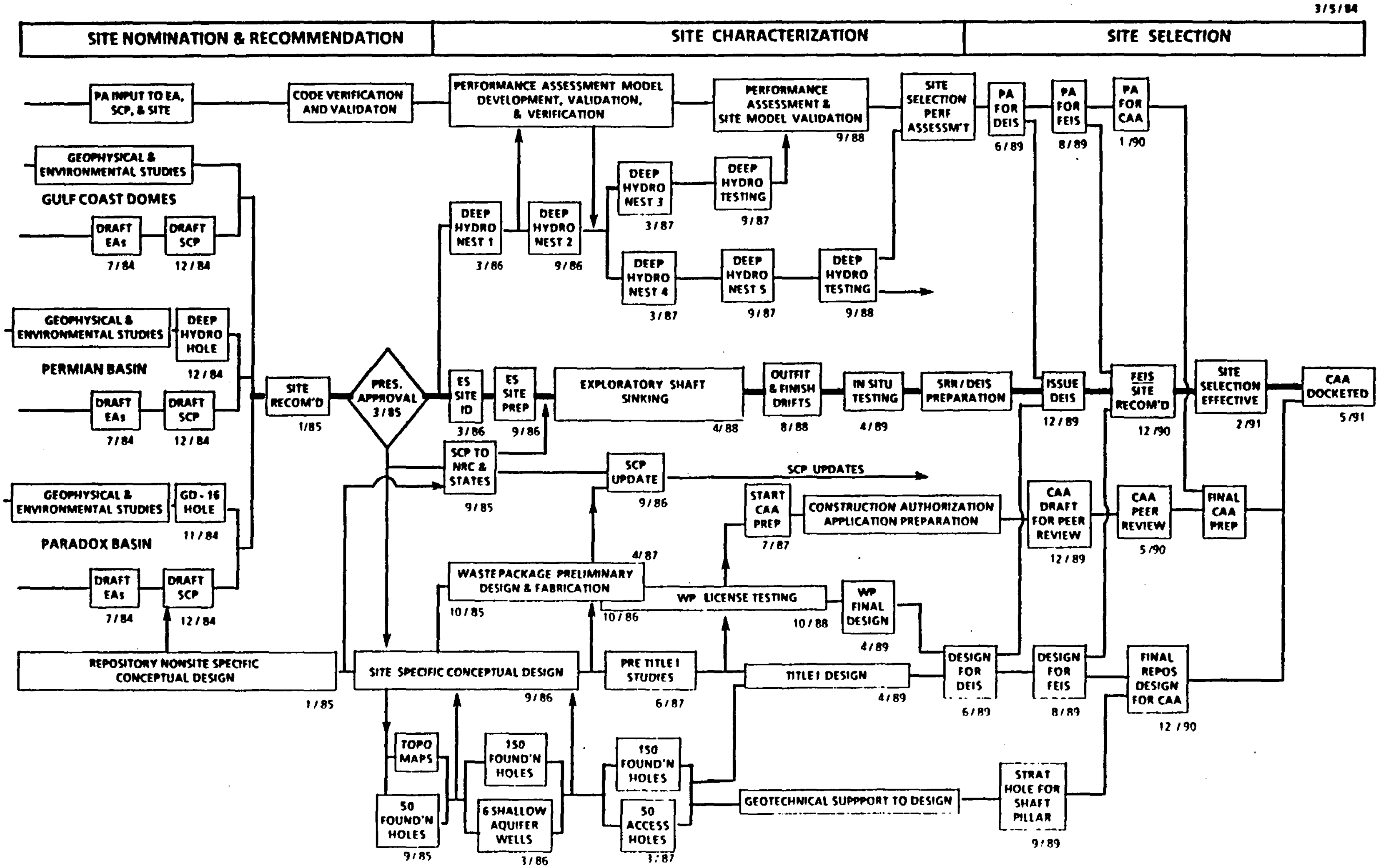


Figure 1-3. Salt Repository Project Strategy

The logic of the overall performance assessment activities, as defined by the completion milestones in Table 1-1, is shown in Figure 1-4. In this figure the milestone indicated in a given block is keyed to the Table by the in a very simplified manner, the milestones are also tied to activity lines for other SRP activities, such as Site Characterization Plan (SCP) preparation, engineering design, and testing. Such interfaces are shown in greater detail in Figures 1-5 through 1-9 and indicate where analyses support major documents, e.g the SCP or Draft Environmental Impact Statement (DEIS), or design activities such as repository Title I, a preliminary design which goes into the Construction Authorization Application (CAA). In all cases it is the nature of the required analysis which drives the performance assessment activity.

The sequence of events that must take place is similar for each of these analyses. First, a baseline set of data must be selected and formalized, so that all related analyses will be consistent with respect to data and design assumptions. Then, analyses of subsystems will be performed over the range of inputs appropriate to the particular assessment. In most cases, overall combined system performance will be assessed. This will be done either using a total system model or by linking the individual subsystem analyses and iterating to account for interdependency among the subsystems. The results of the calculations will be compared to the system or subsystem performance targets and regulatory criteria or limits. The entire process will be carefully documented to show all assumptions and to provide a highly visible and trackable account of the analysis. This is normally done by summarizing the analyses in the program document, e.g., the DEIS, and preparing one or more topical reports with details of the analysis for separate publication. These topical reports contain input data, boundary conditions, and limiting assumptions used for the analyses, details of the analytical techniques (or references to code documentation), and discussions of input and output uncertainty.

The next major SRP activity requiring heavy performance assessment participation is preparation of the Site Characterization Plan (SCP). The specific PA input called for by Regulatory Guide 4.17, the NRC document that specifies the SCP format and content (NURC, 1982), is a section of SCP Chapter 10 on PA status. In addition, performance analyses will be very important to the identification of issues determining critical data needs and to geoscience

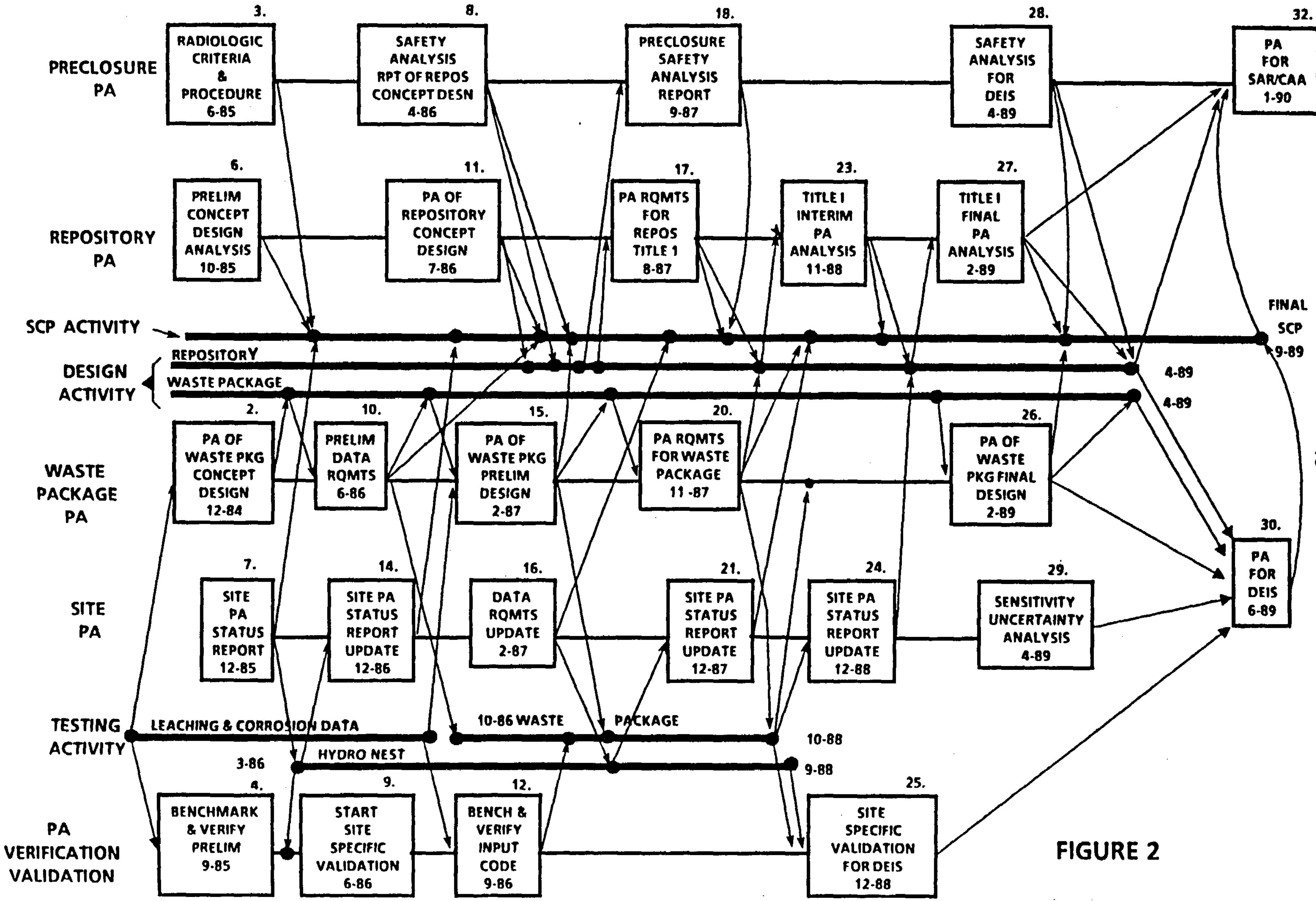
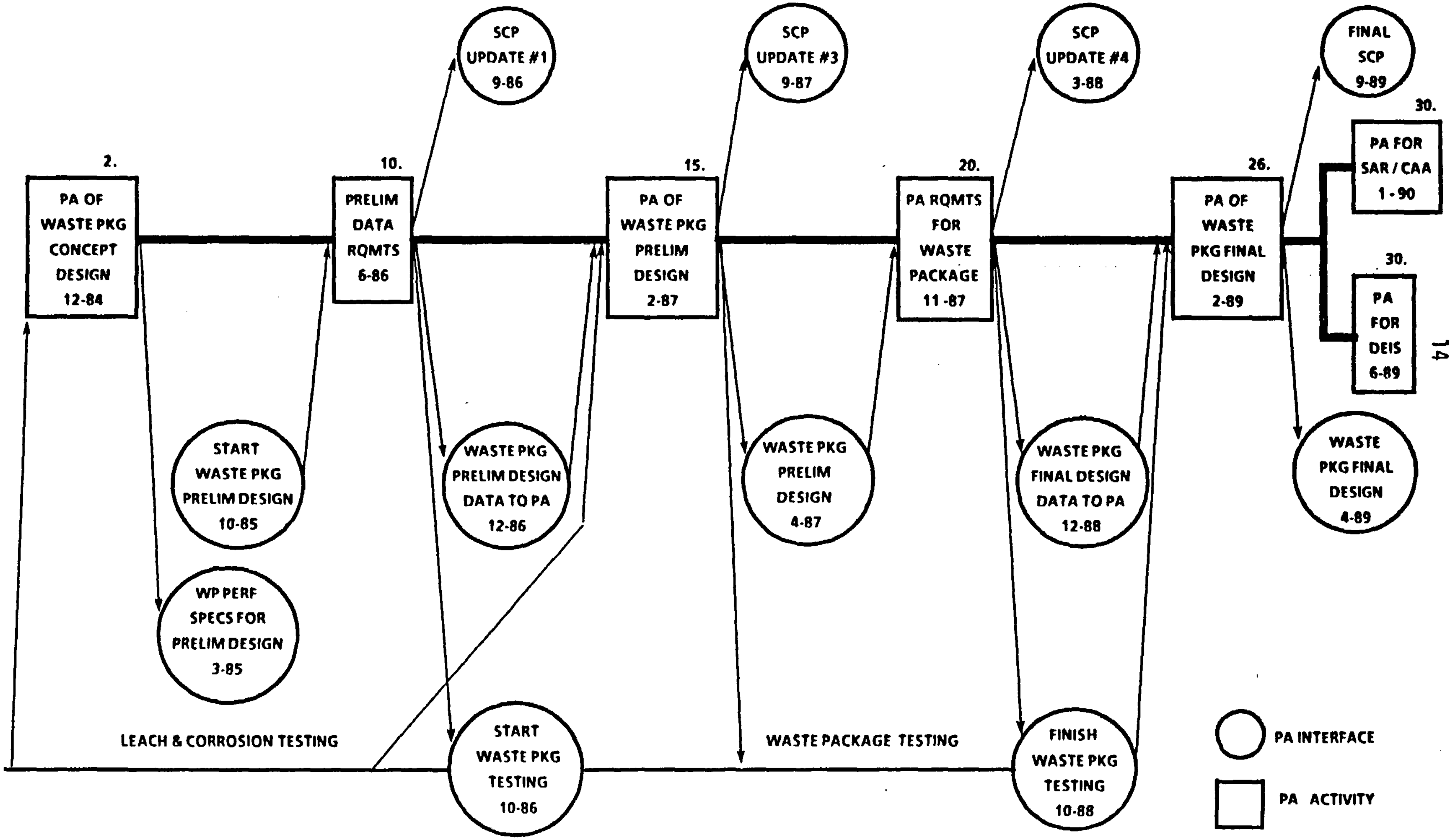
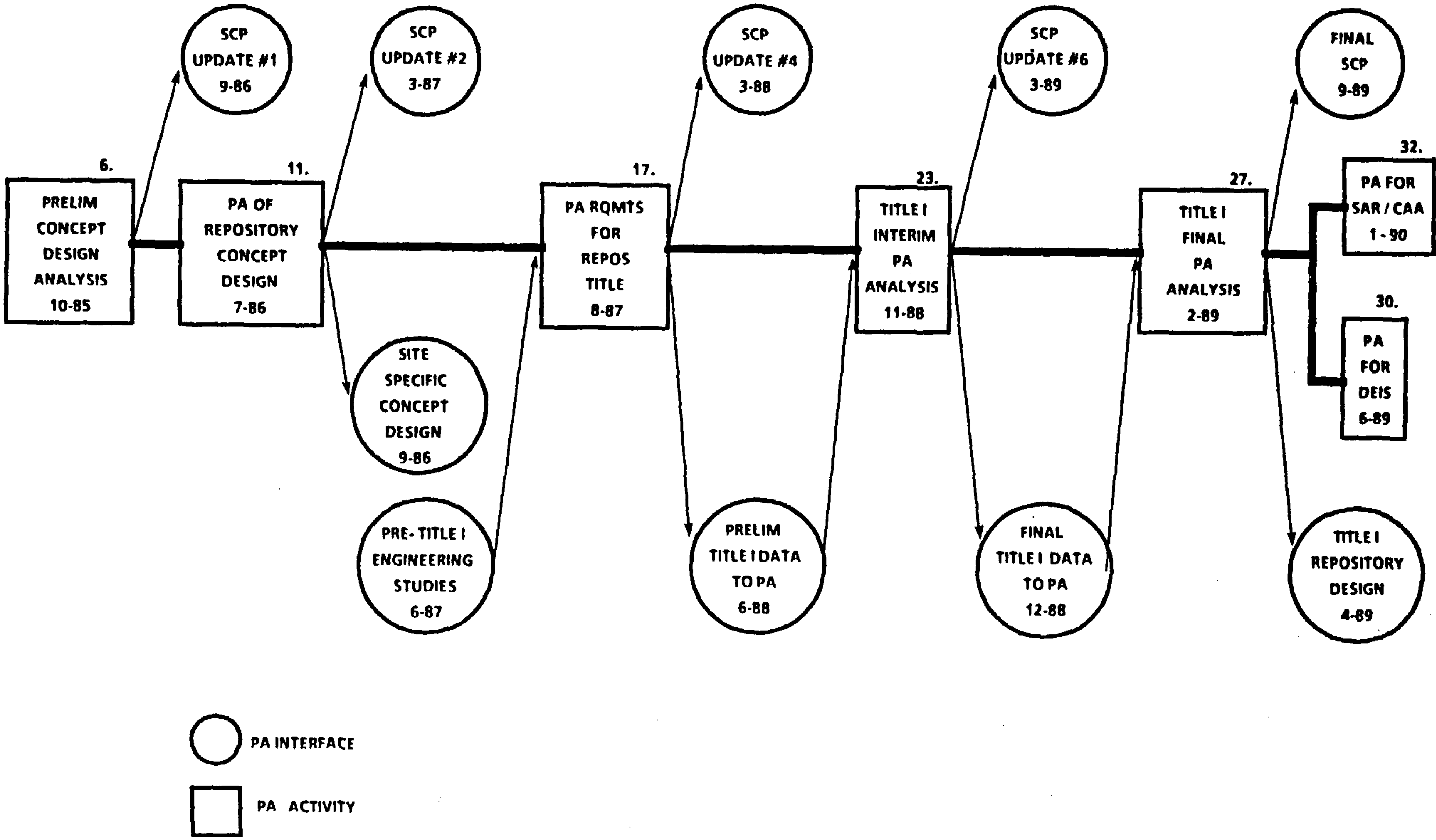


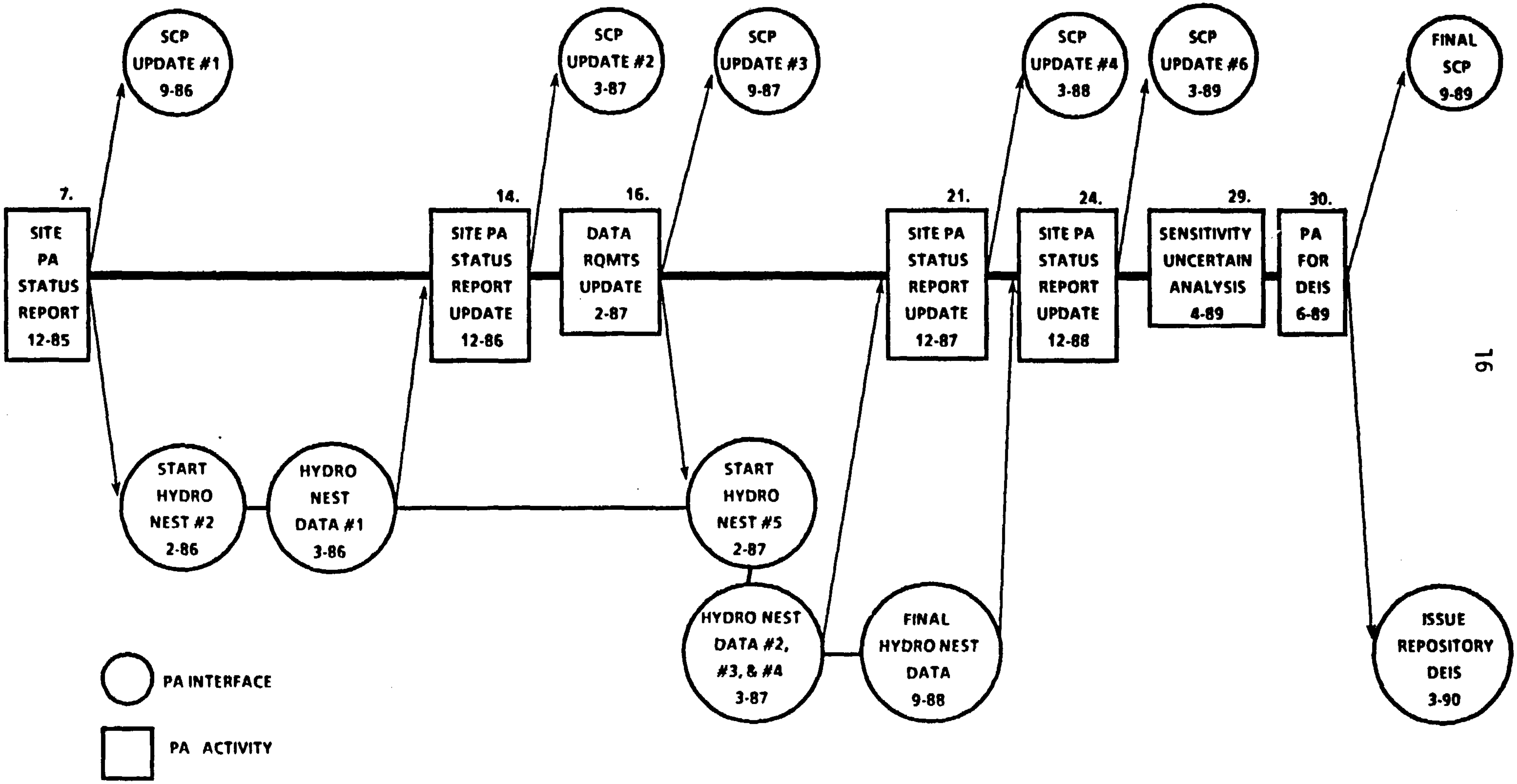
Figure 1-4. Performance Assessment Logic (Completion Milestones)



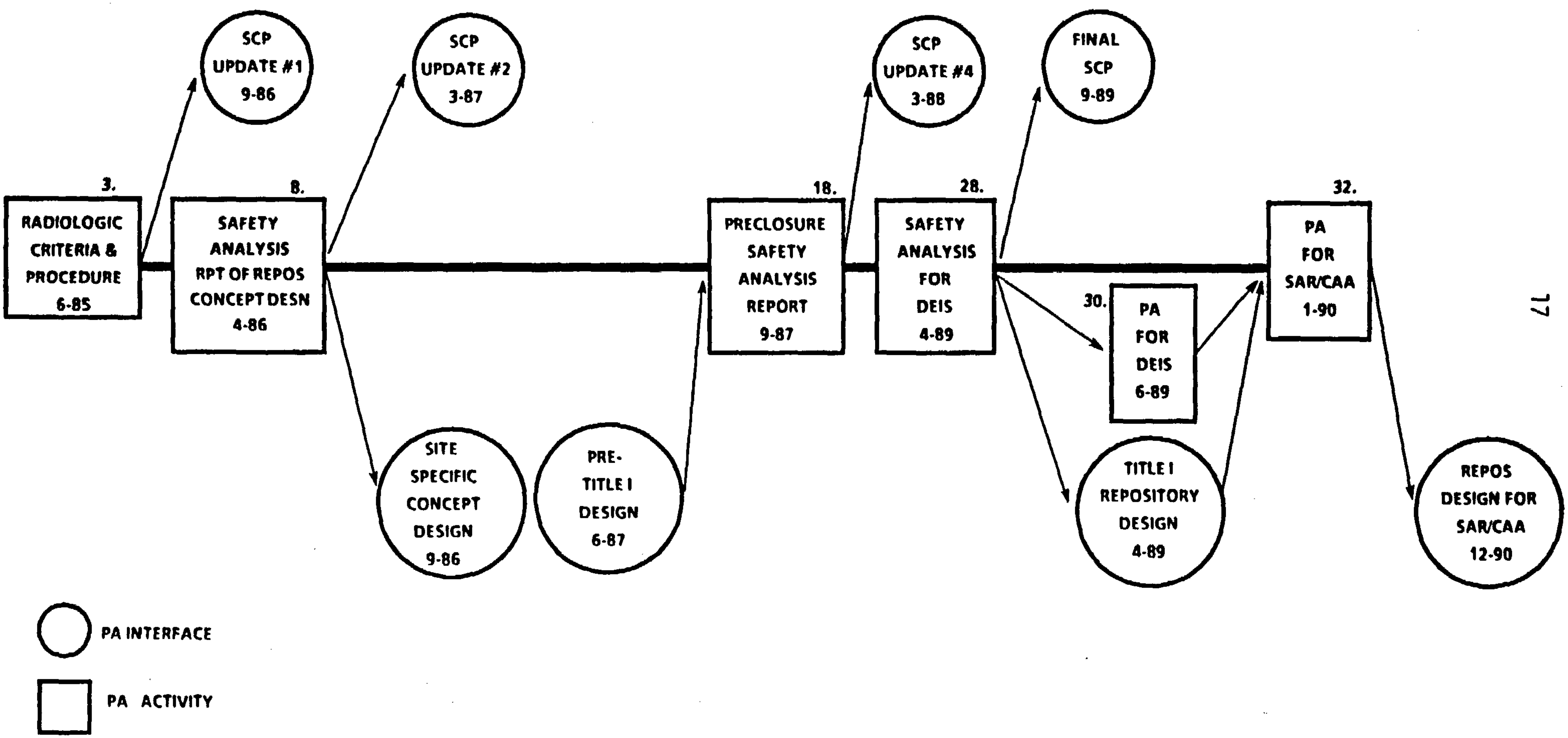
Figures 1-5 and 8-12. Waste Package Performance Assessment Logic
(Completion Milestones)



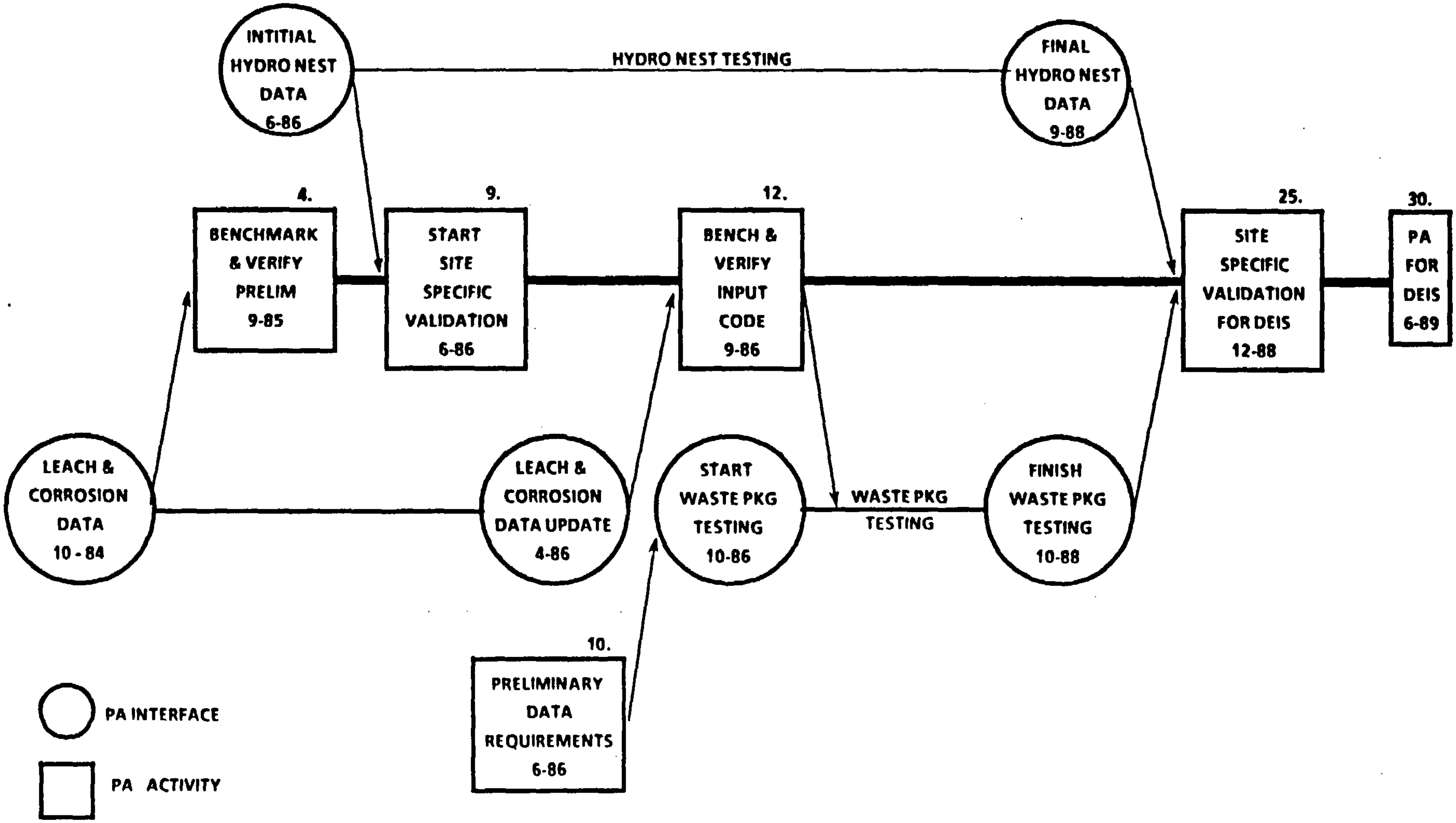
Figures 1-6 and 9-6. Repository Performance Assessment Logic
(Completion Milestones)



Figures 1-7 and 10-12. Site Performance Assessment Logic
(Completion Milestones)



Figures 1-8 and 11.9. Preclosure Performance Assessment Logic
(Completion Milestones)



Figures 1-9 and 12-2. Performance Assessment Verification/Validation Logic

(Completion Milestones)

data collection plan development. These efforts in support of the SCP are described in greater detail in the Activity Plan for the Development of Site Characterization Plans (ONWI, 1984). Figure 1-10 illustrates the SCP planning logic which involves performance assessment at the issue identification stage and shows schematically how analyses and sensitivity and uncertainty studies encompass and define the needs for specific data, types of codes and models, and their verification and validation. These then lead to further updates of this Performance Assessment Plan as well as to specific plan documents for the SCP.

The analytical activities in support of the SCPs will be based on those recently completed for the Environmental Assessments (EAs). For the most part the SCP activity will consist of sensitivity studies around the EA "base" calculation. The SCP will be revised periodically to reflect progress in site characterization and other SRP activities. Such revision will require revised performance analyses based on data and design improvements as indicated in Figures 1-5 through 1-8.

Performance analyses of each subsystem (as described in Chapters 8-10 of this Plan) will be used to investigate the types, quantities and acceptable uncertainties of data needed to demonstrate confidently that each subsystem will meet regulatory criteria and standards. These analyses will include geostatistical evaluations and uncertainty and sensitivity analyses, as discussed in Section 4.2.2 of this document. In addition to subsystem analyses, performance analyses will be used to investigate the nature and the extent of symbiosis and synergism among the subsystems, including compatibility of assumptions and commonality of data needs and data collection activities. As shown in Figures 1-5 through 1-9, the major analytical activities are planned to support design activities as well as do the SCP and its updates with a minimum of duplication. The analyses performed for the first SCPs will use existing models and codes. Future efforts, such as analyses required for the DEIS, Final Environmental Impact Statement (FEIS), and Safety Analysis Report (SAR) may require further model and code development and will certainly need extensive validation, verification, and documentation. The following chapters describe these activities in detail.

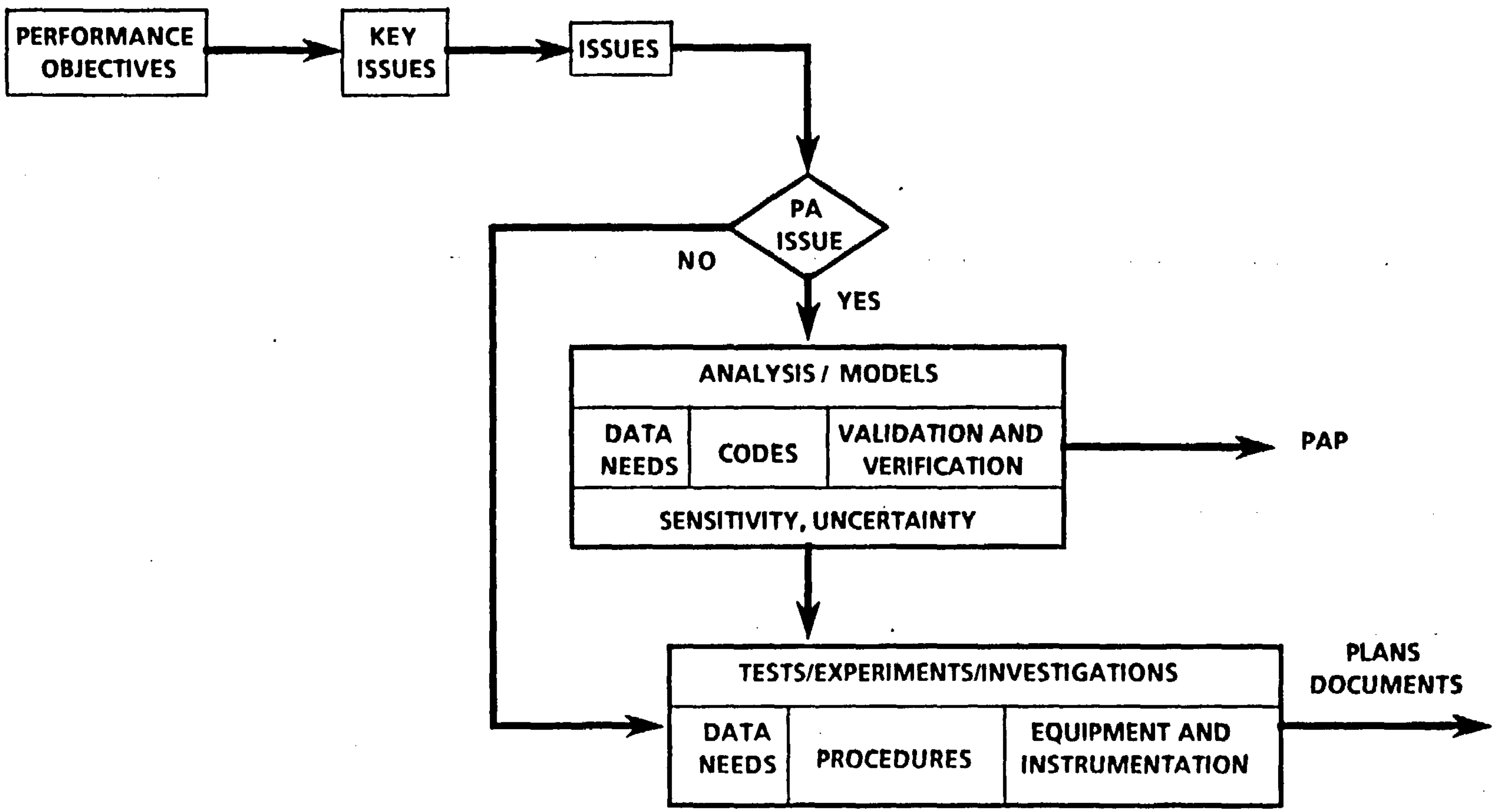


Figure 1-10. SCP Planning Logic

2 TECHNICAL APPROACH TO SALT REPOSITORY PROJECT PERFORMANCE ASSESSMENT

Preclosure performance assessment analyzes the radiological impacts of a repository during its operational phase. Postclosure performance assessment for the Salt Repository Project occurs on two levels. The first level addresses the total system and system uncertainties, and assures that subsystem interactions are well understood. The second level deals with the subsystems. Separate subsystem assessments are made necessary by the complexity of the MGDS and by the needs within the project for detailed analytical results, primarily for design purposes. On both levels, performance assessment is approached through modeling. The lengths of time over which predictions must be made (10,000 years or more) makes direct experimental demonstrations of feasibility impossible.

To begin an analysis, the physical process being modeled must be carefully defined. Where applicable, a preliminary bounding analysis is performed to determine whether the process warrants detailed modeling. If detailed analysis is needed, either because of concern that the process might lead to radionuclide release or because detailed analyses are required to aid design, a model must be developed to represent the process.

Generally two types of models are used. Empirical models are based on observation of experimental data. Theoretical models are based on application of sound physical principles. A drawback to empirical models is that at best they are valid only for the specific conditions under which the data were gathered; predictions of behavior under any other conditions are risky. To compensate for this uncertainty, extremely conservative estimates of behavior are often postulated when empirical models are used. Where the theory behind a process is well understood a theoretical model may be preferred, because the behavior of the system under conditions which have never been observed may be predicted with some confidence. However theoretical models often require knowledge of physical parameters for which no data are readily available. In practice, most models rely on both empirical and theoretical features.

This chapter outlines the technical approach to preclosure radiological assessments and to system and subsystem analyses for expected postclosure conditions, and introduces the concept of the release scenario. The ideas presented here are expanded in later chapters.

2.1 TOTAL SYSTEM POSTCLOSURE ANALYSIS

Total system analysis, as used in this plan, refers only to postclosure system assessment. The SRP intends to develop a system model to perform system assessments based on individual process computer codes. The codes may be combined into a single, complex code, or they may be developed and run separately. A system model does not imply a single system code.

System analysis is discussed further in Chapter 7.

2.2 SUBSYSTEM POSTCLOSURE ANALYSIS

Section 1.3 introduced the subsystems used in postclosure performance assessment. This section explains the technical approach which the SRP will use to model these subsystems, and points out the unique concerns of performance assessment for a repository in salt. Details of subsystem analysis are given in Chapters 8 through 10.

2.2.1 Very Near-Field Analysis (Waste Package Assessment)

Very near-field analysis is concerned only with a single waste package, the borehole that contains it, and the salt immediately surrounding the borehole. In general, any salt which is close enough to contribute to brine migration to the package is included in the very near field.

The goal of very near-field analysis is to assess the ability of a waste package to contain nuclear waste under repository conditions. Therefore the properties of the waste package and the conditions under which a waste package will operate need to be understood. Waste package properties will be specified as part of a waste package design. These properties will be used in analyses to assess the ability of a particular design to contain waste.

Waste package performance will depend on two things. First is the ability of the package to withstand lithostatic pressure at repository depth. Second is its ability to tolerate moisture. Salt is essentially nonporous, so groundwater flow past the waste package will not occur under normal conditions. The expected mechanism for transport of moisture to the waste package is brine migration.

Under the influence of a thermal gradient, brine has been observed to migrate toward a heat source. In a repository, the waste package will generate heat, so brine is expected to travel to the waste package and corrode the package surface. If sufficient brine migrates, package failure can occur. The leaching characteristics of the waste form will then have to be studied, so that the potential for radionuclide release from the waste form may be understood. Finally a mechanism for movement of radionuclides through the solid salt will need to be established. Solid state diffusion is presently under investigation.

Clearly a great number of models are needed to represent the very near field. A thermal analysis is needed as input to a brine migration analysis, which becomes part of a waste package corrosion and failure analysis. Lithostatic stress analyses are also needed to understand waste package failure. Geochemical analyses are needed to understand effects of the local geochemistry on corrosion and leaching. Once failure conditions are determined, a radionuclide transport analysis is required to make possible a prediction of radionuclide release.

The self-healing properties of salt need to be understood. When lithostatic pressure and elevated temperatures are applied to the crushed salt used to backfill the borehole, the salt will resolidify. The condition of the salt around the waste package will affect the way migrating brine is able to attack the waste package surface. Nonuniform corrosion could result in early package failure if voids near the waste package fill with brine. Waste package analyses are discussed in detail in Chapter 8.

2.2.2 Near-Field Analysis (Repository Assessment)

Near field analysis evaluates the performance of the repository and surrounding salt. The objectives of repository assessment are (1) to determine how design features affect repository performance so that appropriate modifications to the repository design can be made, (2) to determine how the repository subsystem contributes to waste isolation, and (3) to evaluate the effects of the repository subsystem on the waste package and the site. To meet these objectives, the repository environment must be evaluated in terms of the thermal, thermomechanical, geochemical, and fluid flow conditions the repository will experience. Models will have to be developed to analyze all these parameters and their effects on radionuclide containment. Because of the dependent nature of the three subsystems, repository assessment must interact heavily with waste package assessment and site assessment.

One specific concern of repository assessment is shaft seal behavior. All shafts leading to the repository must be backfilled and sealed so that water cannot enter the repository through the shaft system. Water is a concern because it dissolves salt and corrodes the waste package materials. The seal design must therefore be carefully studied and its adequacy assured. Another way in which moisture can enter the repository is with the backfill material used. The crushed salt placed in the repository as backfill may have to be carefully protected from moisture if its moisture content is found to be important to containment. Near-field analyses are discussed in detail in Chapter 9.

2.2.3 Far-Field Analysis (Site Assessment)

Far field analysis studies the effects of the repository on the site, both above ground and below ground. Again the self-healing, plastic nature of salt becomes important. As the crushed salt used to backfill the tunnels resolidifies, subsidence of the repository region may occur. At the same time, the heat generated by the waste material will bring about thermal expansion of the salt. The net effect can only be determined by modeling the processes involved. The possibility of fracturing of the rock layers due to these thermal and mechanical stresses must be carefully studied. Effects on groundwater flow must be assessed.

Site assessment is directly involved in site screening and characterization. The ability of a site to limit radionuclide release must be understood before the site can be recommended for repository placement. Groundwater flow patterns, geochemistry, rock properties and local climate all need to be understood. If the possibility of erosion or salt dissolution exists, the extent to which it might occur will have to be predicted. Far-field analyses will be discussed in detail in Chapter 10.

2.3 POSTCLOSURE SCENARIO ANALYSIS

Scenario analysis begins with the identification of credible events which might affect the ability of the repository to contain radioactive waste. Detailed scenarios will be developed for each event and the consequences of each will be studied. Finally, preventive or mitigative measures will be established where possible to reduce the consequence or the occurrence probability of each event. The scenario will relate either to human intrusion, design failure or natural phenomena. Details of postclosure scenario analysis are presented in Chapter 5.

2.4 OPERATIONAL ANALYSIS (RADIOLOGICAL ASSESSMENT)

Operational analysis is concerned with an evaluation of preclosure conditions. As part of operational analysis, the SRP will assess the radiological impact of both normal repository operations and accidents. Transportation of the waste packages to the repository is considered part of repository operation. Worker exposure and population exposure will be examined where appropriate. Operational analysis is discussed in detail in Chapter 11.

2.4.1 Normal Operations

To approach the problem of radiological assessment under normal operating conditions, all operations representing potential hazards will first be separated into clearly delineated unit operations. Each unit operation will be evaluated for potential consequences, including dose assessment where necessary. Then preventive or mitigative measures for each unit operation will be established.

2.4.2 Accident Conditions

Although the types of scenarios hypothesized for preclosure and postclosure conditions are very different, the treatment of scenarios in each case will be very similar. As discussed in Section 2.3, credible events will first be identified, detailed scenarios will be developed, the consequences of each will be determined, and preventive or mitigative measures will be established where possible. The credible events will consist of (1) accidents within the facilities, (2) transportation-related accidents, and (3) events caused by natural phenomena.

2.5 UNCERTAINTY AND SENSITIVITY ANALYSES

Results of performance assessments are by nature uncertain. This uncertainty must be characterized before model results become useful. Part of this uncertainty is due to reliance on input parameters which have various uncertainties associated with them. Uncertainty and sensitivity analyses is used to determine (1) the degree of uncertainty in the results based on uncertainties in the input parameters, and (2) the sensitivity of the results to the various input parameters. In this way key parameters may be identified for more refined analysis. In addition to the uncertainty associated with input parameters, the models themselves contribute uncertainties to the results. Uncertainty and sensitivity analyses model uncertainty by making changes in the model, for example, by changing the assumptions upon which the model is based, and examining the sensitivity of the results.

Two major approaches are used in sensitivity and uncertainty analyses. The first is based on a statistical design. The design may be derived using classical statistical experimental design theory or statistical sampling (Monte Carlo) methods. The advantages and disadvantages of each are given in ONWI-444 (Harper, 1983). The second major method is a deterministic first order approach typified by the adjoint method.

It should be emphasized that the SRP has not chosen a single technique or approach for sensitivity and uncertainty analysis. The SRP will utilize the approaches that are best suited to the particular model. Often double checks will be made using more than one technique. In some cases advantage will be taken of the comprehensive screening capabilities of the adjoint sensitivity method to help define and construct a simplified model which can be handled more efficiently by one of the sampling techniques such as Latin Hypercube Sampling. Details of sensitivity and uncertainty techniques are given in Section 4.2.2.

3 PERFORMANCE CRITERIA AND MEASURES

The technical requirement that must finally be met by the entire MGDS and each of its subsystems relates to the performance of the total system and subsystems. Performance criteria have been established by DOE for the MGDS (NWTS-33(1)) and for the three major subsystems: the site (NWTS-33(2), the repository (NWTS-33(3)), and the waste package (NWTS-33(4a)). These criteria contain the general preclosure and postclosure performance requirements, and contain by reference the specific performance targets that the MGDS and its subsystems must meet. The performance targets are contained in the various applicable regulations and standards, and in the Nuclear Waste Policy Act of 1982 (U.S. 97th Congress, 1983). Performance assessment analyses will result in calculated system and subsystem performance measures which will then be compared to the performance targets to determine compliance. The DOE performance criteria are summarized in Table 3-1.

3.1 STANDARDS AND REGULATORY REQUIREMENTS

The MGDS must satisfy the legal requirements placed upon it by congress and federal agencies and commissions. Not all of these bodies have promulgated performance requirements. The major performance-related requirements are contained in NRC regulations (10 CFR 60; NRC, 1983) and in EPA standards (draft 40 CFR 191; EPA, 1982). In many cases, the regulations and standards are accompanied by formulas or conditions for calculation of performance measures. Neither the NRC nor the EPA has generated performance requirements specific to disposal in a salt formation; repositories in all geologic media are subject to the same requirements.

TABLE 3-1. PERFORMANCE CRITERIA

1.0 SYSTEM PERFORMANCE CRITERIA (DOE/NWTS-33(1))

1.1 Operational Safety

1.1.1 Public Health and Safety

Applicable federal public health and safety criteria issued by the Nuclear Regulatory Commission (NRC) and the Environmental Protection Agency (EPA) shall be satisfied during the operational phase of the mined geologic disposal system.

1.1.2 Occupational Safety

Occupational radiological exposure to the repository personnel shall be maintained to within the limits specified in 10 CFR Part 20 and below these limits to as low as reasonably achievable levels. Applicable regulations of the Mining Safety and Health Administration (specifically, 30 CFR Part 57) and Occupational Safety and Health Administration shall be used to ensure the protection of repository personnel from mining and other occupational hazards.

1.2 Long-Term Safety

The mined geologic disposal system shall meet all applicable standards and shall contain and isolate radioactive wastes to the extent necessary to ensure that releases of radionuclides to the biosphere do not result in unacceptable doses to individuals and to the general population. Reasonable assurance shall be provided that adequate isolation will be achieved for at least 10,000 years with no prediction of unacceptable decrease in isolation beyond that time.

1.3 Environmental Requirements

Siting, developing, and operating the mined geologic disposal system shall be conducted in a manner that preserves the quality of the environment to the extent reasonably achievable and complies with current environmental legislation. The environmental impacts associated with the mined geologic disposal system shall be mitigated to the extent reasonably achievable.

2.0 SITE PERFORMANCE CRITERIA (DOE/NWTS-33(2))

2.1 Site Geometry

The site shall be located in a geologic environment that physically separates the radioactive wastes from the biosphere and that has geometry adequate for repository placement.

(Continued)

(1) The minimum depth of the repository waste emplacement area shall be such that credible human activites and natural processes acting at the surface will not unacceptably affect system performance.

(2) The thickness and lateral extent of the geologic system surrounding the waste emplacement area shall be sufficient to accommodate the repository and a buffer zone and to ensure that impacts induced by construction of the repository and by waste emplacement will not unacceptably affect system performance.

2.2 Geohydrology

The geohydrologic regime in which the site is located shall have characteristics compatible with waste containment, isolation, and retrieval.

(1) The site shall be located so that the present and probable future geohydrological regime will minimize contact between ground water and wastes and will prevent radionuclide migration or transport from the repository to the accessible environment in unacceptable amounts.

(2) The site shall be located so that the hydrological regime can be sufficiently characterized to permit modeling to show that present and probable future conditions have no unacceptable impact on repository performance.

(3) The site shall be located so that the geohydrological regime allows construction of repository shafts and maintenance of shaft liners and seals.

(4) The site shall be located so that subsurface rock dissolution that may be occurring, or is likely to occur, can be shown to have no unacceptable impact on system performance.

2.3 Geochemistry

The site shall have geochemical characteristics compatible with waste containment, isolation, and retrieval.

(1) The site shall be located so that the chemical interactions between radionuclides, rock, ground water, or engineered components will not unacceptably affect system performance.

2.4 Geologic Characteristics

The site shall have geologic characteristics compatible with waste containment, isolation, and retrieval.

(1) The site shall be located so that the subsurface setting can be sufficiently characterized to permit identification and evaluation of conditions that are potentially adverse or favorable to waste containment, isolation, or retrieval.

(Continued)

(2) The site shall provide a geologic system which can be shown to accommodate anticipated geomechanical, chemical, thermal, and radiological stresses caused by waste/rock interactions.

(3) The site shall be located so that development, operation, and closure of underground areas can be accomplished without undue hazard to repository personnel.

2.5 Tectonic Environment

The site shall be located such that credible tectonic phenomena will not degrade system performance below acceptable limits.

(1) The site shall be located so that its tectonic environment can be evaluated with a high degree of confidence to identify tectonic elements and their impact on system performance.

(2) The site shall be located so that Quaternary faults can be identified and shown to have no unacceptable impact on system performance.

(3) The site shall be located so that the centers of Quaternary igneous activity can be identified and shown to have no unacceptable impact on system performance.

(4) The site shall be located so that long-term, continuing uplift or subsidence rates can be shown to have no unacceptable impact on system performance.

(5) The site shall be located so that ground motion associated with the maximum credible earthquake will not have unacceptable impact on system performance.

2.6 Human Intrusion

The site shall be located to reduce the likelihood that past or future human activities would cause unacceptable impacts on system performance.

(1) The site shall be located so that the exploration history or relevant past use of the site or adjacent areas can be determined and can be shown to have no unacceptable impacton system performance.

(2) The site shall be located on land for which the federal government can obtain ownership, control access, and obtain all surface and subsurface rights necessary to ensure that surface and subsurface activities at the site will not cause unacceptable impact on system performance.

2.7 Surface Characteristics

The site and its surrounding area shall be such that surface characteristics or conditions can be accommodated by engineering measures and can be shown to have no unacceptable impacts on repository operation and system performance.

(Continued)

(1) The site shall be located so that the surficial hydrological system, both during anticipated climatic cycles and during extreme natural phenomena, will not cause unacceptable impacts on repository operations or system performance.

(2) The site shall be located in an area where surface topographic features do not unacceptably affect repository operation.

(3) The site shall be located where meteorological phenomena can be accommodated by engineering measures and can be shown to have no unacceptable effect on repository operation.

(4) The site shall be located where present and projected effects from nearby industrial, transportation, and military installations and operations can be accommodated by engineering measures and can be shown to have no unacceptable impacts on repository operations.

2.8 Demography

The site shall be located to minimize the potential risk to and potential conflict with the population.

(1) The site shall be located in an area of low population density and at a distance away from population concentrations and urban areas.

(2) The site shall be located such that risk to the population from transportation of radioactive wastes and from repository operation can be reduced below acceptable levels to the extent reasonably achievable.

2.9 Environmental Protection

The site shall be located with due consideration to potential environmental impacts; air, water, and land use; and ambient environmental conditions.

(1) The site shall be located with due consideration to potential environmental impacts.

(2) The site shall be located to reduce the likelihood or consequence of air, water, and land use conflicts.

(3) The site shall be located with due consideration to normal and extreme environmental conditions.

2.10 Socioeconomic Impacts

The site shall be selected giving due consideration to social and economic impacts on communities and regions affected by the repository.

(Continued)

(1) The site shall be located so that adverse social and/or economic impacts resulting from repository construction and operation can be accommodated by mitigation or compensation strategies.

3.0 REPOSITORY PERFORMANCE CRITERIA (DOE/NWTS-33(3))

3.1 Performance of Design

The design of repositories shall be performed in accordance with current, applicable DOE design criteria and applicable provisions in 10 CFR 60, and shall give consideration to requirements for radiological safety, mining safety, long-term containment and isolation, operations, and decommissioning.

3.2 Radiological Safety

Occupational radiological exposure at repository factilities shall be maintained to within the limits specified in 10 CFR 20 and as low below those limits as reasonably achievable. Exposure of the public from repository activities shall not exceed the limits specified in 40 CFR 19, when adopted.

3.3 Mining Safety

Undergound activities at the repository shall be conducted in accordance with current, applicable provisions of 30 CFR Part 57 - "Health and Safety Standards - Metal and Nonmetallic Underground Mines".

3.4 Long-Term Containment and Isolation

Repository development and waste emplacement activities shall, to the extent practicable, pose minimal adverse effects on the long-term containment and isolation capabilities of the mined geologic disposal systems.

3.5 Operations

Repositories, either individually or collectively, shall be capable of receiving and disposing of all commercial and defense solidified high-level waste, spent fuel, and transuranic (TRU) waste, including those generated by repositories themselves, in a safe manner regardless of the amount of nuclear waste produced and of the specific fuel cycle that produced it.

3.6 Decommissioning

Activities associated with decommissioning of repository facilities shall not adversely affect the system's ability to perform its containment and isolation function.

(Continued)

4.0 WASTE PACKAGE PERFORMANCE CRITERIA (DOE/NWTS-33(4a))

4.1 Operational Safety

4.1.1 Safe Handling

4.1.1.1 Public Health and Safety

The waste package, in conjunction with the repository subsystem, shall provide for the safe handling of the waste at the repository such that applicable federal public health and safety criteria issued by the Nuclear Regulatory Commission (NRC) and the Environmental Protection Agency (EPA) shall be satisfied during the repository operational period.

4.1.1.2 Occupational Safety

The waste package, in conjunction with the repository subsystem, shall provide for the safe handling of waste at the repository such that the occupational radiological exposure of repository personnel shall be maintained to within limits specified in 10 CFR Part 20 and below these limits to as low as reasonably achievable levels. Applicable regulations of the Occupational Safety and Health Administration shall be used to ensure the protection of repository personnel from other occupational hazards.

4.1.2 Retrieval

4.1.2.1 Public Health and Safety

The waste package, in conjunction with the repository subsystem, shall provide for the retrieval of waste during the repository operational period, if necessary, such that applicable federal public health and safety criteria issued by the Nuclear Regulatory Commission (NRC) and the Environmental Protection Agency (EPA) shall be satisfied.

4.2.2.2 Occupational Safety

The waste package, in conjunction with the repository subsystem, shall provide for the retrieval of waste during the operational period, if necessary, such that the occupational radiological exposure of repository personnel shall be maintained to within limits specified in 10 CFR Part 20 and below these limits to as low as reasonably achievable limits. Applicable regulations of the Occupational Safety and Health Administration shall be used to ensure the protection of repository personnel from other occupational hazards.

4.1.3 Identification

The portion of waste package that is handled, transported, emplaced, or retrieved shall be identifiable throughout the repository operational period (to the end of the period of retrievability) such that if retrieval is necessary, the waste content of the package can be described through permanent records associated with the waste.

(Continued)

4.1.4 Criticality

The waste package shall limit the potential for criticality of the waste contained within it such that k_{eff} for the package does not exceed a specified limit under credible operational or operational accident conditions.

4.2 Long-Term Safety

4.2.1 Containment

The waste package shall contain the waste within it such that only very small quantities of radionuclides are released for a specified time period. Any loss of containment during the specified time period shall not lead to radionuclide releases that result in unacceptable doses to the public.

4.2.2 Controlled Release

The waste package shall control release of radionuclides from its boundaries. This control, in combination with characteristics of the repository and site shall provide reasonable assurance that the waste disposal system will perform as required by System Performance Criterion 1.2 - Long-Term Safety.

4.2.3 Criticality

The waste pakcage shall limit the potential for criticality of the waste contained within it such that k_{eff} does not exceed a specified limit for the package under expected repository conditions, assuming credible degradations of package components.

3.2 DEMONSTRATION OF COMPLIANCE

Performance analyses will be conducted to calculate various performance measures. Many of these performance measures can be compared directly to corresponding performance targets contained in the DOE criteria, NRC regulations, and EPA standards. This approach will not demonstrate compliance, however. The performance measures will have associated uncertainties, which will result from input and model uncertainties. Uncertainties will be characterized as described in Chapter 4. Such uncertainties must be taken into account in determining compliance.

The NRC and EPA recognize the problem of performance measure uncertainty in their requirements of "reasonable assurance". The NRC has not offered a definition of reasonable assurance, stating instead that it will decide if reasonable assurance has been provided by the DOE in formal submissions by DOE to the NRC.

The EPA has attempted a formal definition. The third draft of 40 CFR 191 (EPA, 1984), in subsection 191.16, "Guidance for Implementation," has imposed a statistical requirement of a confidence level of 85%, corresponding to one standard deviation in the estimated value, for establishment of reasonable assurance of acceptability of a performance measure. This position has been the topic of considerable comment, and may be different in the final published rule, due during the last half of FY 1984. What this requirement says, in essence, is that the performance measure is a range of values, not a single-valued number. The range is determined by the required level of confidence. It is this range of numbers that must be compared to the performance target to determine compliance.

4 MODELING

Performance assessments are used for demonstrating compliance with the criteria presented in Chapter 3. Because of the long time over which the repository must operate, compliance can be demonstrated only by calculating performance measures and comparing them to the performance criteria. Models which describe the appropriate physical processes are needed to calculate the performance measures. These models will either need to be adapted from models available in the literature, or they will have to be developed by the Salt Repository Project.

4.1 CONCEPTUAL MODELS

A MGDS may be looked upon as consisting of a series of physical processes. This is true on the system, subsystem, and individual process levels. To develop a model on any of these levels, the first step will be to conceptualize the process to be modeled. This conceptualization will consist of a description of the physical process, including a definition of the limits of the process; a listing of the physical parameters believed to be relevant to the process; and a statement of the parameters which the model will be used to predict.

A model is by nature a simplified representation of a physical system; every detail of system behavior cannot possibly be included in a conceptual model. The simplifications decided upon during conceptualization have a bearing on the results obtained from the model. Great care must therefore be taken to consider all important processes and parameters in the conceptual model, so that the results closely approximate reality.

4.1.1 Functional Requirements

The requirements of a conceptual model are (1) that it adequately describe the process being modeled over the range of conditions for which the model must operate, and (2) that it be solvable mathematically. Computer codes are the means by which SRP conceptual models are executed.

The adequacy of a model is determined by its ability to perform calculations for the range of conditions required, and by the correctness of its results. The latter is discovered through the processes of validation and verification described in Chapter 12.

4.1.2 Development and Modification

Model development begins with the conceptualization of a physical process. The level of sophistication of the conceptualization depends on the purpose for which the model is intended. A total system model cannot represent individual processes with the same level of detail as a model designed to study a single process. On the other hand, a total system model can incorporate the interactions between processes in a way that no single process model can. Once a conceptualization has been developed at the appropriate level of sophistication, a process of evolution begins, whereby the important features of the model are retained and the inconsequential features are eliminated. Inconsequential features may be discovered by

(1) Comparing a model with others incorporating different levels of sophistication
(2) Modifying the model to test the assumptions made
(3) Performing a sensitivity analysis to determine how an output parameter changes as a function of changes in input parameters
(4) Performing an uncertainty analysis to determine how much confidence may be placed in a predicted output parameter based on uncertainties in input parameters.

The first two methods deal with model uncertainty. The others deal with parameter uncertainty. Model uncertainty has to do with uncertainties resulting from the way the model is conceptualized; it is discussed further in Section 4.4.1. Parameter uncertainty is a result of the uncertainty in the input parameters; input parameter estimates may consist of subjective or objective estimates of the parameter values and their associated uncertainties. Sensitivity and uncertainty analyses, which quantify parameter uncertainties, are discussed in Section 4.2.2. Parameter uncertainty is described in detail in Section 4.4.2.

An important aspect of model development and modification has to do with model verification and validation. The validity of results predicted by a model will be tested against similar models (verification) and against available data (validation). When discrepancies appear, the model may undergo modification and further verification and validation until the code predicts system behavior with acceptable accuracy. The processes of verification and validation are discussed in Chapter 12.

A model will also undergo modification as special needs arise; for example, to predict how an event might affect a physical process (as described in Chapter 5), or to allow a model to be coupled with another so that interactions of physical processes may be examined.

4.2 MODELING APPROACH

4.2.1 Deterministic vs. Stochastic Models

The models used for performance assessment can be classified as either deterministic or stochastic. Both types of models use physical laws and scientific theory to model a particular phenomenon. Deterministic models do not explicitly account for uncertainties; stochastic models do. Deterministic models therefore require sensitivity and uncertainty analyses. Stochastic models incorporate such techniques directly into the model; in addition to accounting for parameter and spatial correlations, stochastic models can include discrete event probabilities such as those discussed in Chapter 5. Stochastic models can propagate uncertainties by multiple iterations (Monte Carlo techniques) or they can employ direct uncertainty propagation techniques. ONWI-398 (Harper and Waite, 1983) provides examples of this latter form of stochastic model.

The choice between deterministic or stochastic models often is a question of feasibility. The complexity of stochastic models increases exponentially as more detail is incorporated into the model. A simple deterministic model might therefore reasonably be converted to a stochastic form; however a more complex deterministic model would be better treated with uncertainty and sensitivity techniques. Most performance assessment models used by the SRP are deterministic.

4.2.2 Sensitivity and Uncertainty Techniques

The two major approaches to sensitivity and uncertainty analyses are
(1) a statistical design approach

(2) a deterministic first order approach.

Both are discussed in this section.

The statistical design approach may be derived using statistical experimental design theory or statistical (Monte Carlo) methods. This discussion will focus on the sampling methods. These methods typically treat the model as a black box and randomly generate input parameter settings for a specified number of computer runs. The input values are generated based on probability distributions. The model is run for each collection of generated inputs. A technique such as stepwise regression is then used to identify the key parameters and to approximate the functional relationship of the outputs to the inputs. These techniques are easily applied for computationally efficient models with less than roughly 100 parameters. The SRP will use such techniques to analyze the system level models.

Latin Hypercube Sampling (LHS) is the most well suited of these sampling approaches for performance assessment models. Its advantages over other sampling techniques is given in McKay, Conover, and Beckman (1979) and also in ONWI-444. Examples of this approach are available in Iman and Conover (1980) and ONWI-516 (Harper and Gupta, 1983).

The deterministic first order approach is typified by the adjoint method. This approach does not treat the model as a black box, but transforms the model equations into a related system of adjoint equations. This is done using the mathematics found in the calculus of variations and the theory of perturbations. First partial derivatives of a performance measure or response R, $\frac{dR}{d\alpha}$, are derived for every parameter (α is a generic parameter) in the original model. There is no limit to the number of parameters that can be handled by this approach. Normalized sensitivity coefficients, $\frac{dR}{d\alpha}\frac{\alpha}{R}$, show the predicted percent change in the performance measure R for a given percent change in the generic parameter α. A first order uncertainty analysis is then computed by combining the partial derivatives with the model covariance matrix. The covariance matrix accounts for both parameter and spatial variability as well as any correlations. These methods are extremely useful for codes with thousands of parameters such as those employing large finite difference or finite element grids. Examples of this technique are found in ONWI-515 (INTERA, 1983) and ONWI-516 (Harper and Gupta, 1983).

The analytical application of the adjoint method to a complex model has often taken several person-years in the past. Because of the comprehensiveness of such a technique, the Salt Repository Project realized its importance for licensing. As a result, the SRP has funded Oak Ridge National Labs to develop a special compiler for FORTRAN source codes to expedite this process. GRESS, Gradient Enhanced Software System, uses computer calculus to process a FORTRAN code and take the appropriate partial derivatives (Oblow, 1983a, 1983b). This will decrease the application time of these first order deterministic techniques significantly.

4.3 SOLUTION METHODS

Once a conceptual model has been developed, it must be described by a series of equations which relate the descriptive parameters to the desired performance measures. By developing a computer code, executing the code, and calculating the results, the performance measures may be determined. Two general forms exist for describing a process mathematically: an analytical solution or a numerical method.

4.3.1 Analytical Solutions

An analytical solution is an exact, noniterative solution to an equation or series of equations. For a very simple process, a single equation may accurately describe the system. A more complex process can sometimes be approximated by a simple set of equations. Because of its ease of solution and associated low computer cost, a direct analytical solution is the preferred method for describing a physical process. Unfortunately, a system requiring a large number of descriptive parameters often cannot be simplified sufficiently to permit the use of an analytical solution. Where this is the case, a numerical method is required.

4.3.2 Numerical Methods

A numerical method is an iterative, approximate method of solution. Iterations are made on a series of equations which slowly converge on a solution, or which follow a process over time or space. The key to a numerical method is that calculations occur in discrete steps. At each step, the equations or parameters describing the system may therefore change to coincide with changing process conditions. The flexibility which this provides permits many complex systems to be described with relative ease. The disadvantages of numerical methods are (1) the expense of calculation, and (2) the possibility with some numerical methods that the system of equations will not converge to a solution.

4.4 TREATMENT OF UNCERTAINTY

Mathematical models are symbolic abstractions of reality that can be used for description and prediction. The conception that a particular phenomenon is not well understood until it is mathematically expressed in a formal quantitative model must be tempered with an appreciation of available modeling limitations. In the validation of a model the following issues must be addressed:

1. Is the proposed model reasonable?
2. How precise are predictions made by the model?

As these questions illustrate, various levels of uncertainty are involved in every modeling exercise. The first item deals with the adequacy of the model itself. This issue was introduced in Section 4.1.2, and will be further discussed in Section 4.4.1. The second item involves not only the adequacy of the model, but also the uncertainties in model input parameters. The uncertainty of the data used to estimate these parameters must be quantified so that this uncertainty can be propagated through the models to calculate uncertainties in the performance measures of interest. Data uncertainty is discussed in Section 4.4.2.

4.4.1 Model Uncertainties

As mentioned previously, models are abstractions of reality. The mathematical models used by the SRP cannot capture every detail of the physical situation being modeled; instead, they attempt to cover the key processes and parameters. The uncertainty in model adequacy is divided into conceptual model uncertainty and solution uncertainty and is discussed in the following two subsections. Model adequacy is also addressed during the validation and verification process (see Chapter 12).

4.4.1.1 Conceptual Model Uncertainties

A major factor in the confidence which may be placed in predicted performance measures is the ability of the conceptual model to capture the key processes and parameters of a physical system over the time period being modeled. Different conceptual models may describe the physical system adequately. As long as the essential features are covered in a given conceptual model, the choice as to which conceptual model to use can be a function of the ease of model solution. Sensitivity and uncertainty analyses and "goodness of fit" statistical criteria will be used to validate a conceptual model.

As explained in Section 4.1, model conceptualization recognizes that both detailed subsystem and first-order-accurate system level models are required for performance assessment. The evaluation of these two-tiered conceptual models results in a better understanding of the significance of various parameters to the process being modeled.

4.4.1.2 Solution Uncertainties

Solution uncertainties arise during the conversion of a conceptual model to a computer code. The solution method selected, analytical solution or numerical method, will affect the uncertainty in model results.

Analytical solutions generally rely on simplifying assumptions that must be tested. The sensitivity of the desired performance measures to these simplifying assumptions determines whether the analytical solution is capable of modeling the physical situation accurately. Using sensitivity analysis techniques, the SRP will determine if the analytical solution properly models the physical situation. If it is not a good solution technique, the analytical solution will either be improved or replaced.

Numerical methods allow considerably more computational flexibility than analytical solutions. However the set of equations used to describe the system may be quite large and complex. Numerical methods rely on iterative procedures that terminate when specified convergence criteria are met. Truncation and round-off errors caused by computer hardware limitations become a potential source of error in these iterative schemes. The SRP will use a variety of computational schemes to measure and reduce such errors. For example, double precision will be used where appropriate to compensate for potential truncation and round-off difficulties. Known analytical solutions will be used to verify that the numerical methods have not introduced a large source of uncertainty.

4.4.2 Data Uncertainties

Data uncertainties fall into two categories: measurement uncertainties and natural variability. Both contribute uncertainty to model input parameters. The SRP will use sensitivity and uncertainty analysis techniques in its performance assessments to determine the impacts of data uncertainties, and to identify the areas in which additional data collection should be focused.

The input parameters used in performance assessment models are sometimes based on expert opinion. For such subjective data the SRP will use Bayesian techniques, which are explicitly designed to incorporate subjective estimates. These Bayesian techniques, as applied by the SRP, will blend subjective "prior" parameter estimates and uncertainty with the available data and knowledge of the model in which they are used to arrive at "posterior" estimates which should have a reduced uncertainty. These methods are extremely useful when objective site-specific data are very limited in availability.

4.4.2.1 Measurement Uncertainties

Measurement uncertainties relate to the mechanism by which measurements are taken. Measurements are subject to a variety of influences that contribute uncertainty to measured values. The major influences are

(1) the accuracy with which a reading may be taken,

(2) the reliability and accuracy of the experimental method used, and

(3) external factors which affect the measuring apparatus.

Sometimes the method of calculation becomes important. For example, reported permeabilities are calculated values rather than direct measurements. Universal agreement does not exist on the correct procedure for calculating this parameter.

To minimize measurement uncertainties, the Salt Repository Project follows specific quality assurance (QA) guidelines for data collection. The QA procedures are designed to assure repeatability of the results obtained and to record any unusual occurrences that might impact the data.

4.4.2.2 Natural Variability

Natural variability relates to the naturally occurring differences in a property through time or space. A stream flow rate varies with time. Moisture content measurements for a bed of salt vary over geographical space. Different methods of averaging can be used to summarize a collection of data to obtain a parameter value and associated uncertainty. The choice of averaging method requires knowledge of the data collected and its intended use in performance assessment models.

Many earth science parameters can be characterized by their distributions in space. These parameters are called regionalized variables, and can be characterized by their local mean values, their drifts or regional trends, and their spatial variabilities. The variation in space of each parameter is locally random, so each observation must be treated as a realization of a random variable. However, these realizations are spatially correlated and usually exhibit a perceptible pattern.

The procedure for handling such data is first to estimate the drift or trend of the data. Then the spatial correlation of the phenomenon is studied. Typically one can estimate the parameter well for a location close to observed values, and less well as the distance increases between the observed values and the location where the prediction is desired. A simpler one-dimensional version of this can be used in time series analysis. Using a technique such as kriging this spatial correlation structure is used to provide optimal estimates of the parameter over a geographic area. In addition, kriging provides the associated standard errors of these estimates. Kriging is also useful for data screening. If the difference between the predicted and observed values is large for a particular point, then further examination is warranted. Based on other scientific knowledge, one must determine whether the identified points are providing new insights or are anomalous data that should be excluded from further analysis.

5 SCENARIOS

Any radionuclide release to the accessible environment requires that one or more pathways be established connecting the waste in the repository to the surrounding hydrogeologic system. Scenarios describe natural or man-induced events or processes which, acting alone or in concert, create pathways for groundwater flow, and therefore potentially for radionuclide transport. There are many scenarios, each with its probability of occurrence, from the natural extremely slow movement of brine through an undisturbed salt mass, to the extremely rare impact of a very large meteorite causing significant fracturing at the site.

To model the effects of specific events on a physical process, different conceptual models are required. The results of each conceptual model are conditional on the event examined. To arrive at overall estimates, the NRC requires that a probabilistic weighting be attached to each event. Then the expected results are to be found using risk assessment methods to sum, over all possible events, the product of the probability and the consequence for each event. For each event examined the confidence in the predicted performance measures (or consequence) will be evaluated.

The SRP approach to scenarios analysis focuses on the potential radionuclide release pathways rather than on the individual mechanisms that create such pathways. This minimizes the number of scenarios that need to be analyzed because the assessments concentrate on the analysis of bounding scenarios for each of the events identified. In this manner, human intrusion scenarios and natural events and processes may be considered together, since they could create similar potential release pathways. Conformance to the requirements of NRC's 10 CFR 60 and EPA's proposed 40 CFR 191 is required.

This chapter provides a summary of the strategy to be used in determining how natural anomalies, construction or waste emplacement activities and postclosure human activities could affect long-term repository performance. The approach focuses on systematically identifying these effects and properly accounting for them in establishing the boundary conditions to be used in assessing repository performance.

5.1 SCENARIO REQUIREMENTS

A general approach for evaluating the long-term performance of a repository has been outlined by DOE (1980c). This approach, somewhat modified, forms the basic strategy described in this section of the Performance Assessment Plan. This strategy consists of the following four steps:

1. Identification of processes and events which could contribute to release of radioactivity.
2. Evaluation of the likelihood of occurrence of each scenario.
3. Selection of a list of scenarios for further analysis.
4. Demonstration of conformance to the requirements of proposed 40 CFR 191 and 10 CFR 60.

The processes and events which could contribute to release of radioactivity include natural phenomena, waste and repository-induced phenomena and human intrusion. Koplik, Kaplan and Ross (1982) and Claiborne and Gera (1974) provide comprehensive listing of such processes and events. The identified phenomena can result in various scenarios by which release of radioactivity from a repository may occur. As indicated by Bingham and Barr (1979), a complete scenario for a repository in salt includes specifications for six elements:

1. An event that breaches the repository; without a breach there can be no release from a repository in salt.
2. A mechanism for moving radionuclides through the breach.
3. The time between burial and the breaching event.
4. The response of the salt to the breach.
5. The nuclide inventory in the waste.
6. The physical and chemical condition of the waste.

The above elements will be analyzed using the tools of performance assessment to demonstrate compliance with licensing requirements using site-specific characteristics.

5.2 SELECTION OF SCENARIOS

Depending on site characteristics and the level of detail desired, the number of scenarios to be analyzed can be very large (Bingham and Barr, 1979; Guiffree et al, 1980). The approach taken in this plan, as illustrated in

Figure 5-1, is to focus not on the individual mechanisms that create a potential pathway for release of radionuclides but on the release pathways that can be created by many release mechanisms; this approach simplifies the consequence analysis by limiting the number of scenarios which are to be analyzed. To accomplish this, a general model of the radionuclide transport pathway can be used to assess the consequences of the various potential scenarios by varying the transport parameters to simulate the actual scenarios. Using this approach, bounding calculations are performed to demonstrate the acceptability of the results for all the contributing scenarios. Such an approach was used in the WIPP Safety Analysis Report (DOE, 1980a) to reduce a large number of potential scenarios to only four bounding events. These four events form the basis for the scenario selection process for performance analyses and are as follows:

1. Connection to a single hydrostratigraphic unit with water flow through the repository ("u-tube" scenario).
2. Connection to a single hydrostratigraphic unit through a stagnant water pool.
3. Connection between upper and lower hydrostatigraphic units.
4. Direct exposure to radioactive material brought to the surface.

Long-term performance assessment of a repository in salt will require the analysis of these events. Since these events are general, they can be used to model various potential repository breach scenarios.

For example, the first event can account for the following types of scenarios:

1. Multiple drill holes penetrating the repository.
2. Several shaft or borehole seal failures.
3. Fracture of the rock strata extending from the repository to the upper hydrostratigraphic unit.
4. Combinations of the above.

The second event can account for:

1. A single borehole or a single failed shaft or borehole seal.
2. Flooding from a solution mine above the repository with a hydraulic connection to the repository by an integrated fracture network.

The third communication event can account for the following phenomena which could result in water flow between the two hydrostratigraphic units (through the repository horizon):

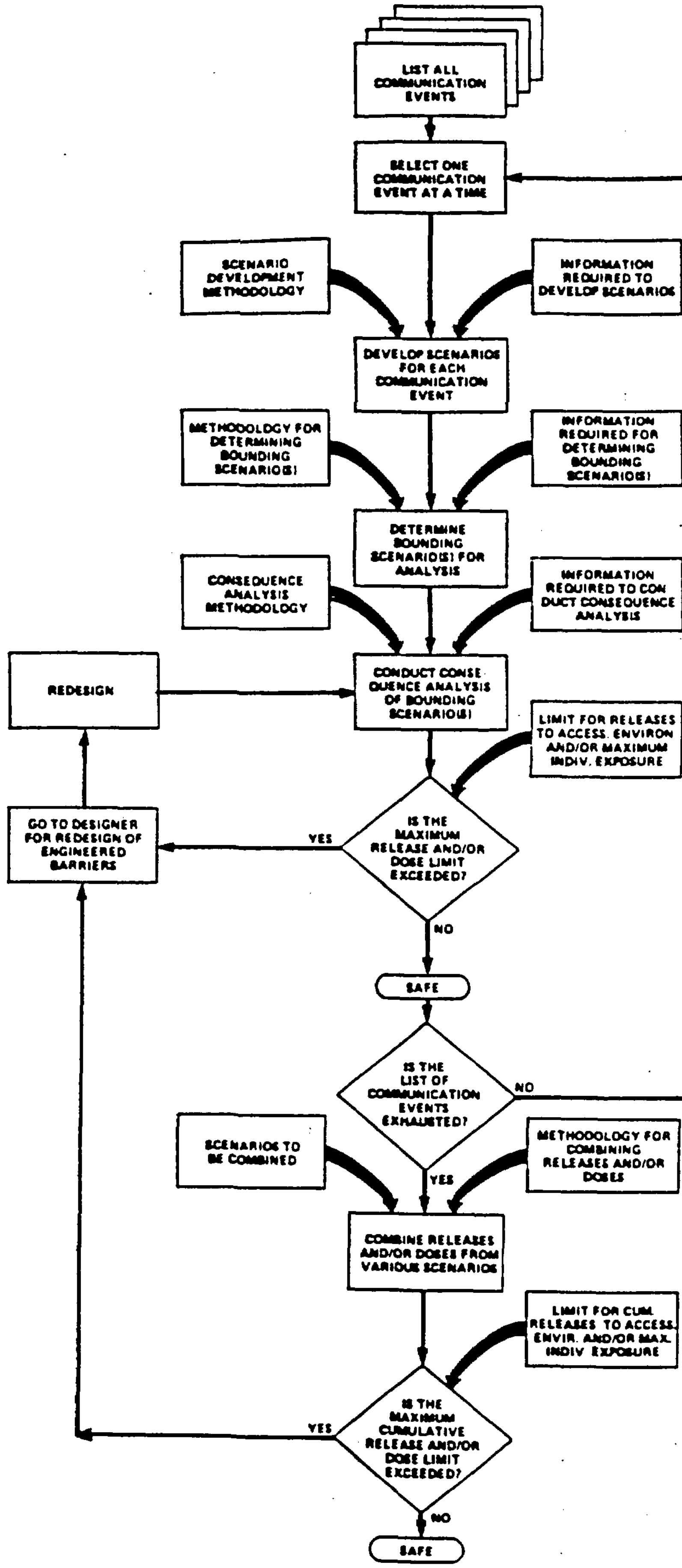


Figure 5-1. Strategy for Performance Assessment of Postclosure Release Scenarios

1. Development of an integrated fracture system connecting the two units.
2. Failure of drill hole seals.
3. Future drilling through the upper aquifer and the repository to the lower aquifer.
4. Formation of a brecchia pipe through the repository connecting the two units.

The fourth event can account for scenarios such as:

1. Direct exposure to radioactive material brought to the surface through exploratory drilling.
2. Excavation of the repository by a meteorite strike.
3. Excavation of the repository by volcanism.

By analyzing the important parameters that determine the amount and timing of radioactivity release (such as postulated time of occurrence, fraction of repository affected, flow area, etc.), bounding scenarios will be selected for each communication event.

The choice of processes and events which are selected for the bounding calculations is of critical importance in the licensing of a repository. As required by 10 CFR 60, identification of processes and events must include both those "anticipated processes and events" which are reasonably likely to occur during the intended period of waste isolation as well as those "unanticipated processes and events" which are not likely to occur, but which are sufficiently credible to warrant consideration. Those processes and events which are reasonably likely to occur will be identified in the process of performance assessment. For unanticipated processes and events, judgement must be made of both their probabilities of occurrence and the levels of probability below which no consideration is warranted. The EPA has established definitions of the two probability classes of events in 40 CFR 191.

For events such as a meteor strike or volcanism, where the probability of occurrence has been shown to be extremely low (Claiborne and Gera, 1974; Logan and Berbano, 1978), the choice of selection is easy. Clearly these probabilities are so small that these events do not have to be considered. Estimates of the likelihood of occurrence of those unanticipated processes and events which are more likely must, to a large extent, rely on expert judgement. In some cases, a simplified qualitative analysis may be an appropriate method for eliminating scenarios regardless of their probabilities of occurrence because other scenarios would be clearly bounding.

The selection process for determining the scenarios to be used for the bounding calculations will be documented in a formal report. This report will include: 1) a listing of all scenarios considered for each type of event, 2) the criteria used in comparing the scenarios, 3) inputs to any comparative qualitative or quantitative analyses performed, and 4) the results of such analyses.

5.3 SCENARIO ANALYSIS APPROACH

For scenarios which are found to be sufficiently credible to warrant consideration, long-term safety is demonstrated by showing compliance with the requirements of 10 CFR 60 and proposed 40 CFR 191. Thus, the scenarios will be related to licensing assessment. The communication event method of scenario categorization and evaluation is particulary suited to this objective because the scenarios can be structured in terms of barriers which correspond to the various components and boundaries of the engineered system and geologic setting. In this framework, the results of the scenario evaluations can be directly related to the numerical performance targets required for licensing.

The time between burial and the breaching event shall be varied in the scenario evaluation. This is important due to the changing radiological characteristics of the waste, the time-dependent nature of the transport processes and the time limit of the EPA standard. Since, for unanticipated events, the time at which the event could occur cannot be predicted in advance, the consequences of the event shall be evaluated at a number of specified times. These times may be keyed to significant changes in the composition of the radionuclide inventory in the repository and the time constants of the mobilization and transport processes such as corrosion, leach rate, and groundwater transport to the boundary of the accessible environment. Alternately, a Monte Carlo or other probabilistic variation might be desirable.

Uncertainties will also be assessed in the scenario evaluation. This shall be done by treating the effectiveness of the containment and geologic barriers parametrically and model parameters probabilistically. The communication event method is well suited to this type of analysis.

The steps involved in the evaluation of the bounding scenarios are described below. This evaluation will be documented in a formal report that addresses: 1) all assumptions used in the performance assessment calculations, 2) a description of all models and computer codes used, 3) all input parameters (along with their levels of uncertainty), and 4) analysis results.

5.3.1 Source Term Determination

The first step in the analysis is to determine the radionuclide inventory in the emplaced waste. The waste inventory is dependent on the nature of the waste (age, processing, and so forth). The radionuclide flux from one barrier can be used as the source term for the analysis of the subsequent barrier. That is, the flux from the waste package is used as the source term for the repository analysis; the flux from the repository boundary is then used as the source term for site assessment.

5.3.2 Release Pathways

The next step involves the determination of the various pathways by which radionuclides could reach the accessible environment. Each should fall into one of the four types of events indicated in Section 5.2. It is expected that, while the release pathways may be similar for scenarios of the same event type, the physical characteristics that define the pathways will vary, depending on the specific scenario being analyzed. These characteristics need to be defined on a site-specific basis, taking into account the properties of the salt host rock, the surrounding geology, and the nature of the subsurface and surface hydrologic regime.

5.3.3 Scenario Analysis

After all the required parameters (along with associated uncertainties) have been quantified, a consequence analysis will be performed for each of the bounding scenarios. A consequence analysis may include the determination of radiological releases to the accessible environment, the dispersion and transport of these releases via different environmental pathways (air, water, soils, and food chains), and the resulting potential radiation doses to humans. However, as discussed in Section 5.3.4, the regulatory requirements applicable to assessment of postclosure performance of a mined geologic repository are currently in terms of radiological releases rather than doses. Therefore, the consequence analysis to be performed for each bounding scenario will be limited to determining the radionculide releases to the accessible environment and across each of the engineered barriers.

5.3.4 Comparison with Regulatory Limits

For each of the bounding scenarios analyzed, the radiological releases to the accessible environment and across each of the engineered barriers must be compared to the performance targets of 10 CFR 60 and proposed 40 CFR 191. These regulatory requirements are tied to the likelihood of occurrence of either the processes and events (10 CFR 60) or the radiological releases (40 CFR 191), as discussed in Chapter 3.

The strategy for postclosure safety assessment includes a design feedback mechanism, in the event that the limits are exceeded for a particular scenario. In such cases, the designer shall re-evaluate the engineered barriers for design modifications and the analysis will be redone until all releases are within the regulatory limits. Then the repository system can be considered safe with regard to that scenario.

It should be noted that the proposed EPA release limits are based on cumulative releases over 10,000 years. Therefore, after all the scenarios have been evaluated individually, the cumulative releases to the accessible environment for the more likely scenarios may need to be combined and compared to these limits. The determination of which scenarios need to be considered in combination will be based on the likelihood of the occurrence of the different releases.

5.4 HUMAN INTRUSION SCENARIOS

Reducing the likelihood of future inadvertent human intrusion into a high-level waste repository requires DOE to seek sites which should not be attractive to future generations. Once a repository has been built, DOE must establish effective institutional controls and permanent markers informing future generations of the presence of the repository and its associated hazard. These are basic site performance criteria of the CRWM program for mined geologic disposal of nuclear waste (as discussed in Chapter 3) as well as requirements of the NRC and proposed EPA regulations.

In proposed 40 CFR 191, the EPA requires avoidance of sites where there has been mining for resources or where there is a reasonable expectation of future resources. In addition, proposed 40 CFR 191 requires that disposal systems be identified by "the most permanent markers and records practicable to indicate the dangers of the wastes and their location" (40 CFR 191.14(e)). The regulations state that active controls, such as markers, public records or archives, Federal ownership and control of land use, or other methods of communicating knowledge of the existence of the repository, can keep the chance of inadvertent human intrusion very small.

The NRC approach to the issue of inadvertent human intrusion is specified in 10 CFR 60 and discussed in the supplementary information for the rule. As stated in the supplementary information, "everything that is reasonable should be done to discourage people from intruding into the geologic repository." Those measures which it believed to be reasonable included directing site selection toward sites having little resource value, and marking and documenting the site. Beyond that, the Commission felt there would be no value in speculating on the virtually unlimited possibilities for human intrusion and whether or not they would result in violation of the EPA standard.

Appendix B of the third draft of 40 CFR 191 (EPA, 1984) prescribes limits on probability of occurrence and on possible consequences of a borehole penetrating a repository. These limits are described in Section 10.8.

The NRC requires the consideration of the potential for inadvertent human intrusion as a siting requirement. 10 CFR 60 requires that human intrusion be explicitly considered at sites where there is evidence of subsurface mining or drilling, or potential natural resources which could be attractive for exploitation in the future. Such "adverse conditions" render the site unsuitable for a repository unless it can be demonstrated that future human intrusion would not compromise the ability of the repository to isolate the waste or that the potentially adverse human activity can be remedied.

In addition, the NRC requires consideration of human intrusion scenarios on a case by case basis as "unanticipated processes and events" which are sufficiently credible to warrant consideration. The NRC provides further guidance that: "Processes and events initiated by human activities may only be found to be sufficiently credible to warrant consideration if it is assumed that (1) the monuments provided for by this part are sufficiently permanent to serve their intended purpose; (2) the value to future generations of potential resources within the site can be assessed adequately under the applicable provisions of this part; (3) an understanding of the nature of radioactivity and an appreciation of its hazards have been retained in some functioning institutions; (4) institutions are able to assess risk and to take remedial action at a level of social organization and technological competence equivalent to or superior to that which was applied in initiating the processes or events concerned; and (5) relevant records are preserved and remain accessible for several hundred years after permanent closure."

The above criteria should be used to determine which human intrusion scenarios are sufficiently credible to warrant consideration. However, in assessing the consequences of the intrusion, the pathways for radioactive release which are created by the intrusion are the vital component. The most likely scenarios can be reduced to the four event types discussed in Section 5.2. Therefore human intrusion for each event type will be assessed according to Section 5.2 in order to determine if these scenarios are bounding.

6 DATA REQUIREMENTS

Performance assessment models generate data requirements which must be met by the SRP. Data are needed for (1) the selection of input parameter values, (2) the determination of uncertainties associated with the parameter values selected, and (3) model validation efforts as described in Chapter 12. The nature of each model therefore dictates the data needs for a specific performance assessment. As the models evolve, data requirements will change.

6.1 DATA AVAILABILITY

Data are available from many sources. Considerable data are already in the public domain. NUREG/CR-3066 (Mercer et al, 1982) documents the generic data available in the literature. This report provides means and ranges for the data and thus can be used as a guideline when site specific data are limited. Where the necessary data are lacking, the SRP will perform its own analyses to generate data for use in its models. Site-specific data are a particular concern of the SRP.

All data used by the SRP for licensing activities must meet strict quality assurance requirements. Two systems were recently established within the SRP for ensuring that QA requirements are met. The Technical Database Management System (TDMS) is a computerized technical database which will eventually contain all data approved for use in licensing activities. The Records Information System (RIS) handles paper or microfiche copies of relevant reports, data and maps.

The TDMS will ensure the validity, consistency, timeliness, and traceability of SRP technical data. For all data in the TDMS, references to the original source documents will be given. A technical expert will be listed who can answer questions concerning the acquired data. The TDMS will provide a QA-approved change control procedure to manage new data entries and modifications. The requirements for acceptance of data into the TDMS are currently being established by an interdisciplinary group.

At present, preliminary analyses are being performed with whatever data are available. Eventually these analyses will help to determine which data belong in the TDMS.

6.2 USE OF PERFORMANCE ASSESSMENTS TO GENERATE FURTHER DATA REQUIREMENTS

One vital role played by performance assessment relates to data acquisition. The requirementsof performance assessment models to a large extent determine the types, amount, and quality of data which the SRP must gather. Data need to be gathered to quantify input parameters and their associated errors. Data are also needed to provide model validation. As models evolve based on improved knowledge, data needs will change. The data gathering efforts of the SRP will evolve to reflect the new needs.

The first real opportunity to direct data gathering efforts based on PA needs will be the SCP activities (see Section 1.4). The SRP will need to gather data based on the most recent performance assessment needs. The data gathered as a result of the SCP efforts will aid in the development of more refined models, which will eventually lead to more refined data requirements.

7 TOTAL SYSTEM ANALYSIS

Section 2.1 introduced the subject of system postclosure analysis. Clearly some type of analysis is required on the system level to demonstrate compliance with the performance targets described in Chapter 3. Less clear is what form that analysis should take. A single system code would be convenient but might be too restricted by simplifying assumptions to be meaningful. Although cumbersome, a series of individual process codes would be less restricted by simplifying assumptions, and would be flexible. One code could be substituted for another to make calculations, or a code could be added to the series to account for a previously neglected process. The SRP is presently using a series of individual codes to perform system analyses. The development of these codes into a single system level code is being considered; the need for such a code has not yet been established.

7.1 METHOD

The general method for performing system assessments is illustrated in Figure 7-1. A series of process codes is selected from the three major subsystems and chained together to represent the system. The necessary input parameters for each code are then selected. The codes are run on a computer, each generating numbers that will feed into the next code in the chain, until the entire series of computer runs is complete. This series of runs will generate performance measures to be compared to the performance targets of Chapter 3.

The sensitivity and uncertainty analysis techniques described in Chapter 4 will be used for system assessments. The process codes will be analyzed separately and together, and both model and data uncertainties will be assessed. Alternate codes which model the same processes will be studied to assess model uncertainty. Chapters 8, 9 and 10 offer a selection of processes and codes which might be used on the system level.

Validation and verification (discussed in Chapter 12) will be performed for each code used. The system as a whole will also undergo validation and verification.

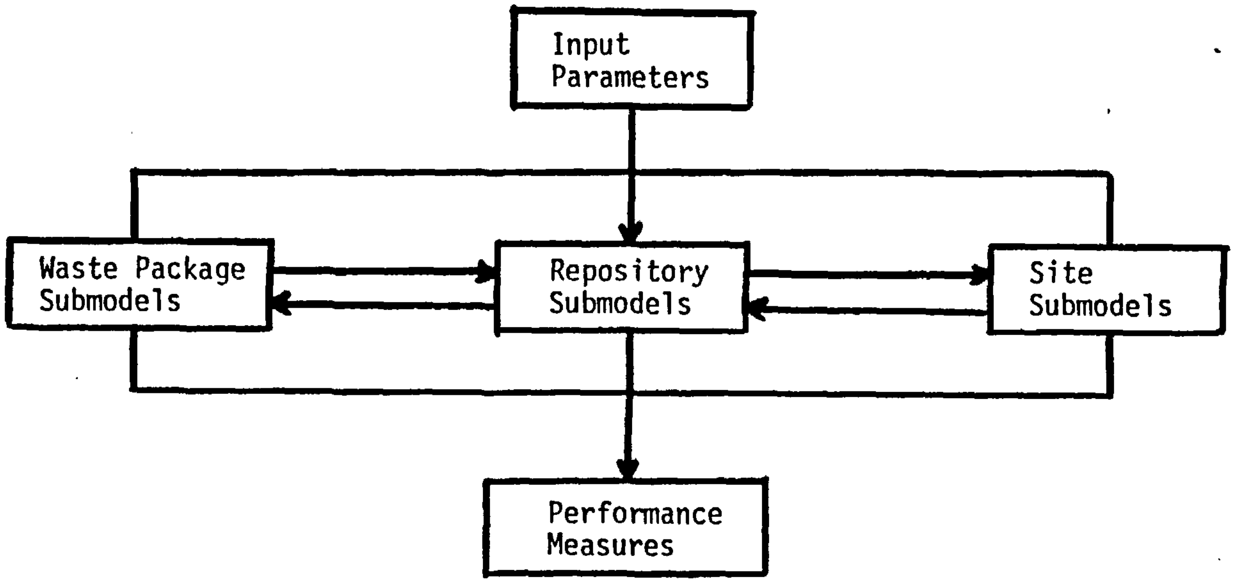


Figure 7-1. General Method for Total System Analysis

7.2 SCENARIO ANALYSIS

Scenario analysis will be needed on the system level. The approach will usually be the same as that described in Chapter 5. Since scenarios generally introduce new pathways for radionuclide release, they may require specialized process codes and input parameters to be incorporated into the system model. This will in turn require new sensitivity and uncertainty analyses, and new validation and verification exercises.

For some scenarios, single codes have been developed which model all, or nearly all, of the disturbed system. One example is BORHOL (see Appendix), a code which models the penetration of a salt repository by a single borehole.

8 VERY NEAR-FIELD ANALYSIS

Performance assessment of the very near field requires analysis of a single waste package and the surrounding disturbed zone during postclosure operation of a repository. The objective of very near-field analysis is to predict the performance of a proposed waste package design and to give direction for changing the design if it is inadequate. Radionuclide release to the geologic medium must be limited to a value prescribed by the NRC. In addition, the waste package must be retrievable during the early years of postclosure repository operation. The specific requirements are presented in Chapter 3.

This chapter describes the very near-field subsystem and the strategy which will be used for performance assessment of the very near field. Descriptions and references for all computer codes mentioned in this chapter are given in the appendix.

8.1 DESCRIPTION OF WASTE PACKAGE SUBSYSTEM

The very near field is pictured in Figure 8-1. The waste package, the rock salt backfill, and the salt immediately adjacent to the borehole are the three main components of the very near field. The waste form, the canister and the overpack are the three components of the waste package. According to present plans, the backfill material will be the rock salt which was excavated to form the repository. The backfill will help to minimize subsidence.

Several different waste forms are being studied for possible placement in a salt repository: commercial high-level waste (CHLW), defense high-level waste (DHLW), which consist of radioactive material encased in glass matrices; transuranic waste (TRU); and spent fuel (SF), which consists of the unprocessed, spent fuel rods from a commercial nuclear power plant. Two types of spent fuel may be studied: spent fuel, pressurized water reactor (SFPWR) and spent fuel, boiling water reactor (SFBWR). Package conceptual designs for these waste forms differ at present only in package dimensions, which will depend in part on the dimensions of the original waste form.

Present conceptual designs call for the overpack to be made of steel. The overpack will be designed to provide the structural strength needed to withstand expected lithostatic pressure; a corrosion allowance is added to

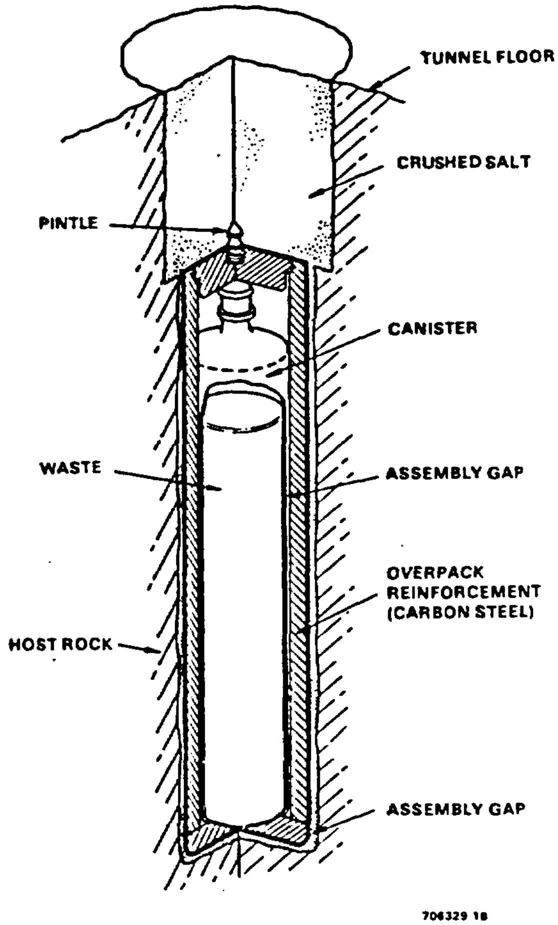


Figure 8-1. Generic Waste Package Design for Emplacement in Boreholes Below the Water Table

provide package integrity. The performance of the package will be assessed to assure that the package design can withstand both these factors sufficiently to provide the required radionuclide containment. After package failure, should it be predicted, the performance of the waste form and salt in retarding radionuclide release and migration will be assessed.

Figure 8-2 is a simplified flow diagram for waste package performance assessment. As it shows, the first requirement is for a detailed description of the proposed package design and the package configuration within the repository. This information must come from the waste package and repository components of the SRP. These components must also supply data on material properties. All this information will then be analyzed using performance assessment models.

A crucial part of the definition of the waste package is a detailed description of the waste form itself. Radionuclide inventory data, including the expected heat and radiation to be emitted, must be provided. Leaching data for the waste form will also be needed.

Once a detailed description of a waste package design has been provided, models will be used to describe the behavior of the waste package in a repository setting. The behavior of the package surroundings will also be described with models. Parameters and processes which will be described by models include:

(1) Temperatures
(2) Stresses
(3) Local fluid flow
(4) Geochemistry
(5) Canister and overpack corrosion
(6) Local radionuclide transport.

These will be treated in the following sections of this chapter. Because these parameters are interrelated, Section 8.8 will discuss the coupling of these various models.

8.2 THERMAL ANALYSIS

Temperatures in the salt surrounding a waste package will be calculated at both the repository and individual package levels. Temperatures of package components will be determined at the individual waste package level. The

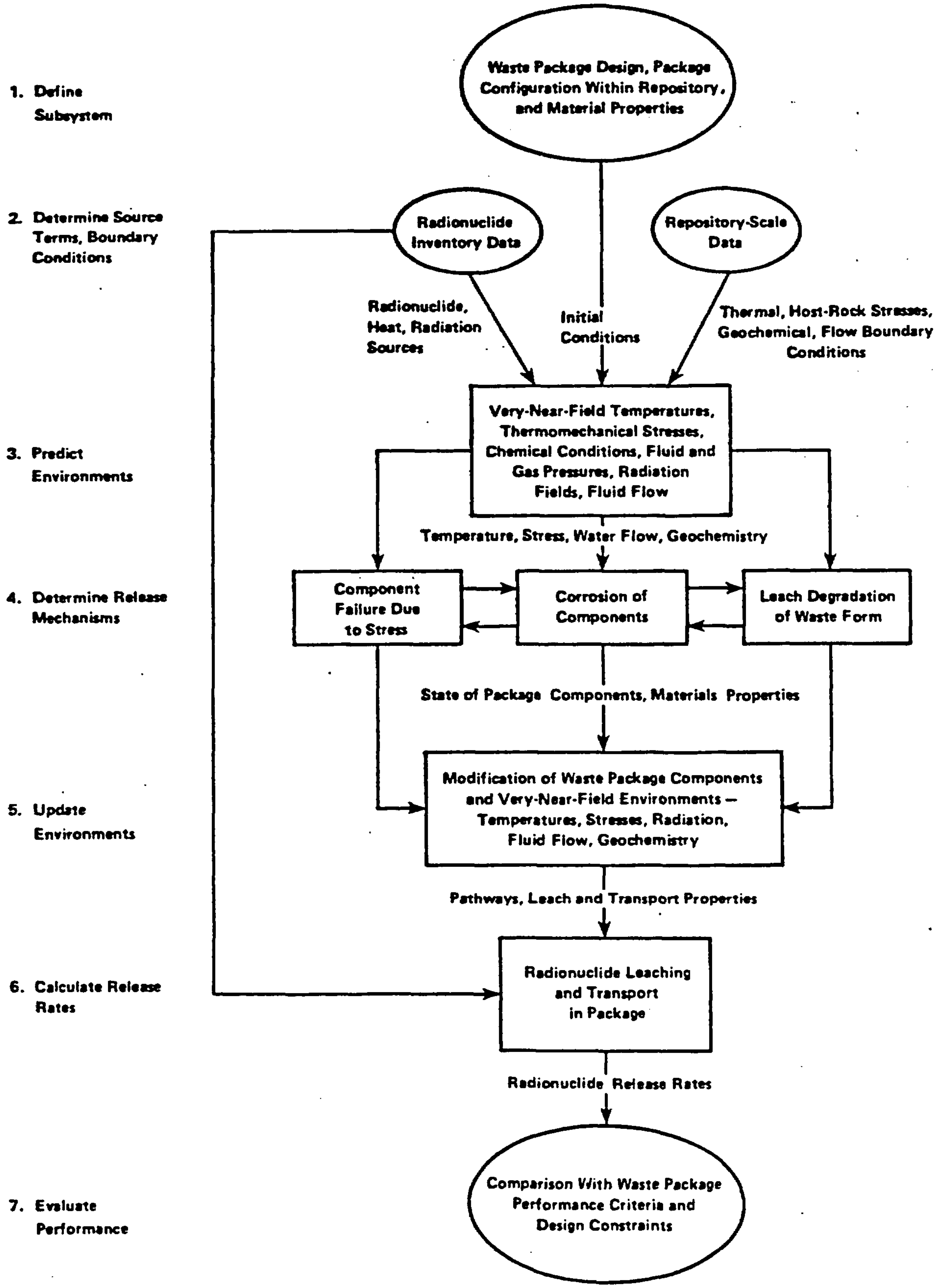


Figure 8-2. A General Step-Wise Approach for Waste-Package Subsystem Performance Assessments

first set of temperatures will provide the boundary conditions for the second, and will enter into brine migration calculations. The second set of temperatures will enter into calculations of package component behavior, specifically corrosion and leach rates and reaction to thermomechanical stresses.

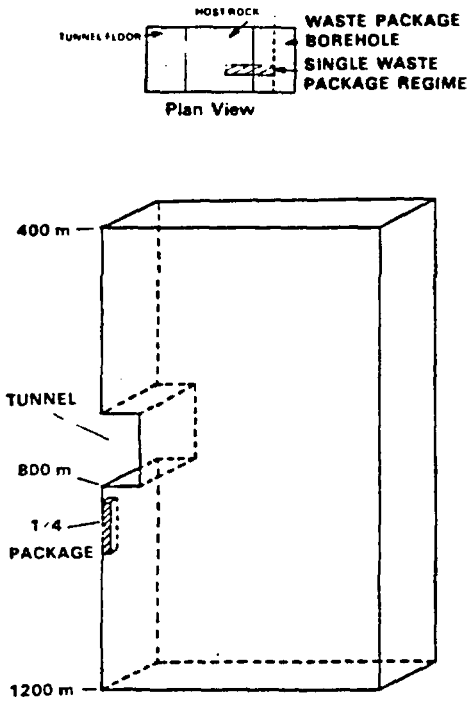
8.2.1 Temperatures in the Salt Adjoining a Waste Package

The waste package thermal output, package dimensions, material properties, package arrangement, and spacing within the repository are the major parameters affecting the temperature distribution in the salt adjoining a waste package. A two- or three-dimensional simulation of the salt surrounding a single waste package will be used for very near-field thermal analyses. Codes which perform this type of simulation are listed in Figure 8-3. In addition, temperature profiles in the salt surrounding a waste package are being determined from thermal models of the entire repository, such as TEMPV5. These thermal analyses require as input:

- Geometry and thermal conduction and capacitance properties of:
  - waste package components
  - local salt and relevant engineered barrier materials
  - geologic media beyond the repository
- Time dependent thermal output of the waste
- Regional thermal parameters including:
  - geothermal heat flow
  - ground surface temperature.

8.2.2 Temperatures of Waste Package Components

The waste package can be treated as radially symmetrical and modeled in one dimension as depicted in the most general form in Figure 8-4. The barriers depicted in this figure can be solid or air filled. In the latter case, heat transfer across the gap will occur by a combination of conduction, convection, and radiation. The gap will be assumed to be sealed at the ends. Heat generation will occur throughout the waste form. The temperature differential between the waste centerline and canister as well as temperature-dependent thermal properties will be accounted for.



BOREHOLE PACKAGE – 1 ROW/TUNNEL

Repository Thermal Model
3-D Views

Computer Codes

- CFEST — Coupled Flow, Energy, and Solute Transport
- HEATING6/5 – Thermal Conduction Code
- SWENT — Coupled Flow, Energy, Solute and Radionuclide Transport

Input Data

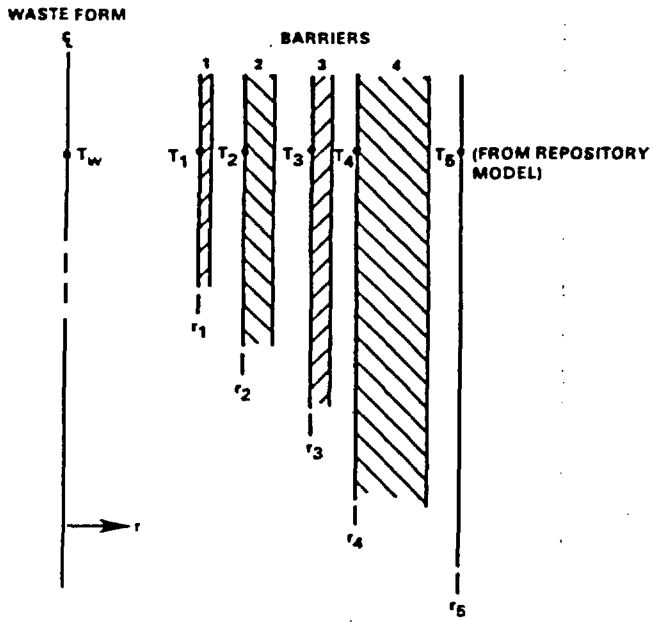
- Heat Source From Waste (Type and Amount) in Each Canister
- Design of Canister and Backfill (Thermal Properties of Each Component)
- Emplacement Plan Spacing and Layout Plan
- Boundary Conditions Defined From Single Unit Cell Analysis
- Host Rock Properties

Output

Temperature Distribution Within Waste Package Components as a Function of Time for:

- Mechanical and Thermal Stress/Strain Analysis
- Geochemical and Leach Rate Analysis

Figure 8-3. Waste Package Thermal Boundary Analyses - Computer Codes, Input and Output



Variables

- Heat Load Per Unit Length
- Barrier Radii — r_1, r_2, r_3, r_4, r_5, and Thicknesses
- Barrier Thermal Conductivities
- Emissivities (if Gaps Between Barriers are Air-Filled)
- Filler Thermal Conductivities (if Gaps are Solid-Filled)
- Corrosion Constants

Figure 8-4. A General One-Dimensional Waste Package Thermal Model

Initially the effect of corrosion product buildup on temperature distribution will not be considered. In the sensitivity analysis the effects of the lower thermal conductivity of the corrosion product will be considered. If the impact of corrosion product buildup proves to be significant, it will be included in further detailed analyses. Similar analyses will test the importance of such other factors as the type of fluid present in the gaps.

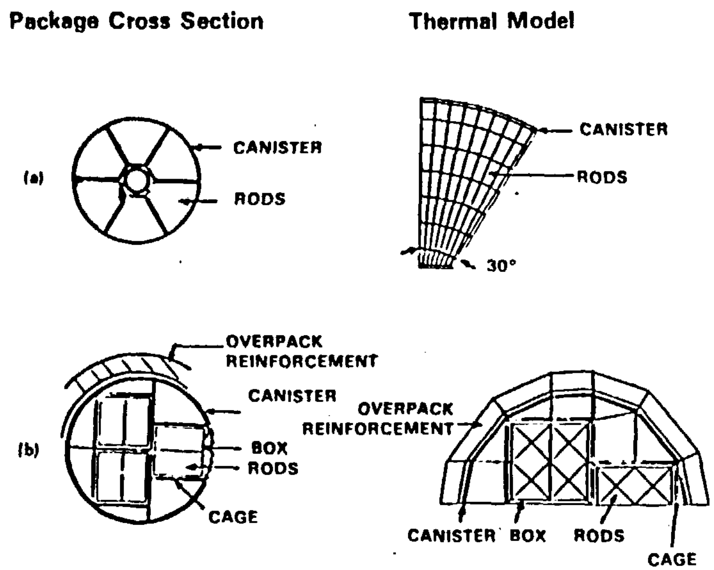
For waste forms which are radially symmetrical, the results from a one-dimensional radial model will be compared with results from two- and three-dimensional analyses. For spent fuel, for which radial symmetry is not appropriate, peak fuel temperatures will be calculated by using two-dimensional steady-state models that consider either boxed or bundled fuel elements and include heat transfer effects of package structural members such as box walls and box supports. Within a bundle of close-packed fuel rods, heat transfer by combinations of radiation, convection, and conduction will be considered. The radiation heat transfer will be represented by the effective conductivity which will depend on the temperature, a coefficient which is a function of the rod emissivity and the physical characteristics of the rod bundles (Westinghouse Electric Corporation, 1983). For detailed thermal analysis of each component of the waste package, will be modeled as illustrated in Figure 8-5 or by a similar method.

8.3 THERMOMECHANICAL STRESS ANALYSIS

Like temperature analyses, thermomechanical analyses must be performed for both the salt surrounding and acting upon an individual waste package, and for the waste package components. These analyses are discussed in this section.

8.3.1 Thermomechanical Stress Boundary Analysis

The thermomechanical behavior of the host rock adjoining the waste package will be analyzed to provide the stress boundary conditions needed to assess the mechanical behavior of the waste package components. This behavior will be modeled for a single waste package regime, as well as on the repository level. On the single waste package level, the repository stress field in the vicinity of the waste package will be described for a vertical



Computer Codes

- CFEST — Coupled Flow, Energy, and Solute Transport
- HEATING6/5 – Thermal Conduction Code
- SWENT — Coupled Flow, Energy, Solute and Radionuclide Transport

Input Data

- Heat Source From Waste (Type and Amount) in Each Canister
- Design of Canister and Backfill (Thermal Properties of Each Component)
- Emplacement Plan Spacing and Layout Plan
- Boundary Conditions Defined From Single Unit Cell Analysis
- Host Rock Properties

Output

Temperature Distribution Within Waste Package Components as a Function of Time for:

- Mechanical and Thermal Stress/Strain Analysis
- Geochemical and Leach Rate Analysis

Figure 8-5. Temperature Analyses Within Waste Package Components - Computer Codes, Input and Output cross section of the package. Figure 8-6 lists computer codes which perform stress boundary analyses. These simulations will require

- o the geometry and temperature-dependent mechanical properties of
  - the waste package components
  - the salt and relevant engineered barrier materials
  - geologic media beyond the repository
- o the time-dependent distribution of temperature throughout the single waste package regime
- o the regional stress state.

To make reasonable estimates of waste package boundary stress values, the effects of tunnel closure on the repository stress field in the vicinity of the waste package will also need to be considered.

8.3.2 Stress and Strain Within the Waste Package

Stress and strain within the waste package may result from:

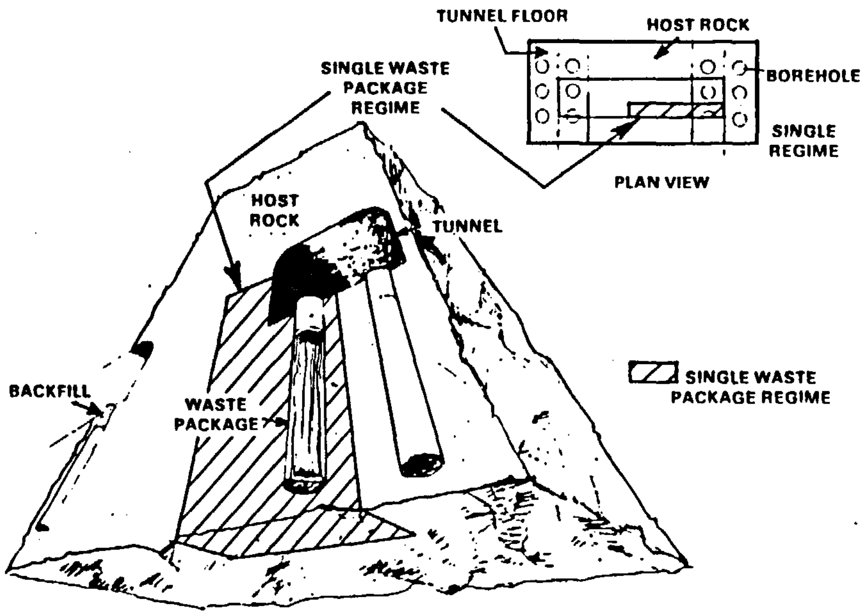
- o material incompatibilities (deformation stresses)
- o thermal gradients
- o repository boundary stresses.

Internal stress from these sources may affect the behavior of the package by:

- o causing breaching or collapse of the canister and other metallic barriers
- o initiating or increasing the rate of stress corrosion
- o increasing the surface area of the waste itself by fracturing and, hence, increasing the potential leach rate.

The mechanical behavior of the waste package will be analyzed using an axisymmetric generalized plane strain formulation. Like the approach to thermal modeling described above, this structure takes advantage of the cylindrical geometry of the waste package. Five types of elements will be considered:

- o a solid elastic/brittle core to represent the waste form
- o elastic or elastic/plastic hollow cylinders to represent metallic barriers
- o compressible elastic hollow cylinders to represent backfill barriers
- o incompressible zero strength hollow cylinders to represent liquid-filled layers, corrosion product layers, or failed barriers



Perspective View of Detail Region

Computer Codes:

- VISCOT — Visco- and Elastic-Plastic Thermomechanical Analysis

Input Data

- Waste Package Emplacement Plan and Repository Tunnel Design
- Thermal and Mechanical Properties of Host Rock
- Excavation Method
- Overburden Loading
- Time Dependent Temperature Distribution Throughout the Single Waste Package Regime
- Regional Stress Slag

Output:

Spatial and Temporal

- Stresses
- Deformation
- Failure Zone

For use in

- Stress and Strain Analysis in Metallic Canister and Clad
- Thermal and Hydraulic Properties of Host Rock

Figure 8-6. Waste Package Thermomechanical Stress Boundary Analysis—Computer Codes, Input and Output

- o hollow cylinders which transfer no pressure to represent gas gaps.

To carry out the mechanical analysis will require:

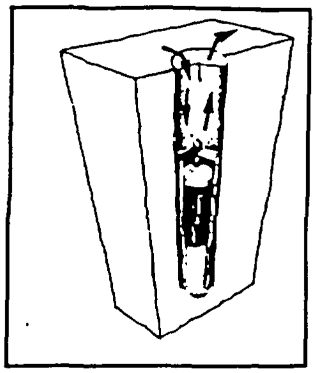
- o the temperature-dependent values of the mechanical properties of each waste package component
- o time dependent values of the external stresses from the surrounding salt, as described in Section 8.3.1
- o time dependent temperatures within the waste package itself, as described in Section 8.2.2.

8.4 LOCAL FLUID FLOW

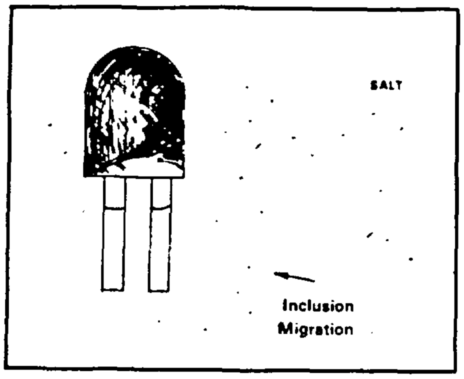
Fluid flow is of interest because moisture which comes in contact with the waste package will corrode it, and may cause it to fail. Should package failure occur, leaching of the radionuclides from the waste form by the fluids present is the only means by which significant numbers of radionuclides could escape the waste form. Two types of fluid flow will be modeled. The first is brine migration, which is the only expected means for transport of fluid to the waste package. Brine migration analysis will be performed on the individual waste package level, and will be discussed in this section. The second is fluid flow through the repository, which is part of scenario analysis. This type of flow will primarily be analyzed on the repository level, and the results applied to individual waste package analyses. It will be discussed in Chapter 9. Figure 8-7 lists the codes to be used to analyze local fluid flow.

Salt crystals contain small inclusions filled with brine. Under the influence of a thermal gradient, these brine inclusions migrate toward a heat source; at the crystal boundary, the brine from the inclusions enters the intercrystalline network and continues to migrate toward the heat source. Because nuclear waste generates heat, brine will migrate in this manner to the waste package surface. Models will be used to predict the amount of brine expected to reach the waste package surface with time.

Brine migration of all-liquid inclusions is the expected means by which moisture will reach the waste package. It is not a means by which moisture could leave a waste package surface. Gas-liquid inclusions migrate away from a heat source, but since inclusions cannot cross a crystal boundary, this does not present a potential for migration of radionuclides from the waste package.



Schematic Representation of Flow Caused Due to Seal Leakage and Density Currents



Schematic Representation of Brine Migration

Computer Codes

- BRINEMIG – Brine Migration
- SPECTROM-58 – Brine Migration

Input Data

- Waste Package Design and Emplacement Details
- Temperature Distribution
- Water Source* (Amount, and Location Brine Pockets, Resaturation)
- Properties of the Materials

Output and Its Interface With Other Processes

Flow Rate and Travel Time for Leach Rate and Radionuclide Transport

*Salt is impervious and flow around waste is only possible under disruptive events or brine migration.

Figure 8-7. Fluid Flow in the Vicinity of the Waste Package--Computer Codes, Input and Output

Movement of brine through the intercrystalline network does need to be examined as a potential pathway for radionuclide release, since it seems to be controlled by pressure gradients. Pressure gradients could conceivably reverse, forcing brine away from the waste package.

Two approaches to brine migration modeling are currently under investigation for use by the SRP. One employs empirical equations which overpredict in situ migration. This is the approach of BRINEMIG. The other method relies on a theoretical development. The program SPECTROM-58 takes this approach.

Two other sources of moisture exist in a salt repository and will have to be dealt with. The first is moisture introduced with the salt backfill. The second is moisture released by hydrated minerals. The latter is a particular concern with bedded salts, which are more likely to contain layers of impurities. The quantities of hydrated minerals present and the amount of moisture available through dehydration will have to be determined on a site-specific basis.

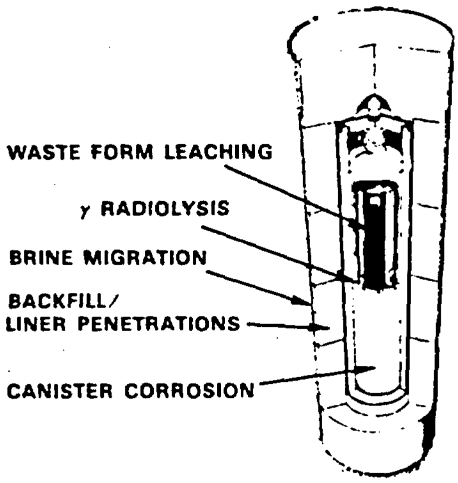
8.5 GEOCHEMISTRY

At least as important as the quantity of fluid which reaches the waste package is its chemical composition. The corrosive and leaching properties of brine depend greatly on the geochemistry of the waste package environment. Figure 8-8 illustrates the geochemical interactions which need to be considered in a waste package assessment.

The SRP will rely on EQ3/EQ6 as its primary tool for modeling the geochemistry of the very near field, the near field and the far field. The SRP is presently financing efforts to modify EQ3/EQ6 for high ionic strength calculations, so that it may be used for calculations involving brines. Extensive laboratory data will be gathered to verify the computer code, including studies of radiolysis, gas phase formation, clay mineral alterations, and formation of new solid phases. The code will be used to model changes in brine composition expected during brine migration, geochemical interactions at the waste package surface, and changes in composition of intruding fluids as they pass through the various subsystems.

Processes Considered

1. Brine-Host Rock Interactions
2. Brine-Canister Interacting
3. Brine-Waste Form Interactions
4. Radiolysis Effects on Above



Computer Codes

- EQ3/EQ6 — Aqueous Speciation and Mass Transfer Models of Chemical Processes With Upgraded Versions for Brine Environment

Input Data

- Identities and Thermodynamics Properties of Species
- Temperature Distribution in Waste Package Regime
- Spatial Salt Mineralogy Distribution in Repository Horizon
- Radionuclide Solid Phase Stability Data

Output and Its Interface With Other Processes

- Radionuclide Solubilities in Brines Developed in the Repository for Use in Radionuclide Transport

Figure 8-8. Geochemistry Affecting the Waste Package

8.6 CANISTER AND OVERPACK CORROSION

As mentioned in Sections 8.4 and 8.5, waste package corrosion is a function of both the quantity and the composition of the brine contacting the waste package. Waste package assessments will determine whether the corrosion allowance proposed for a particular site is sufficient to assure the integrity of the overpack. If the corrosion allowance is insufficient for the overpack material proposed, appropriate recommendations will be made to waste package design components of the SRP.

Several types of analyses will be carried out. The influence of temperature, geochemistry, fluid quantities, and time on corrosion will be considered. Figure 8-9 lists corrosion processes to be studied. As with geochemistry, extensive laboratory work is being conducted by the SRP to support these modeling efforts.

8.7 LOCAL RADIONUCLIDE TRANSPORT

Two processes determine the nuclide release rate from the waste package to the repository. These are:

- the rate of mass transfer of a nuclide from the solid state in the waste form to the dissolved state in the fluid in contact with the waste form
- the rate of transport in that fluid from the point of dissolution at the waste form through the other waste package components to the salt.

Both leaching and transport depend on the presence of fluid within the waste package. Before either process can begin, it is necessary that:

- fluid from the repository has invaded the waste package
- the canister has been breached, either by mechanical failure or corrosion, so that the fluid is also in contact with the waste form.

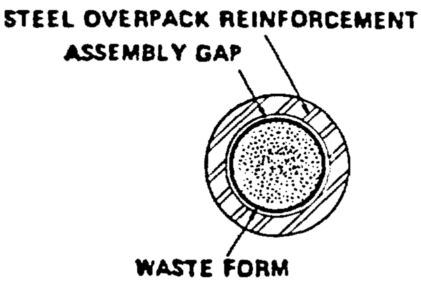
Figure 8-10 describes the input and output for release rate modeling.

The processes which affect the transport of nuclides in solution across the waste package and hence determine the rate of release to the repository include:

- the rate of diffusion of the nuclides in the waste package fluid
- the remaining cross-sectional areas of such breached barriers as the canister

Corrosion Processes Considered

- General Corrosion
- Localized Corrosion Including Pitting and Crevice Corrosion
- Stress Corrosion Including Active Path Stress Corrosion Cracking and Hydrogen Embrittlement
- Galvanic Corrosion
- Dry Oxidation



Computer Codes

- WAPPA   Corrosion Process Submodel

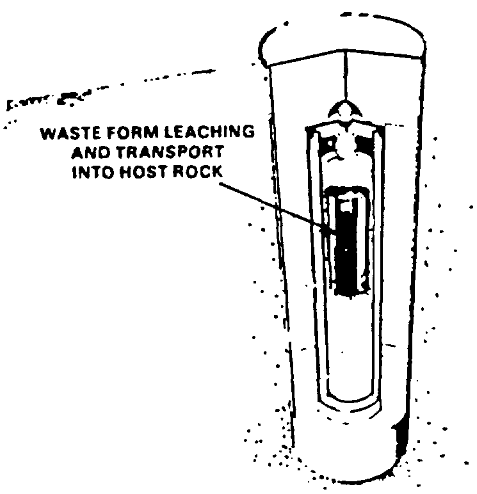
Input Data

- Temperature as a Function of Time
- Pressure (Hydraulic and Caprock Mass Loading)
- Geochemistry (pH, Free O, Fluid Phase Composition)
- Stress-State (Corrosion Cracking, Residual Stress from Processing)
- Sensitization (in Welding and From Storage at High and/or Changing Temperature)
- Electrochemistry Due to Overpack Metal and Prevailing Electrolytic Environment
- Radiolysis Products
- Available Water in Near-Field Domain

Output

- Corrosion Rates for Estimation of Time to Canister Failure
- Predominant Failure Mode
- Effective Confinement Period of Waste
- Leach Rate Analysis

Figure 8-9. Corrosion Rate of Metallic Canister and Overpack



A Waste Package

Computer Code

WAPPA Axisymmetric Radiation, Thermal, Mechanical, Corrosion and Leach Model

Input Data

- Radionuclide Inventory and Other Properties
- Waste Package Design and Material Properties
- Data from Other Analyses
- Stress
- Temperature
- Flux of Fluid
- Time to Repository
- Resaturation

Output

Decay Power

Barriers Wetting Times

Barriers Failure Times

Nuclide Fluxes to Repository

Total Nuclides Mass to Repository

Radial Nuclides Concentration Profile

For Use in Repository Boundary Conditions

Figure 8-10. Radionuclide Leach Rate From Waste Form, and Release Rate from the Waste Package - Computer Code, Input and Output

- o sorption and other reactions between the nuclides and backfill
- o the concentration gradient between the repository boundary and the fluid at the waste form.

The waste package performance assessment code WAPPA will calculate releases of radionuclides from the very near field. WAPPA takes boundary conditions from other codes and models the performance of the waste package during the postclosure phase of repository operation. It calculates radiation shielding, internal package temperatures, package corrosion and failure, and waste form leaching to produce these release rates, which are used as source terms for near field radionuclide transport. For conservatism, they will also be used as source terms for far field release calculations.

Many of the effects accounted for by WAPPA are modeled on a superficial level. Individual codes will be used to study the processes in detail; WAPPA will then be made to mimic the behavior predicted by these more sophisticated codes.

8.8 COUPLING OF THERMAL, MECHANICAL, FLUID, AND CHEMICAL MODELS

Figure 8-11 illustrates the complex, coupled nature of the processes of the waste package subsystem. Detailed analyses of each process along with sensitivity analyses of coupled processes will assist in identifying the strength of the coupling between parameters and processes. Examples of considerations which may influence the manner in which coupling is treated include:

- o That analyses of individual processes to provide a basic understanding of each component of the subsystem should precede coupled overall system analyses.
- o That strain, creep, geochemical reaction, and corrosion rates are temperature dependent, but that these processes do not significantly influence temperature.
- o That the heat generation rate is a function not only of nuclide inventory but of the rate of heat transfer, and the resulting canister component temperatures will depend on the properties of the waste package materials and on the properties and geometry of the repository.

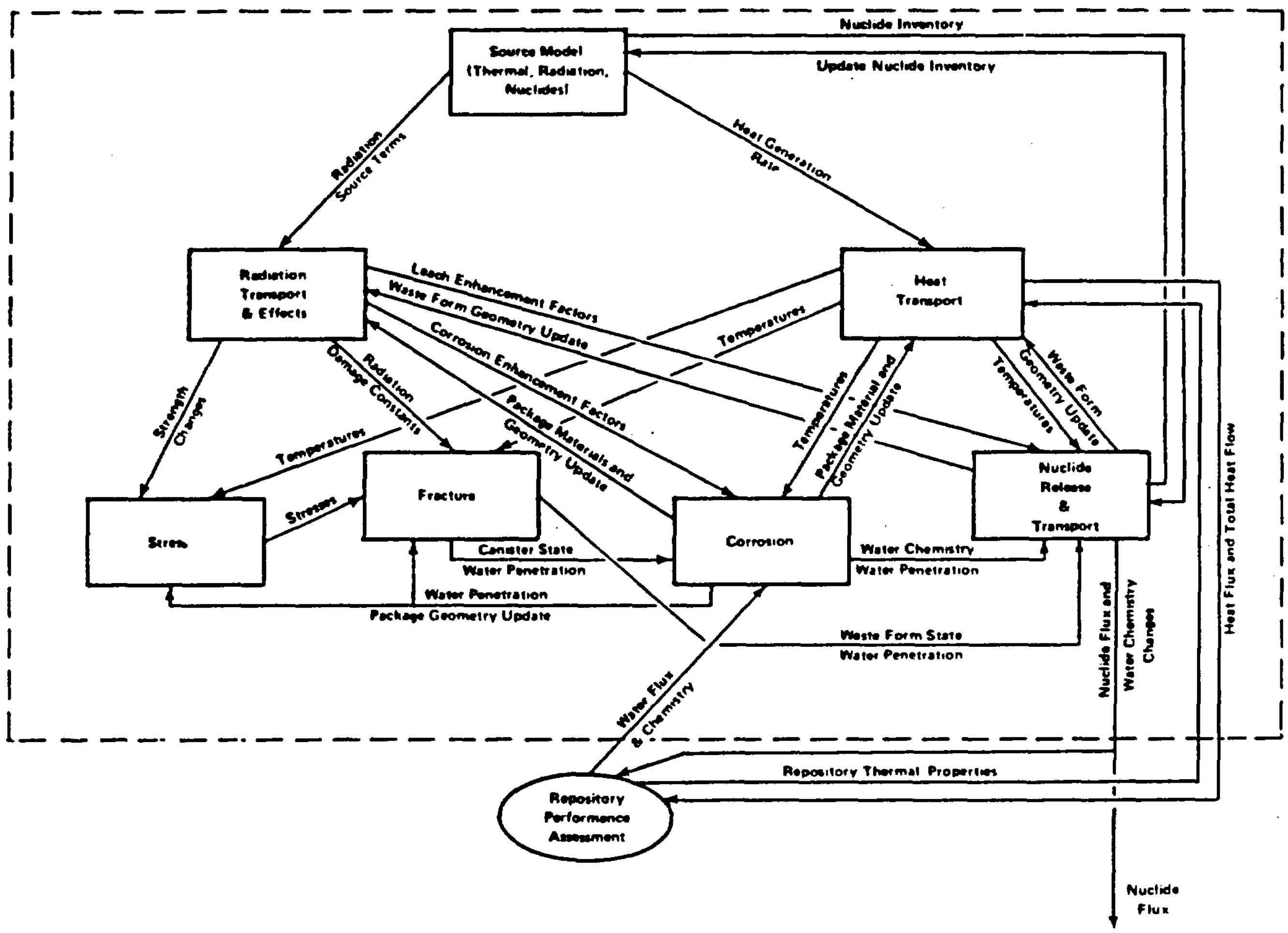
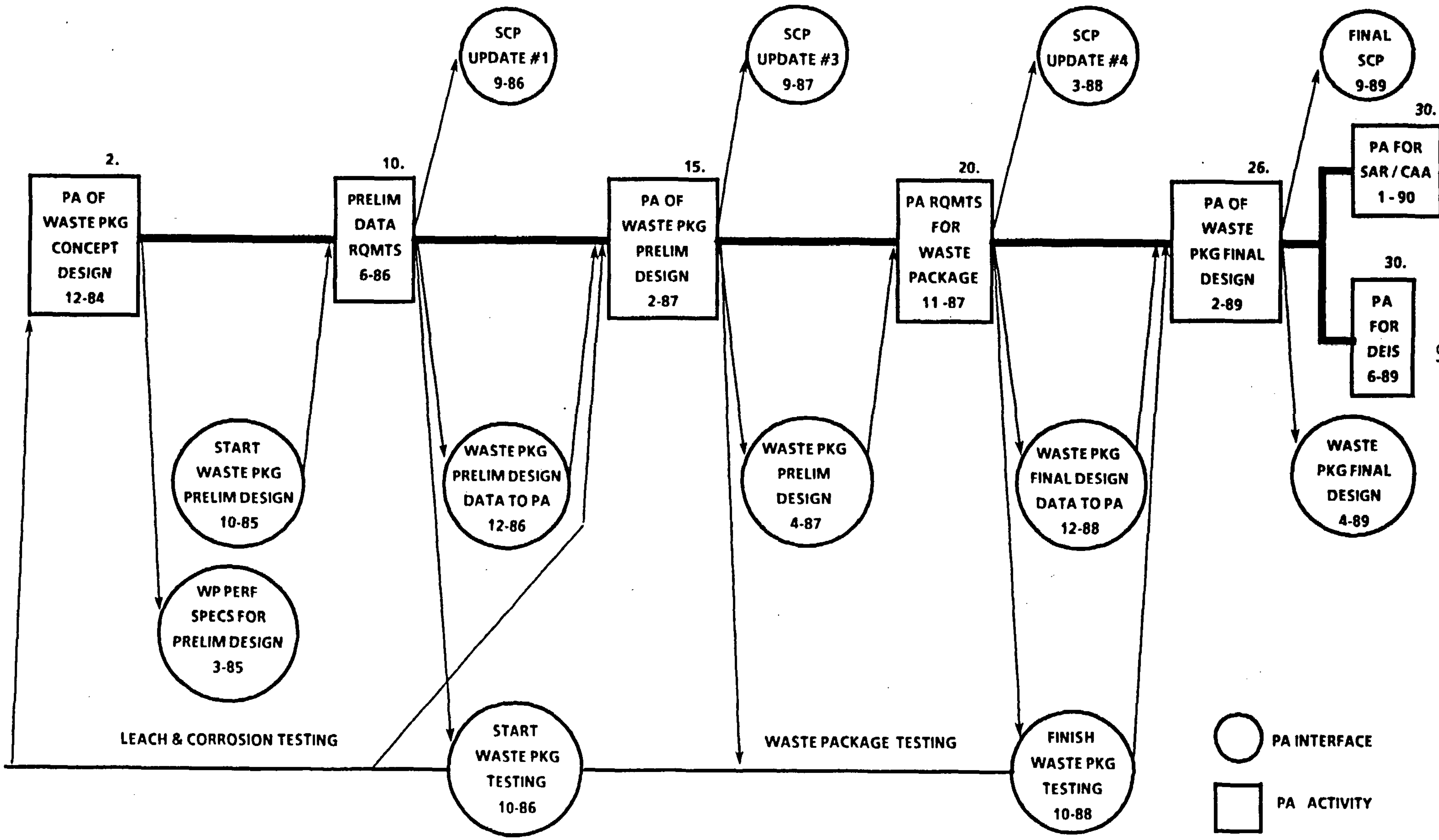


Figure 8-11. Information Flow Diagram for Waste Package Assessment

- That the mechanical behavior of the waste package will depend on the mechanical stress imposed on it by the repository. The repository mechanical behavior will in turn be influenced by its temperature.
- That corrosion, leach, and nuclide transport rates will be influenced by the geochemistry and flow of fluid impinging on the waste package from the repository.

8.9 MILESTONES

To emphasize its relationship to this chapter, Figure 1-5 is repeated here as Figure 8-12. Its place in the SRP program is described in Section 1.4.



Figures 1-5 and 8-12. Waste Package Performance Assessment Logic (Completion Milestones)

9 NEAR-FIELD ANALYSIS

The repository subsystem (DOE, 1982b) has been defined as all human-made structures and components of the disposal system, including engineered barriers not associated with the waste package, and the local host rock. The repository subsystem provides the surface and subsurface facilities that allow emplacement of the waste and contribute to the ability of the disposal system to contain and isolate waste in the long term. For the purpose of postclosure analysis, only the subsurface facilities are of interest. Therefore surface facilities will not be considered in this chapter.

The repository subsystem will contribute to long-term containment and isolation in two ways (DOE, 1982a)

1. By limiting the impacts of activities such as excavation, waste emplacement, and introduction of boreholes and shafts on the containment and isolation capabilities of the natural and human-made system, and
2. By limiting the degradation of the natural containment and isolation capabilities of the repository subsystem through the use of engineered barriers such as sealing and backfilling materials.

The purpose of the assessment on the repository scale is at least three-fold:

- o To determine key features of the design affecting repository performance and to recommend design parameters and modifications to conceptual designs that will ensure satisfactory performance of the system;
- o To evaluate effects of repository performance on the waste package and the site; and
- o To determine the role of the repository subsystem in overall system performance.

These assessments involve (1) evaluation of the system environment such as thermal, thermomechanical, geochemical, and fluid flow conditions; and (2) calculation of radionuclide containment within the system and migration of radionuclides through the system. The repository subsystem assessments will provide more appropriate interfacing boundary conditions between the waste package, repository and site subsystems for specific release scenarios.

The repository itself, independent of the waste package and the geologic barriers, plays a significant role in system performance. The repository contributes to system performance by providing a dilution factor for the waste in the geology, due to the separation and distribution of the waste packages through the repository. In scenarios for release involving a penetration of the repository, such as a borehole, the disposal of the waste through the repository can greatly limit potential releases by minimizing the likelihood that a waste package would be breached by the penetration. The repository also contributes to system isolation by means of the backfilling and sealing procedures, which improve system isolation.

Included in this chapter are brief descriptions of proposed analyses of the thermal and mechanical conditions that can affect the integrity of the host rock and the repository seals and backfill; the potential flow of water into and through the repository under site-specific, physically realizable conditions; and the transport of radionuclides out of the repository. Special scenarios for intrusion of the repository and the constraints on release in such cases will also be investigated. Descriptions and references for all computer codes mentioned in this chapter are given in the appendix.

9.1 DESCRIPTION OF REPOSITORY SUBSYSTEM

According to present proposals, an underground salt repository will consist of a series of long, parallel tunnels. Boreholes will be drilled into the tunnel floors at evenly spaced intervals, and the individual waste packages will be placed in these boreholes. After emplacement, the boreholes and tunnels will be backfilled with salt; when backfilling is complete, all shafts leading from the surface facilities to the repository horizon will be sealed and filled.

The focus of repository subsystem performance analyses is to quantify the radionuclide fluxes at the repository and site subsystem interfaces. A number of factors affect the availability of ground water to transport radionuclides from the emplaced waste package to the natural hydrologic system. Excavation-induced (size and method of excavation) and waste-induced (waste package and areal loading) forces affect the rock temperature distribution and quantity of rock disturbed, which in turn may affect the ground-water movement by modifying the properties of the materials and pathways for radionuclide transport from the repository subsystem to the site subsystem boundary.

The general approach to repository subsystem performance assessment begins with detailed analyses of various individual processes. Two- and three-dimensional analyses of the repository subsystem, including the host rock, will be made for thermal, mechanical, geochemical, hydrologic, and radionuclide transport. Two-dimensional individual tunnel (room scale) and set of tunnel cross-sectional (panel scale) analyses will be performed to determine the disturbed zone stability, room closure rate, and other properties. Three-dimensional simulations of the whole underground repository subsystem including the host rock will be made to determine the long-term thermal stress, thermomechanical stress, geochemistry and ground water flow of the site above and adjoining the repository subsystem. For detailed waste package subsystem analyses (Chapter 8) independent single waste package regime analyses are proposed to provide the conservative interfacing repository subsystem boundary conditions. The repository subsystem analyses will be used to support and quantify the conservatism built into waste package assessment.

In salt repositories, the host medium is essentially impermeable. The availability of ground water to transport radionuclides has to be analyzed by postulating various possible pathways under designed and unexpected conditions. The repository subsystem performance assessment will include flow and radionuclide analyses through the shafts, tunnel network, and drift including backfill, bulk head, and seals.

The following sections describe briefly the individual process analyses proposed for the repository subsystem temperature distribution, disturbed zone, uplift in the repository overburden, geochemistry, ground-water movement, degradation of repository seals, thermo-mechanical effects on the waste and the geologic media, and radionuclide transport.

9.2 THERMAL ANALYSIS

Limiting the impacts of heat generated by the waste is a principal consideration in the design of a repository. Temperature limits need to be imposed to ensure that thermomechanical and thermochemical interactions will not endanger the structural stability of the repository, cause significant impacts on the hydrologic properties, or lead to premature degradation of the waste package.

To design the repository for minimal influence of thermal effects, the following steps are recommended in DOE/NWTS-33(3) (DOE, 1982b):

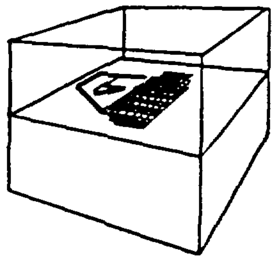
1. The thermal limits are required to be prescribed in terms of allowable temperatures, stresses, and deformations in the system. These limits

should be based on an understanding of the physical processes and failure mechanisms, including design bases, accidents, and natural phenomena controlling the behavior of the system, and on the observation of the response of the system components in both laboratory and in situ tests. Processes and mechanisms of principal interest include:

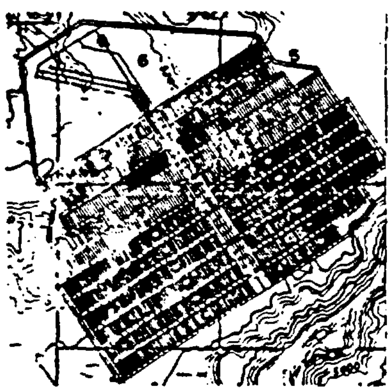
- o Uplift of overlying rock mass due to thermal expansion and subsequent subsidence upon cooling, and their effects on the hydrologic flow regime
- o Thermally induced stress perturbations and their importance to stability, permeability, and waste package integrity
- o Thermally induced incursion of fluids into the waste package vicinity
- o Thermochemical interactions that accelerate degradation of the waste package and the rate of transport of radionuclides.

2. Models that analyze the temperature, stress, and hydrologic perturbations in the rock mass due to excavation, waste emplacement, and sealing are required to be used to develop design specifications (e.g., thermal areal loading) that must be applied to ensure that the thermal limits are not exceeded. Margins related to the limits should be applied in setting the design specifications. Key data needs for modeling include:
   - o The heat-generating characteristics of the waste
   - o The geologic, geotechnical, geochemical, hydrologic, thermal, and mechanical characteristics of the host rock mass.
3. A repository design should be developed that satisfies the prescribed thermal limits and other applicable design constraints. Site-specific design options that must be considered include:
   - o Aging the waste to reduce the amount of heat generated after emplacement
   - o Limiting the amount of waste per package to reduce package thermal output
   - o Limiting the number of waste packages per unit area of the repository.

Figure 9-1 is a general list of the computer codes and their input and output proposed for use in thermal analyses. Both cross-sectional 2-dimensional and full 3-dimensional simulations will be conducted along with sensitivity and uncertainty analyses. Since stresses will occur during the thermal and post-thermal periods, the analysis will be carried out over both entire periods.



3-D Repository Domain For Temperature Simulation



General Layout of Repository Tunnel Network

Computer Codes

- CFEST — Coupled Flow, Energy, and Solute Transport
- HEATING6/5 — Nonlinear Heat Transport Code
- SPECTROM 41 — Heat Transfer Code
- SWENT — Coupled Flow, Energy, Solute, and Radionuclide Transport
- TEMP — Finite-Length Line Source Superposition Model

Input Data

- Repository Design and Thermal Loading
- Geologic Layering and Thermal Properties
- External Boundary Conditions

Output

Spatial and Temporal Temperature Distribution in Repository Region for Use in

- Thermomechanical Analysis
- Geochemical Processes and Radionuclide Transport

Figure 9-1. Repository Subsystem Thermal Environment Assessment--Computer Codes, Input and Output

9.3 THERMOMECHANICAL ANALYSIS

The thermomechanical analyses in performance assessment will involve use of computational methods to identify, based on exploration data, any anomalies which are unacceptable for full-scale excavation, existing in-situ stresses, potential disturbed zone due to excavation and thermal loading, borehole closure, potential subsidence, and effects of alternative excavation methods, designs, and backfilling. The CRWM guidelines (DOE, 1982b) on excavation are mentioned below along with a brief description of the proposed performance assessments.

The exploration of the rock mass before committing specific areas for waste emplacement allows flexibility in repository underground emplacement configuration development and provides a means for avoiding anomalies that might cause the repository to be judged unacceptable if intersected by a full-scale excavation. Computational methods using the exploration data base compiled for the repository subsystem design will be used to evaluate the potential hazards, if any.

During the excavation process, the balance of the forces present in the geologic formation is altered. As equilibrium is reestablished, localized fracturing around the perimeter of the excavated areas can result from stress concentrations. Fracturing around the excavation, if extensive, may provide a potential pathway for ground water flow. The extent of fracturing depends on the host material, the extent of natural jointing or fracturing, the depth of the repository, in situ stress, and the excavation techniques used. Computational methods will be used to quantify the disturbed zone under in situ and excavation stresses.

The excavation of rooms and tunnels underground will induce a new stress state and displacement field in the host environment. The nature of these stresses and displacement fields depends on the cross-sectional geometry and orientation of the excavation, the layout of the tunnels and rooms, and the extraction ratio (the ratio of the volume removed to the total volume). Of interest to long-term containment and isolation in some geologic media is the possibility of subsidence in the strata overlying the repository, which might lead to adverse perturbations in the hydrologic regime. The performance assessment will include estimation of subsidence in the strata overlying the repository and its effects on the hydrologic regime. If significant subsidence is predicted, subsidence may be reduced by limiting the extraction ratio. Backfilling of the excavated areas will also be examined.

Fracturing due to excavation is a function of:

- o Extraction ratios and room geometries affecting the extent of fracturing due to stress concentrations.
- o Designed blasting patterns, charge sizes, and types and sequence of detonation if blasting is used.
- o Mechanical excavation methods used.

The following are some of the specific thermomechanical studies and analyses using site-specific data:

(i) In Situ Stresses: assessment of anomalies (if any) which may be a potential hazard.

(ii) Excavation Techniques: stress and displacement analyses for delineation of disturbed zone as a function of room geometry, excavation techniques, and site-specific information.

(iii) Room Closure Calculations: prediction of room closure rates; estimates of reconsolidation and permeability changes with thermal loading within the crushed backfill.

(iv) Borehole Closure Calculations: evaluation of the mechanical closure of a borehole due to deformation of the rock.

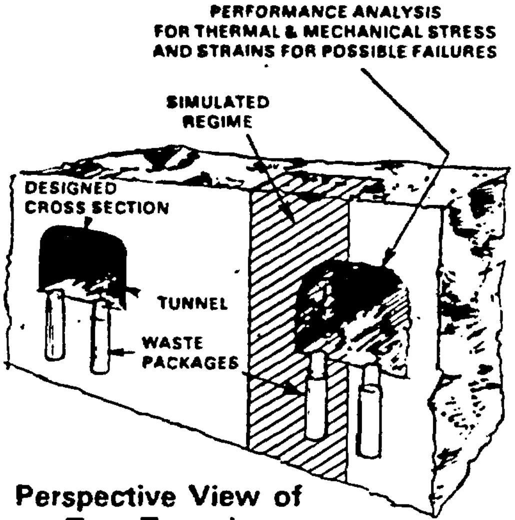
(v) Shaft Seal Calculations: predictions of thermal and mechanical conditions within the seal components and the surrounding rock mass; investigation into fracturing of seals and conditions within backfill.

(vi) Thermomechanical stress and deformation analyses in overlying sediments: for assessing potential tensile fractured zones due to thermal expansion and uplift.

The impact of thermomechanical behavior will be evaluated for the probability of radionuclide transport through the disturbed zone. Figure 9-2 is a general list of codes and their input and output for the thermomechanical analyses.

9.4 FLUID FLOW

The fluid condition in the repository is an important factor describing the environment and pathways within the repository subsystem for radionuclide migration.



Perspective View of Two Tunnels

Computer Codes

- **VISCOT — Visco- and Elastic-Plastic Thermomechanical Analysis**
- **SPECTROM 21 — Thermoviscoelastic Analysis**
- **STEALTH — Thermoviscoelastic Analysis**

Input

- **Repository Design Details**
- **Thermomechanical Properties of Host Rock and Other Parameters**
- **Thermomechanical Properties of Repository Backfill and Seal Material**
- **Thermal Output From Waste in Each Canister and Emplacement Plan**
- **Excavation Method**
- **In Situ Stress State**
- **Temperature Distribution in Repository System**

Figure 9-2. Thermomechanical Response in the Repository Regime--Computer Codes, Input and Output

The performance assessment consists of the evaluation of water ingress into the repository; the flow rate will be quantified and sensitivity and uncertainty analyses will be conducted. The salt deposits are relatively impermeable, and no significant flow is expected under the designed conditions. Due to thermo-plastic properties, the backfilled tunnels and other excavations within the high thermal range will seal as a result of room closure and salt flow, and thereby further reduce the probability of fluid entering the waste isolation system.

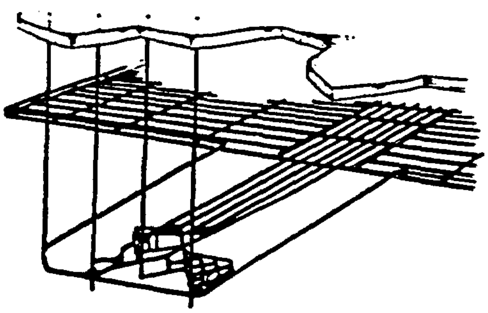
The fluid flow analysis for unexpected events includes flow-through shaft seal failure, exploratory boreholes, and natural fault or brecciation of the salt host rock. These analyses will be conducted in detail considering properties of the backfill, seal materials, interfaces between shaft seals and host material, individual tunnels, and networks of tunnels. The analyses will account for dissolution and precipitation effects, along with closure due to salt creep.

The plan for evaluating fluid conditions consists of the following tasks:

- o Determine the flow parameters in the repository storage rooms and connecting tunnels
- o Determine permeabilities and porosities in the disturbed zones in the repository
- o Determine the flow parameters for the repository seals and backfill
- o Using the regional-scale pressure boundary conditions, evaluate flow into and out of the repository
- o Take into account the dissolution and precipitation of host rock minerals in these flows and include the effects of heat upon these properties and the water density
- o Evaluate special scenarios involving fluid flow in the repository.

Sensitivity and uncertainty analyses will be conducted to identify the important parameters. Figure 9-3 is a general list of the codes proposed for use, and their input and output. Following are brief discussions of three aspects of the flow problem, repository seals, resaturation, and flow through a fault or disturbed zone.

Human intrusion and natural phenomena performance assessments are dealt with under site subsystem performance assessment. A detailed flow and temperature analysis of salt as an idealized, extremely low permeability medium will be conducted as one of the scenarios. This is the expected condition.



Simplified Repository

- Analysis for Shaft Seal Failures
- Resaturation Estimation
- Influence of Human or Natural Disturbance
- Other Scenarios

Computer Codes

- CFEST — Coupled Flow, Energy, and Solute Transport
- SWENT — Coupled Flow, Energy, Solute, and Radionuclide

Input

- Repository Design
- Hydrologic Boundary Conditions
- Geologic Structure and Disturbed Zones
- Hydraulic Properties of Host Rock, Backfill, Seals

Output

- Pressure Distribution
- Quantity of Waste in the Repository
- Flow Rate Through Various Pathways

Figure 9-3. Fluid Conditions in Repository Regime--Computer Codes, Input and Output

9.4.1 Repository Seals

The overall goal of the repository sealing progam is to design seals acceptable for emplacement in boreholes, shafts, and tunnels at or near repositories. A further consideration is the backfilling of repository chambers. The seals and backfill must be capable of controlling the movement of ground water and the release of radionuclides or other contaminants through these penetrations.

The seal must perform these functions under changeable environmental conditions in the seal zone, including variable waste heat loads, for relatively long periods (D'Appolonia Consulting Engineers, 1980). The design effort requires that a series of decisions be reached regarding material selection and emplacement techniques. The hydraulic, mechanical, thermal, and chemical properties are critical to material evaluations. In addition to the intrinsic material properties, the host environment and the properties of the host materials will be considered in the performance assessment. Through sensitivity and uncertainty analyses, the important prarmeters affecting flow rate at specific sites will be analyzed.

9.4.2 Resaturation

Backfilling of rooms and drifts with crushed salt is currently under consideration. Moisture within the backfill or introduced through accidents may migrate towards the reconsolidated crushed salt. This process may be complicated by the mechanisms of salt dissolution and reprecipitation. The rate of dissolution may be influenced by temperature-dependent solubility, dependence of fluid density upon salinity and temperature, and natural convection circulations. The formation of limited resaturated cavities within the crushed salt will depend on the amount of water entering, its origin, temperature, salinity, and so forth. Depending upon the amounts of water available, a brine lens may or may not be formed. If formed, the lens may reasonably be expected to move and deform under the influence of the dissolution-reprecipitation mechanism. The interactions are thus very complex and knowledge about this type of process is very limited.

To quantify resaturation, the simple approach is to do bounding calculations. The consequence of the conservative resaturation rate will be analyzed for effects on radionuclide release rate and transport. A few simulations with the complex modeling will be conducted to quantify the additional safety factor provided by the isolation system.

9.4.3 Flow Through Potential Fault or Disturbed Zone

A fault or disturbed zone can provide one of the conduits for water movement with some diffusive leakage into the rock matrix. Analysis of flow and transport in such a system is complex because the systems are highly heterogeneous. The three commonly used conceptualizations of a fractured system are the equivalent porous medium, double or composite-porosity systems, and discrete fractured systems. The equivalent porous medium treats the fractured system as an equivalent statistical continuum. The tacit assumption is that physical quantities such as porosity, pressure, and other parameters are averaged over sufficiently large blocks that differences due to fractures are averaged out. The double porosity approach is mathematically idealized as a complex of two intersecting media, one representing the fissured regime (high permeability and very low storage) and the other representing the porous regime (low permeability and high storage). In the discrete fracture approach, the fractures and porous matrix are separately discretized. Each method has its advantages and limitations.

The performance assessment capabilities include codes for analysis using the above approaches. Initially, the effect of disturbed and fault zones will be studied using scenarios for the salt site repository regime. The sensitivity and uncertainty analyses will assist in understanding flow and radionuclide transport through the fractured media.

9.5 GEOCHEMICAL REACTIONS

Analyses proposed to be performed under this task are very similar to those described in Section 8.5. The important concerns are:

1. Mineral dehydration-alteration reactions in the repository as a function of the pressure-temperature (P-T) conditions. The temperatures and pressures are expected to be less extreme on the repository scale than on the waste package scale.

2. Brine-host rock-repository and brine-backfill reactions. The analyses are similar to those performed at the individual waste package level. The only difference may arise from brine reactions with nonsalt materials used for repository backfilling. Two cases are of interest here:
   a. Reactions between brine from the very near field with the repository backfill and host rock material, and
   b. Reactions between waters intruding into the repository from above or below the repository salt horizon.

   In both cases, brine compositions will need to be determined and combined with local P-T conditions derived from thermomechanical analyses to predict possible reactions.

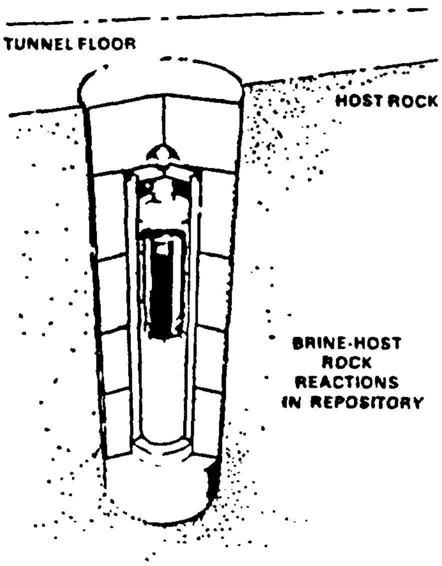
Figure 9-4 provides a tentative list of computer codes and their input and output for geochemical analyses in the repository regime.

9.6 RADIONUCLIDE TRANSPORT

Radionuclide transport through different components of the repository subsystem will be analyzed using local temperatures, potential flow field, and geochemistry. The radionuclide transport estimations will be performed for each postulated flow event. The leach rate from the waste package analysis will be used as input. The radionuclide transport from the repository subsystem will provide the boundary conditions for the site subsystem evaluation.

For radionuclide transport through the repository tunnel network, cumulative flow of one-dimensional radionuclide transport will be estimated. Transport through seal materials, solubility limits, salt solubility, and spatial distribution of the radionuclide release from the waste package subsystem will be considered. The following is an additional description of the radionuclide transport analysis for a repository subsystem.

The flow of water through and out of the repository is described earlier. The transport properties will correspond to conservative values appropriate for brine in the repository environment and both retardation and solubility considerations will be taken into account along with the effect of separation of waste packages. The tunnels will generally have an opening at only one end which will reduce the possible flow from the tunnels. If these openings are



Computer Code:

- EQ3/EQ6 Aqueous Speciation and Mass Transfer Models of Chemical Processes with Upgraded Versions for Brine Environment

Input Data

- Pressure and Temperature Distribution in Repository Subsystem
- Spatial Salt Mineralogy Distribution in Repository Subsystem
- Brine Composition of Inclusions and/or Intruding Waters
- Radionuclide Solubility Data in Brines

Output

For Use in Leach Rate Estimation

- Brine Chemistry Around Waste Package Considering Brine-Host Rock and Package-Brine Interactions, and Brine Radiolysis
- The Effects of Brine Chemistry Around Waste Package on Corrosion Rates, Leaching Rates, and Backfill and Liner Performance

Figure 9-4. Geochemistry Affecting Radionuclide Transport in Repository Regime closed with a bulkhead, the flow will be further constrained. The repository will be constructed of panels of such storage tunnels separated from one another. This separation of panels, storage tunnels, and waste within tunnels will limit the rate at which waste can exit the repository by way of any opening or penetration of the subsystem.

The prediction of the migration of radionuclides down a storage tunnel will take into account the distribution of canisters in the drift. It will be assumed that all waste released from the waste pakages is immediately received into the storage tunnel. This is a conservative assumption since the process of transfer from the emplacement hole to the storage tunnel will provide additional isolation. The releases from each waste package will be convolved with the storage tunnel flow rate to evaluate the rate of release from the storage tunnel. These release rates will be used in turn as source terms for transport through a panel of such storage tunnels. Finally, the convolution of the release rates from the various panels will be used to predict the release of radionuclides from the repository. Two classes of calculations will be performed: (1) release of radionuclides to an opening at the edge of the repository such as the tunnel connecting the repository with a shaft, and (2) release of radionuclides to a penetration in the center of the repository such as a borehole intersecting one of the storage drifts. These two sets of calculations should determine the bounds to the release rates for the intact repository.

The transport of radionuclides in the tunnel leading to the repository tunnel may be affected by fractures intersecting the tunnel. In one sense they provide a dispersive mechanism for the transport; in another sense they provide additional pathways for radionuclide transport. Therefore, analyses are planned to investigate these effects.

9.7 COUPLING OF THERMAL, MECHANICAL, FLUID, AND CHEMICAL MODELS

Figure 9-5 illustrates the coupled nature of the processes of the repository subsystem. As with very-near field performance assessment, detailed analyses of each process along with sensitivity analyses of coupled processes will assist in identifying the strength of the coupling between parameters and processes.

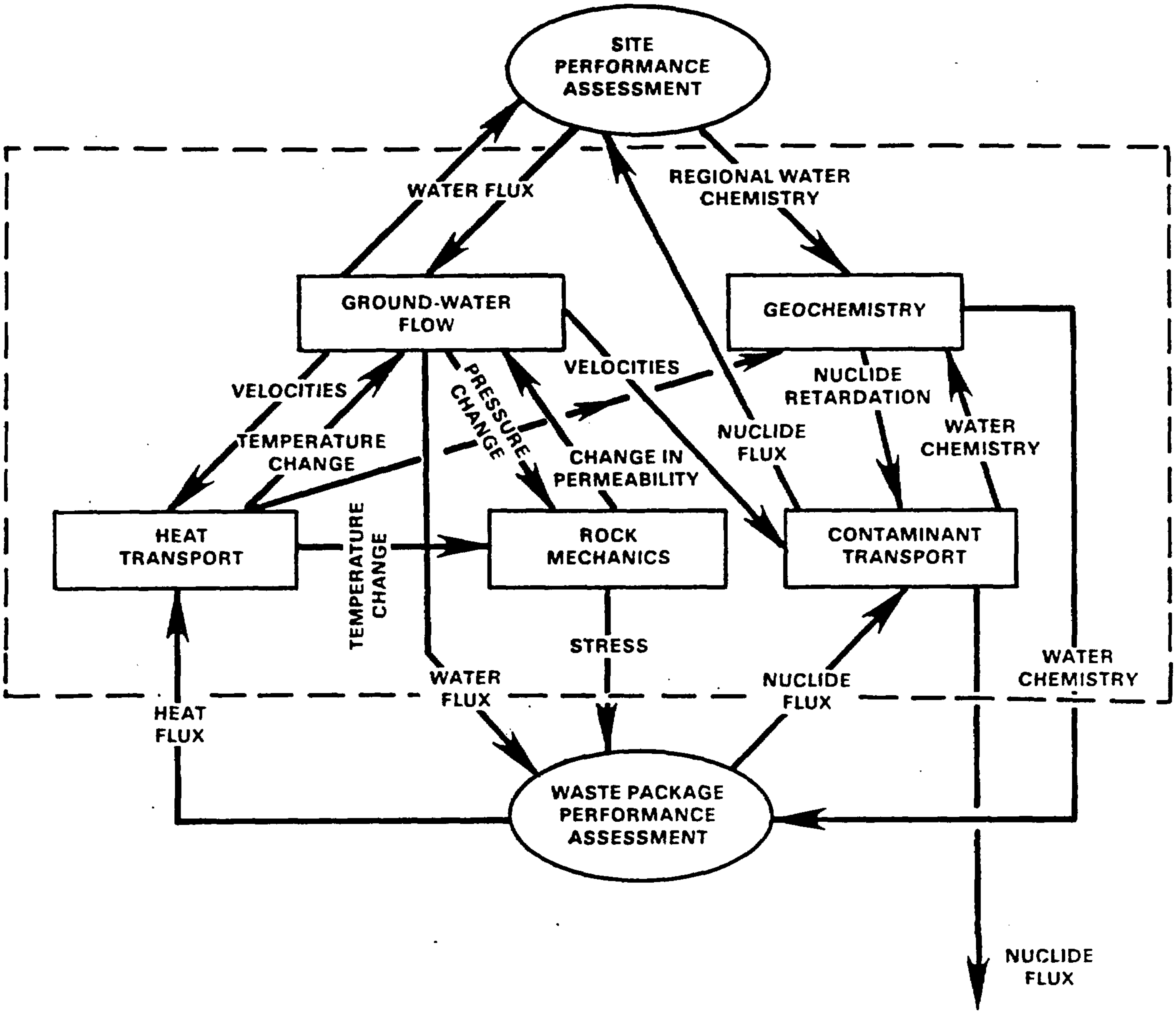
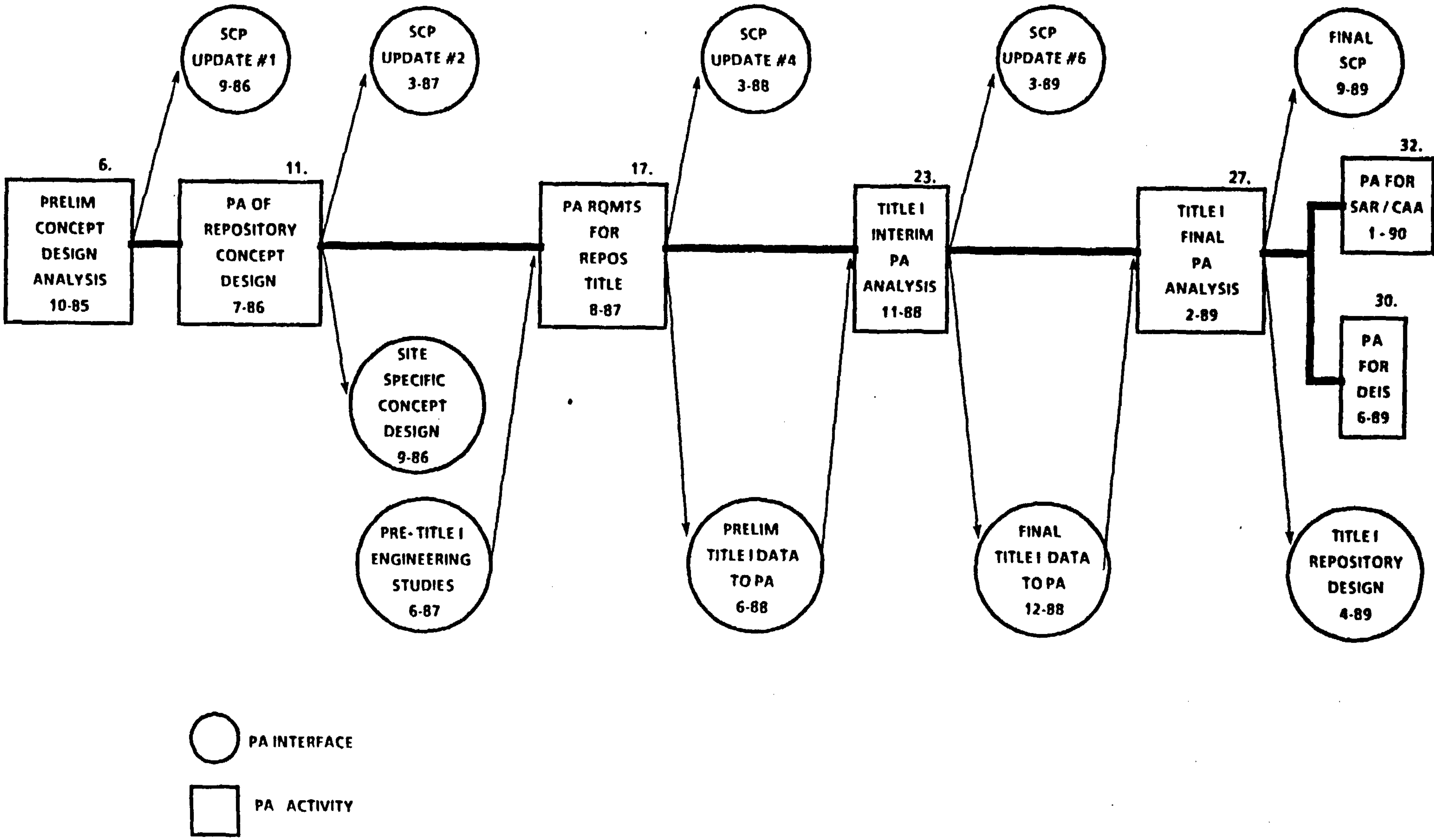


Figure 9-5. Information Flow Diagram for Repository Assessment

9.8 MILESTONES

To emphasize its relationship to this chapter, Figure 1-6 is repeated here as Figure 9-6. Its place in the SRP program is described in Section 1.4.



Figures 1-6 and 9-6. Repository Performance Assessment Logic
(Completion Milestones)

10 FAR-FIELD ANALYSIS

10.1 DESCRIPTION OF THE SITE SUBSYSTEM

The "site" as used here is the surface and subsurface portion of the earth's crust that contains the repository and the natural barriers to radionuclide release. It is therefore defined as the place both at and below the surface containing the repository and auxiliary facilities and the surrounding buffer area (DOE, 1981). Analysis of the site must consider the geologic and geohydrologic regime in which the site is located, inasmuch as the regime influences conditions and processes that determine the performance of the site. The most important aspect of site performance is groundwater flow, as this is the major mechanism for long-term release of waste radionuclides to the accessible environment. For this reason, site assessment relies strongly on modeling of the regional hydrogeologic system.

Site subsystem performance assessments support site screening and site characterization, and define interactions with the repository subsystem. PA analyses may be used in support of site screening by comparing sites on the basis of preliminary estimates of predicted performance, and by examining the consequences of locating a site at various points in a hydrcgeologic system. PA analyses will be used to examine data needs as inputs to the Site Characterization Plans required by the Nuclear Waste Policy Act (U.S. 97th Congress, 1983, Section 113(b), especially by coupling geostatistical analyses with groundwater modeling. The hydrogeologic framework of the repository subsystem is defined by regional groundwater modeling. Site subsystem modeling also provides the means of transferring nuclide releases from the repository to the biosphere or the accessible environment in a performance assessment of the total system. Site assessments must demonstrate that the site presents an effective barrier to radionuclide transport.

The site subsystem (far field) considers the region outside the regime where material properties and the ground-water flow system are not significantly changed by waste and repository-induced effects. The far-field subsystem can be divided into three subgroups based upon the modeling approach. These subgroups are termed geosphere, biosphere, and far-field state. The biosphere models calculate transport of radionuclides within the biosphere; that is, from discharge to surface water bodies to doses to human organs. The objective of the geosphere performance assessment is to analyze nuclide transport in the subsurface geologic media. The far-field state analysis evaluates changes in site geology and climatology as functions of time, and the effects of these changes on site performance.

The site subsystem must meet several objectives, to meet various regulatory requirements. PA analyses will determine how well each site may meet these objectives, and will estimate the level of uncertainty in the calculated performance measures. Specific site requirements are (NRC, 1982):

- o that the pre-waste emplacement groundwater travel time be at least 1,000 years from the disturbed zone to the accessible environment (10 CFR 60.113 (a) 2)
- o that effects of potentially adverse human activities or natural conditions are shown not to cause the repository system to fail to meet the performance objectives (10 CFR 60.122 (a)).

These are in addition to the system performance requirements discussed in Chapter 3 of this plan, mainly from 40 CFR 191 Subpart B, and 10 CFR 60.

Descriptions and references for all computer codes mentioned in this chapter are given in the appendix.

10.2 PROPOSED ANALYSES FOR SITE SUBSYSTEM PERFORMANCE ASSESSMENTS

Figure 10-1 illustrates the major processes and interactions of site performance assessments. Repository performance assessments will provide source terms for radionuclide release; for conservatively high calculations, radionuclide releases from the waste package assessments will also be used in site assessments. Repository assessments will also provide thermal and thermomechanical stress effects needed to model groundwater flow. In turn, the far-field groundwater flow model will provide the source term for groundwater flow into the repository for scenario analyses.

Figure 10-2 shows a stepwise procedure for performing site assessments. The process is iterative, allowing interactions between submodels to be accounted for. Specific analyses proposed for the far field are listed in Figure 10-3. These analyses will be described in the following sections of this chapter. In general, site subsystem modeling will provide:

(1) existing volumetric rates and ground-water travel times to locations of existing ground-water use and surface discharge

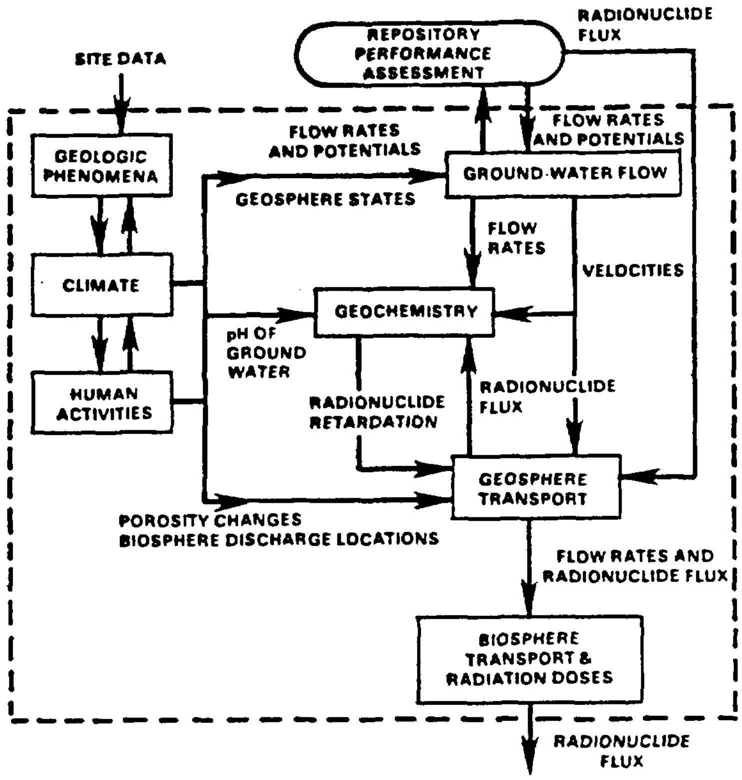


Figure 10-1.Information Flow Diagram for Site Subsystem Assessment

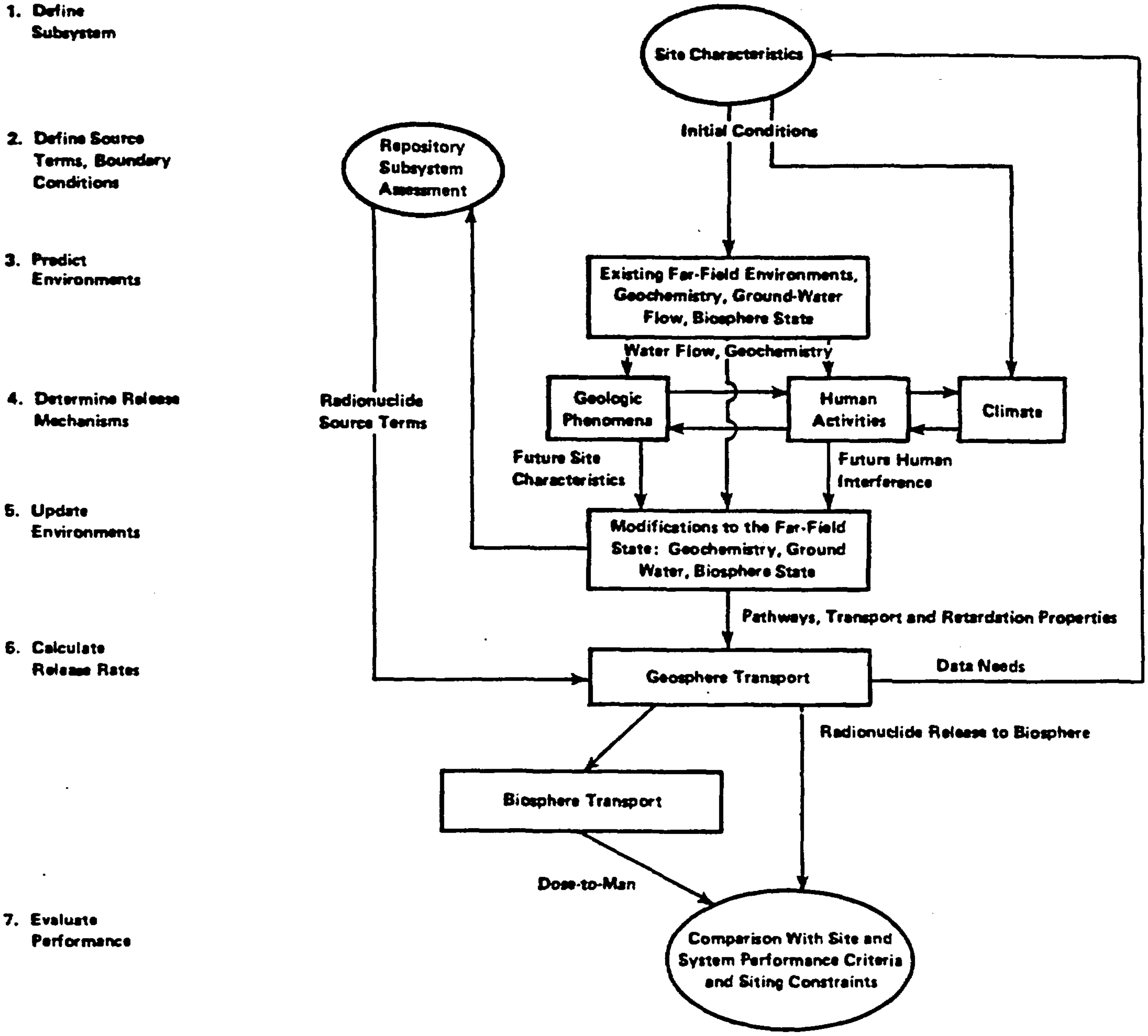
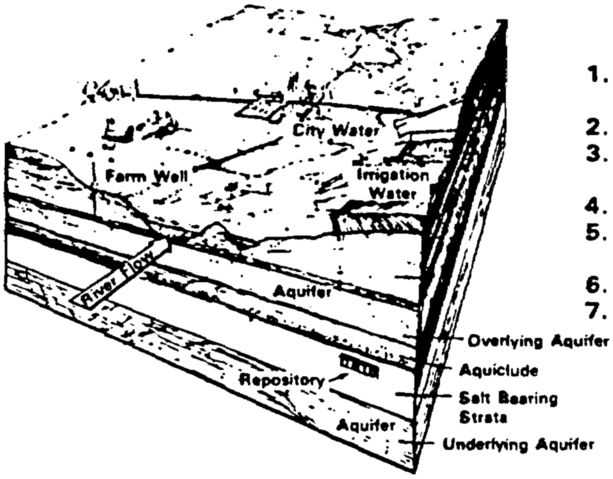


Figure 10-2. Stepwise Procedure for Site Subsystem Performance Assessment



Analyses Proposed for Site Subsystem Assessment

1. Site Data Compilation, Evaluation and Geostatistical Analyses
2. Ground-Water Flow Paths, Rates and Hydrologic Budget
3. Geochemical Reactions Affecting Radionuclide Transport in Site Domains
4. Radionuclide Transport from Repository Boundary to Biosphere
5. Radiation Doses to Human Through Various Environmental Pathways
6. Long-Term Natural Processes and Events
7. Evaluation of Potential Human Interference

Performance Measures

Ground-Water and Radionuclide Travel Times and Rates From Repository to Accessible Environment

Figure 10-3. Analyses Proposed for Site Subsystem Assessment

(2) potential effects of the existing geochemical regime on radionuclide retardation

(3) natural and human-caused phenomena which could change future ground-water flow

(4) expected radionuclide travel times between a given repository site and the accessible environment or locations of potential ground-water use and surface discharge.

Site performance assessments will provide required input to the Location Recommendation Reports (LRR), Exploratory Shaft (ES) site decision document, Site Characterization Plans (SCP), Final Environmental Impact Statement (FEIS), and Safety Analysis Report (SAR) required for construction authorization.

10.3 SITE DATA COMPILATION, EVALUATION AND GEOSTATISTICAL ANALYSIS

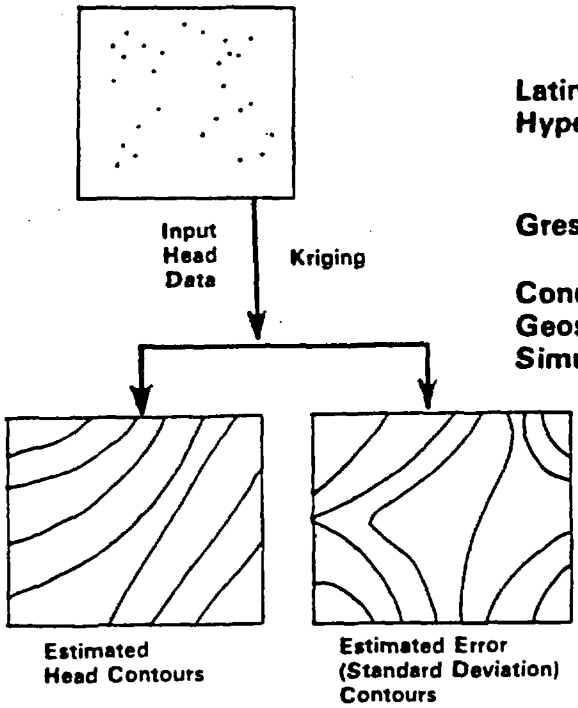
Understanding the geologic, hydrologic, and seismic characteristics of the region are an important part of a site subsystem performance assessment.

Data is collected from available sources in order to:

- o Obtain modeling parameters from field measurements and previous studies
- o Critically examine the data base for consistency
- o Quantify the uncertainty in each parameter.

Hydrogeologic data used for performance assessments are drawn from the SRP Geologic Project Managers, who are responsible for characterization of the various sites. These data result from compilations of published and other sources as well as from field measurements performed by the SRP. The hydrogeological data base compilation process includes well test interpretations and geophysical log verifications. Available flow and trace tests will be analyzed to obtain flow and transport parameters.

The spatially distributed variables will be analyzed for means, standard deviations, and structural drift. Kriging and other geostatistical techniques will be used for optimal interpretation of variables, distributed in two- and three-dimensional space, sampled at points (e.g., wells) scattered through the space. Figure 10-4 is a summary of geostatistical analyses for site performance assessment.



Computer Codes:

GEOSTAT	**Optimal Interpolation of Spatially Distributed Variables (Kriging).**
Latin Hypercube	**Monte-Carlo Like Approach to Sensitivity/Uncertainty (S/U) Analysis.**
Gress	**Adjoint Approach to S/U Analysis.**
Conditional Geostatistical Simulation	**Propagate Kriging Uncertainties Through Hydrologic Models.**

Input:

- **Spatially Distributed Parameters**
- **Modeling Parameters from Field and Laboratory Studies**

Output:

- **Means, Standard Deviations, Drift**
- **Sensitivity to Various Parameters**
- **Uncertainty in a Given Output Parameter**

Figure 10-4. Geostatistical Analyses--A Partial List of Computer Codes, Input and Output

Stochastic hydrogeology deals with the uncertainty in ground-water modeling which can be accounted for by spatial variability and limited sampling of the flow. The complex variability of the important hydrogeologic parameters has required the development of geostatistical computer codes using the theory of random functions. Monte Carlo techniques with and without the spatial correlation structure, and perturbation theory with and without regime spectral analysis have been used. Conditional simulations that incorporate spatial variability based on Kriging analysis have also been applied to hydrogeologic parameters. Using the geostatistical techniques, the spatially distributed data base will be analyzed for estimation of statistical parameters like variance, autocorrelation, and uncertainty. These analyses also will be used for identifying appropriate locations for additional wells for hydrologic characteristics determination.

The far-field state model input parameters probabilistically describe the past history and spatial distribution of climatic variation, glaciation, erosion, deposition, faults, breccia pipes, brine pockets, magmatic events, and drilling and other resource-related activities.

10.4 REGIONAL GROUND-WATER FLOW AND HYDROLOGIC BUDGET

Geohydrologic systems consist of multiple aquifers separated by semiconfining layers. In contrast to surface water supplies, ground-water reservoirs are interconnected over large areas and require difficult and expensive geologic investigations for their definition and analysis. Due to the slow rate of ground-water movement, direct observation of flow rate is generally not possible. Because of the complexity of the physical system, the mathematical model is the most powerful tool available to ground-water hydrologists for predicting the behavior of the reservoir. Performance assessment activities related to ground water flow and hydrologic budget will include characterization of ground-water residence times, travel times, recharge rates, potentiometric surfaces, and path lengths and orientations.

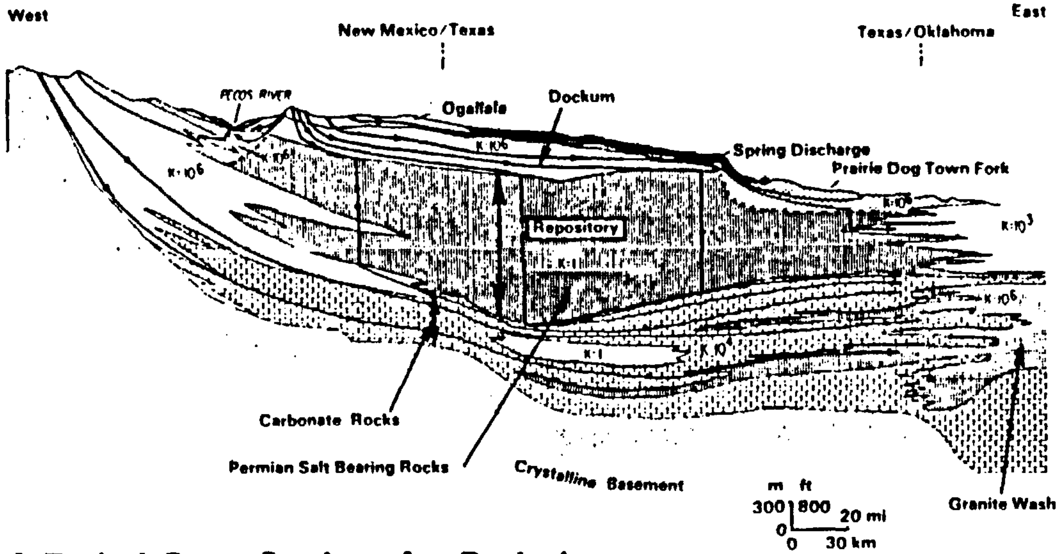
For performance assessment, ground-water flow analyses will involve development of input files for multidimensional analysis and plotting the important parameters, like stratifications, material thickness and extent, and boundary conditions, for interaction with the field geologists and for verification. Appropriate parameter combinations will be developed for effective sensitivity and uncertainty analyses. This will be followed by simulations for pressure head and temperature distributions. Ground-water travel times and volumetric rates from the repository to the accessible environment and to locations of existing ground-water use and surface discharge will be estimated. Sensitivity and uncertainty analysis of flow paramerters and appropriate display of the results and interpretations will be done.

The flow calculations will be performed on regional and local scales. Simulation of the groundwater basin will provide boundary conditions for the region of interest. More detailed analysis of ground-water flow in and adjacent to the repository as well as in the controlled zone (the region needing institutional control according to regulatory guidelines) will be performed using a finer grid than the one used for regional scale ground-water simulation. In these localized analyses the effects of thermal gradients and stress-strain conditions on hydrogeologic properties will be considered. Sensitivity and uncertainty analyses will be conducted to quantify the confidence limits in the prediction.

Figure 10-5 lists some of the computer codes for ground-water analysis, with their inputs and outputs.

10.5 RADIONUCLIDE MIGRATION

The ultimate test of the site is its ability to restrict the release of radionuclides to the accessible environment. Although performance measures such as groundwater travel time from the repository to the accessible environment are made important by the regulatory requirements (see Chapter 3), the performance measure of final concern is the rate at which radionuclides travel to the accessible environment, thence to humans. The pathway for long-term (postclosure) nuclide release is by way of ground water. If radionuclides are released from the waste form and package, and escape from the repository, they may eventually reach one or more aquifers and enter the accessible environment. This section discusses this process and the approach and plans adopted by the SRP for analysis.



A Typical Cross Section of a Geologic System Through Repository

Computer Codes

- CFEST — Coupled Flow, Energy, and Solute Transport
- FE3DGW — Ground-Water Flow
- SWENT — Coupled Flow, Energy, Solute, and Radionuclide Transport
- TRIPM — Saturated and Unsaturated Flow and Transport

Input

- Repository Design
- Hydrologic Boundary Conditions and Disruptive Events (Source, Sink, Brine Pockets)
- Geologic Structure
- Hydraulic Properties of Materials

Output

- Internal Pressure Distribution
- Ground-Water Velocity Distribution and Travel Times

Figure 10-5. Ground-Water Flow and Hydrologic Budget--Computer Codes, Input and Output

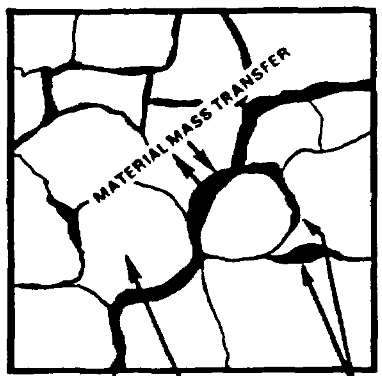
10.5.1 Geochemical Reactions Affecting Radionuclide Transport in the Site Regime

Geochemical analyses must consider species formation, solubilities, and sorption in evaluating radionuclide transport. Geochemical assessments in the far field are based on the principle of thermodynamic equilibrium between rock minerals and chemical species in groundwater. The basic set of equations includes mass balances, mass action equations, electrical neutrality (pH calculation), phase equilibrium expressions, conservation of electrons, and relationships between thermodynamic activity and molality. The partition coefficient (the ratio of nuclide mass on the solid phase to that in the aqueous phase)d will be calculated based on these relationships and available data. Radionuclide retardation factors can then be calculated from the partition coefficient using rock density and bulk porosity. (Retardation is discussed further in the next section.)

Ground water age can be calculated from isotopic ratios, such as carbon-14 to total carbon. The procedure requires knowledge of the source of the isotopes, the path followed by the ground water and geochemical reactions over the path. Isotopes consumed or generated by chemical reactions and radioactive decay from the source to the sampling location are calculated to obtain the water age.

Obtaining retardation factors as functions of time and space, from which species transport may be calculated, requires knowledge of concentrations of major aqueous species as functions of time and space. The poor spatial resolution in species transport calculations, lack of specific knowledge of heterogeneity in rock mineralogy at a fine scale and uncertainties in the thermodynamic data base all contribute to uncertainties in geochemical performance assessment results. Sensitivity analysis will be done using a sampling technique to evaluate the effects of the uncertain parameters. In the far-field analyses, attempts will be made to refine these parameters; conservative values of retardation factors and water travel times will be used. Figure 10-6 lists computer codes that have been tentatively selected for geochemical analysis of the site subsystem.

Far-field ground-water flow paths and rates will be determined from regional potentiometric head distributions using site-specific values for porosity, permeability, and other hydrodynamic properties. Ground-water age



Computer Code:

- EQ3/EQ6 — Thermochemical, Aqueous Speciation, and Mass Transfer and Their Updates for Brine Composition

Input Data

- Ground-Water Compositon, Thermodynamic Properties, and Reaction Rate for Each Benchmark Zone Affecting Geochemical Environment Along the Flow Path

Output

- Major Geochemical Reactions Affecting Radionuclide Transport
- Retardation Factors for Each Benchmark Zone
- Sensitivity and Uncertainties of Geochemical Parameters

Geochemical Processes

Promoting Radionuclide Retention

- Precipitation in Discrete Solid Phase
- Chemical-Physical Sorption on Mineral Phases
- Decay in Stagnant Pores

Inhibiting Retention

- Complexing in the Aqueous Phase
- Colloid and Particulate Movement

Figure 10-6. Geochemistry Affecting Radionuclide Transport -- Computer Codes, Input and Output dating results, if available, will be used to confirm the results of hydrologic flow modeling. Radionuclide migration will be calculated by coupling geochemical effects with the flow model results.

The identification of the geochemical reactions affecting radionuclide retention will delineate zones where changes in the geochemical environment along the ground-water flow path significantly affect radionuclide behavior. The chemical characteristics of each zone will either be based on field studies or interpreted. The geochemical speciation computer codes will be used to define the aqueous species and their saturation states with respect to mineral phases. The models will be run for each bench geochemical zone to determine variations in ground-water speciation and solubility relationships. The resulting knowledge of the ground-water geochemical environment and its variation will be used to:

a. define reactions for mass transfer modeling, such as precipitation and redox reactions
b. determine where, along the migration path, the geochemical mass transfer calculations need to be performed.

10.5.2 Radionuclide Transport

The radionuclide transport assessment will provide radionuclide discharge rates as a function of time at 10 km from the repository (the "accessible environment", 40 CFR 191, EPA, 1982) , input to the biosphere transport models, and distributions in the geosphere for evaluation of other accessible environment releases.

Under expected conditions, radionuclides will not be able to escape the repository. Radionuclide transport analyses will therefore be primarily conducted to evaluate potential breach scenarios (Chapter 5). Radionuclide fluxes across the repository site boundary will be used as source terms for transport calculations in the site region.

The basic set of equations for geosphere transport are equations of conservation of dissolved radionuclides, including advection (bulk flow), diffusion, dispersion, radionuclide decay and daughter-product generation and retention on the rock (sorption or other deposition). Analytical, numerical (finite difference and finite element), and random walk (particle movement) methods are used for radionuclide transport analyses. The transport equations for different radionuclides are coupled through radionuclide decay and generation terms and retardation. Retardation causes the radionuclides to move at lower velocities than the ground water in which they are dissolved. These include such phenomena as adsorption, ion exchange, colloid filtration, reversible precipitation and mineralization. The retardation factor is an equilibrium constant for each nuclide and can be based on laboratory measurements or computed to account for geochemical environment changes in time and space, as discussed in the previous subsection.

Sensitivity analyses will be performed on retardation factors and dispersivity factors using adjoint or direct methods. Formal uncertainty analyses will also be made using a linear perturbation technique.

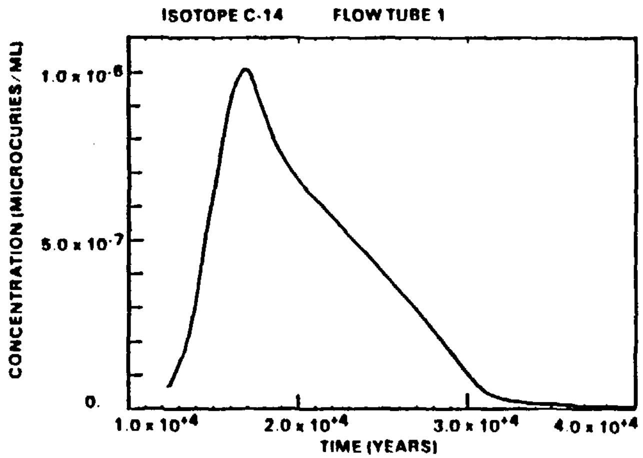
Figure 10-7 lists selected codes proposed for radionuclide transport assessment in the far field.

10.6 RADIATION DOSES TO HUMANS THROUGH VARIOUS ENVIRONMENTAL PATHWAYS

Performance assessments involve estimation of dose to people through external radiation exposure and ingestion of radionuclides transported through the biosphere via water and terrestrial pathways (Figure 10-8). Current EPA standards (EPA, 1982) and NRC Regulations (NRC, 1982) do not specifically require the calculation of doses for compliance. However, the various types of dose calculations are useful in evaluating the effectiveness of the system and its various subparts. The following are the brief details relative to water pathway transport:

- The radiation doses from external exposure to contaminated water and soil are calculated using the basic assumption that the contaminated medium is large enough to be considered an "infinite" volume or plane relative to the range of the emitted radiations. The equations for calculations of the radiation dose from external exposure to shoreline sediments include a correction for the finite width of the contaminated beach.
- Important ingestion pathways (or food products) will be selected with corresponding consumption rates, growing periods, and air or water concentration and deposition rates. Similarly, the external exposure pathways will be selected with corresponding exposure times, and soil or water concentrations. Accumulated doses will

Radionuclide Transport From Repository Boundary to Biosphere



Sample Output at Exist Point

Computer Codes

• LAYFLO	Analytical Solution of Radionuclide Decay Chain Transport
• MMT	Radionucide Decay Chair Transport Using Random Walk Method
• SWENT • SCOPE	Coupled Flow, Energy, Solute, and Radionuclide Transport

Input Data

- Flow Velocity
- Geochemistry
- Retardation Coefficient
- Radionuclide Transport Rate from Repository Subsystem

Output

- Rate and Total Amount of Each Radionuclide Release Into the Biosphere

Figure 10-7. Radionuclide Transport from Repository Boundary to Biosphere--Computer Codes, Input and Output

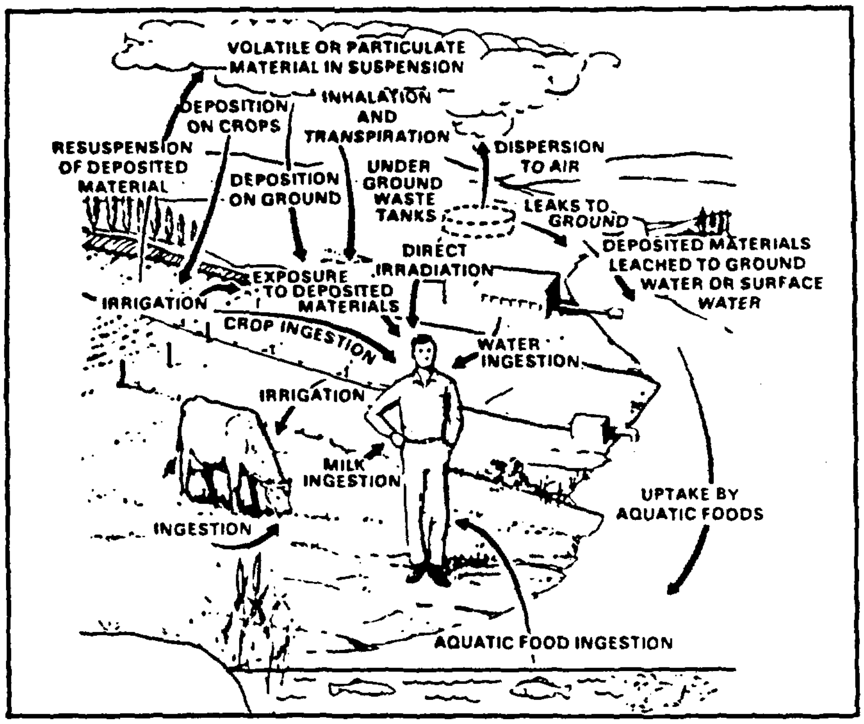


Figure 10-8. Major Pathways by Which Environmentally Dispersed Radionuclides Can Affect Living Organisms (PNL Drawing, Reproduced from Murray, 1982)

be calculated to various body organs or tissues for any one or combination of radionuclides.

- o Radioactive decay will be considered using a chain decay scheme which includes branching to account for transitions to and from isometric states.
- o Exposure pathways will include exposure to radionuclides deposited on the ground or crops from contaminated air or irrigation water, radionuclides in contaminated drinking water, radionuclides in aquatic foods raised in contaminated water, and radionuclides in bodies of water and sediments where people might fish, boat, or swim. For vegetation, the radiation dose model will consider both direct deposition on leaves and uptake through roots.
- o Doses will be calculated for a maximum-exposed individual and for a population group. The doses calculated will be accumulated doses from continuous chronic exposure.
- o The equations for calculating internal radiation doses are derived from those given by the International Commission on Radiological Protection (ICRP) Publication 2 (ICRP, 1959) for body burdens and MPCs (Maximum Permissible Concentrations) of each radionuclide.

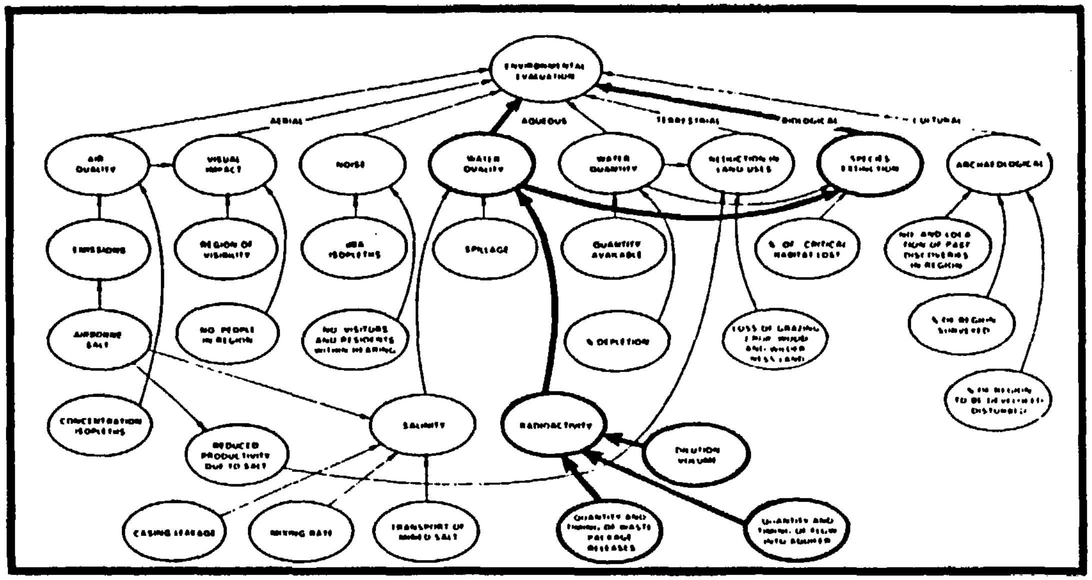
Figure 10-9 lists briefly the computer codes currently considered for dose evaluations.

10.7 LONG-TERM NATURAL PROCESSES AND EVENTS

The EPA specifies in 40 CFR 191 that the performance assessments can be carried out for a period of 10,000 years after disposal based on the following:

1. Because of the slow rate of ground-water travel, 10,000 years of assessment "encourages selection of sites where the geochemical properties of the rock parameters can significantly reduce releases of radioactivity through groundwater."
2. Major geologic changes, such as development of a faulting system or a volcanic region, take much longer than 10,000 years. Thus, the likelihood and characteristics of geologic events which might

disrupt the disposal system are reasonably predictable over this period.



General Bubble Diagram of Environmental Evaluation

Computer Code

- PABLM — A Dose-to-Man Model for Ingestion and External Exposure Through Different Pathways

Input Data

- Terrestrial Parameters
- Aquatic Parameters
- Radionuclide Release Rates in the Environment

Output

- Doses for a Maximally Exposed Individual or a Population Group
- Integrated Long-Term Doses

Figure 10-9. Radiation Doses to Humans Through Various Environmental Pathways--Computer Code, Input and Output

The following are the general guidelines by DOE (DOE, 1981) for long term characteristics.

Quaternary Igneous Activity. "The site shall be located so that the centers of Quarternary igneous activity can be identified and shown to have no unacceptable impact on system performance.

The evaluation of the likelihood and impact of igneous activity on the disposal system will include thorough evaluations of the region's igneous history, with particular attention given to temporal and spatial distribution of activity, character of activity, and analysis of the possibility of migration or expansion of areas of active volcanism."

Quarternary Faults. "The site shall be located so that Quarternary faults can be identified and shown to have no unacceptable impact on system performance.

The evaluation of Quaternary faults will emphasize the determination of the potential for rupture in or adjacent to the site but will include evaluation of the likelihood and consequence of earthquake generation and plausible impacts on the regional hydrology."

Faults, Volcanoes and Geothermal Gradients. "The site shall be located so that its tectonic environment can be evaluated with a high degree of confidence to identify tectonic elements and their impact on system performance. Potentially hazardous geologic elements, including faults of any age, volcanoes, and anomalous geothermal gradients, must be sufficiently investigated to allow determination of their potential effects on system performance and to show that these effects will not unacceptably affect system performance."

Earthquake. "The site shall be located so that long-term continuing uplift or subsidence rates can be shown to have no unacceptable impact on system performance.

Evaluation of the rates of uplift or subsidence is required so that effects of such movement can be shown to cause no unacceptable reduction in repository performance."

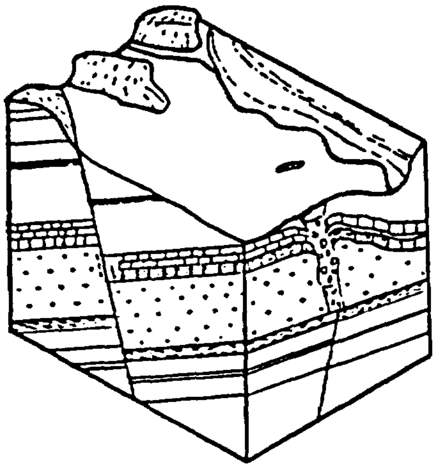
Performance assessments will be conducted to determine compliance with the above site criteria. The objective of far-field state performance assessments is to analyze and understand site integrity and behavior using past history as an indication of future behavior. Far-field state asssessment is a probabilistic representation and evaluation of the site. The processes are modeled empirically and a sampling method like Monte Carlo or Latin Hypercube is used to estimate the associated probability of the event.

Figure 10-10 lists the code currently being considered for long-term geologic simulation of a site.

10.8 EVALUATION OF POTENTIAL HUMAN INTERFERENCE

In Working Draft No. 3 of 40 CFR 191 (EPA, 1984) the EPA devotes an appendix to inadvertent human intrusion. It states that inadvertent intrusion by exploratory drilling for other resources should be the most severe intrusion scenarios considered, and sets limits on the assumed likelihood of such inadvertent drilling (0.003 and 0.0003 boreholes per square kilometer of repository area per year for repositories in sedimentary formations and other geologic formations, respectively). The consequences of inadvertent drilling were limited to "(1) creation of a groundwater flow path with a permeability typical of a filled (but not well-sealed) borehole; and (2) direct release to the land surface of all the groundwater in the repository horizon that could promptly flow into the borehole--or 200 cubic meters of groundwater, whichever amount is greater."

For protection from human interference, DOE/NWTS-33(2) (DOE, 1982, p. 21) specifies that in site selection, resources that would invite human interferences will be avoided. The aquifer systems below potential repository sites are generally not suitable water supplies because of their high salinity and the cost of extracting the water. The probability of drilling for other purposes (oil and gas exploration or recovery, geothermal recovery, brine or other waste disposal) will have to be assessed, as well as the potential impacts of such drilling. Figure 10-11 lists some of the computer codes that will be used. The impacts of various human interference activities can be divided into the four basic scenarios of Chapter 5.



BLOCK DIAGRAM CONCEPTUALIZATION OF HYPOTHETIC STUDY AREA

Climatic Changes
Glaciation
Geomorphic Processes (Erosion, Deposition)
Tectonic Processes (Regional Deformation, Folding, and Faulting)
Natural Salt Dissolutioning
Salt Dome Diapirism
Volcanism and Magnetic Events

Computer Code

- Salt-GSM — Far-Field State Code

Input Data

Area Extent, Details and Time History of Faults

- Faults
- Folding (Uplift, Subsidence, Diapirism)
- Igneous Activity (Volcanic Eruptions, Magmatic Intrusions)
- Seismicity

Climate-General and Long-Term Trends
Continental Glaciation

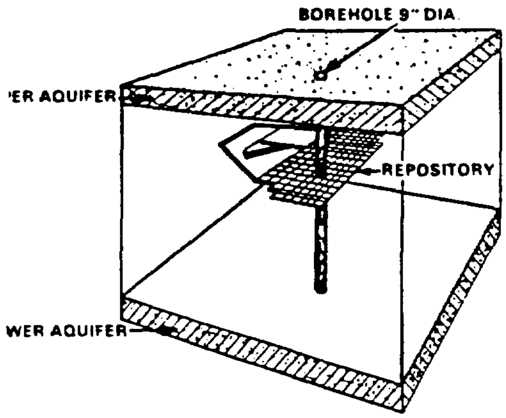
Output

- Climatic and Glaciation State Indicators
- Physical Characteristics of Modeled Events and Processes

For Probability Analysis of Natural Events and Their Effects on Radionuclide Transport

Figure 10-10. Long-Term Natural Processes and Events Analysis--Computer Codes, Input and Output

Drilling Into Repository



Schematic Representation of a Borehole Connecting Two Aquifers and Repository

Computer Codes

- **Salt-GSM** Far-Field State Code
- **CFEST** Coupled Flow, Energy, and Solute Transport
- **SWENT** Coupled Flow, Energy, Solute, and Radionuclide Transport
- **VISCOT** Visco and Elastic-Plastic Thermomechanical

Input Data

Scenarios (Describing Probable Human Interference)

- Location and Number of Wells
- Pumping/Injection Rate Amount

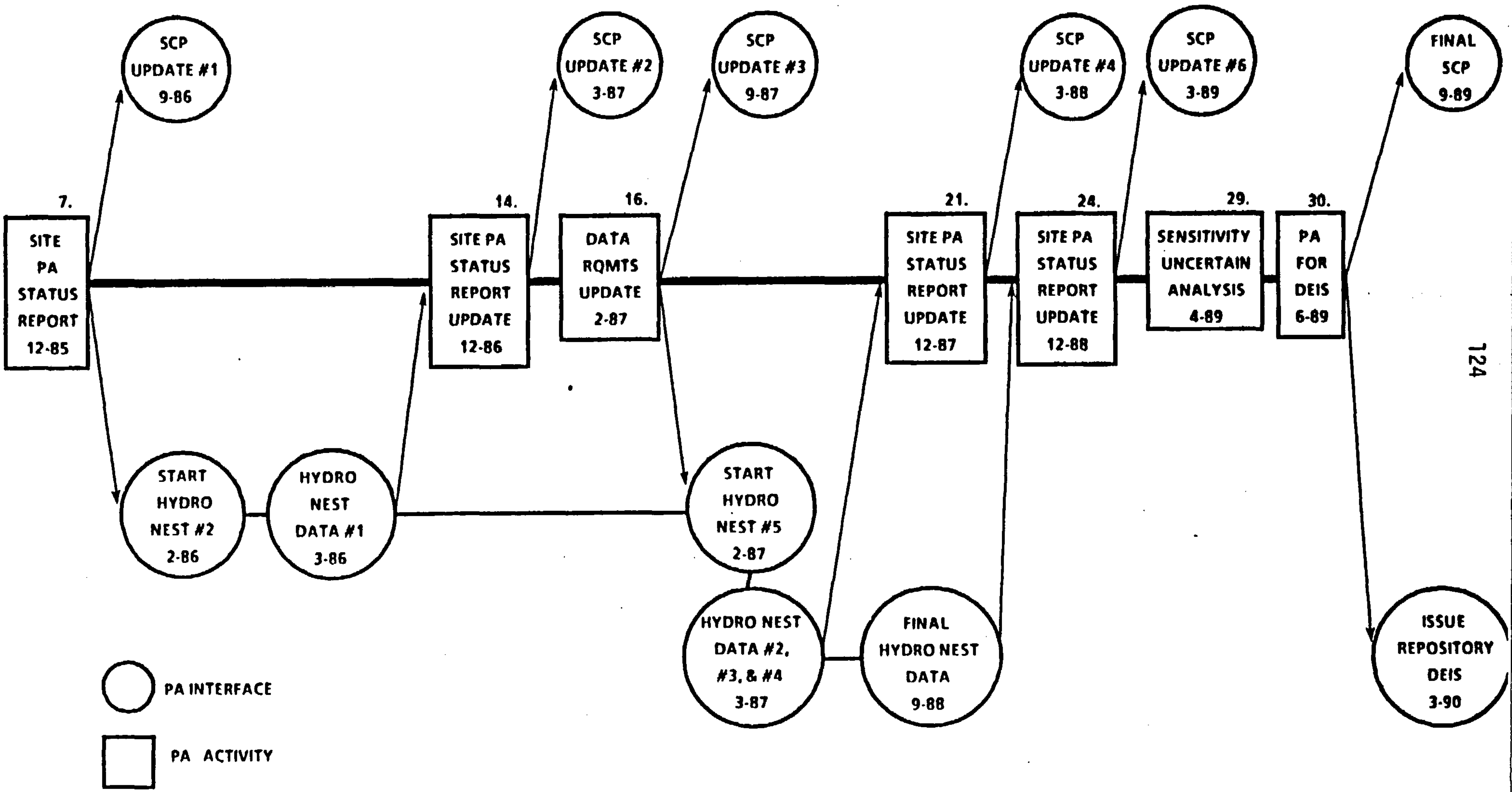
Output

- Flow Rates, Borehole Closure, Travel Path and Travel Time, and Radionuclide Released to Biosphere

Figure 10-11. Evaluation of Potential Human Interference: Computer Codes, Input and Output

10.9 MILESTONES

To emphasize its relationship to this chapter, Figure 1-7 is repeated here as Figure 10-12. Its place in the SRP program is described in Section 1.4.



Figures 1-7 and 10-12. Site Performance Assessment Logic
(Completion Milestones)

11 OPERATIONAL ANALYSIS

This chapter discusses the strategy and requirements for operational phase (preclosure) radiological performance assessment. This phase is defined to include optional retrievability operations and transportation of waste packages from packaging to the repository location. The objective is to protect plant personnel and the general public from potential radiation exposures. Radiological performance objectives include 10 CFR 20 for plant personnel (NRC, 1980), 40 CFR 191 for the general public (EPA, 1982), and an operating philosophy of maintaining all exposures at "as low as is reasonably achievable" (ALARA) levels. The assessment is divided into two steps (Figure 11-1):

(1) Performance assessment of normal operations, including transportation and retrievability operations

(2) Performance assessment of accident conditions.

Strategies for assessing the radiological safety of these two steps and requirements for implementation of the strategies are discussed in the following sections. Descriptions and references for all computer codes mentioned in this chapter are given in the appendix.

11.1 RADIOLOGICAL SAFETY ASSESSMENT FOR NORMAL OPERATIONS

The strategy for assessing repository safety under normal operations (including transportation and retrievability) consists of three steps: (1) identification and classification of all operations involving a potential hazard into separate "unit operations"; (2) evaluation of each unit operation and consequences of its hazard, including dose assessment, where necessary; and (3) development of preventive or mitigative measures for each unit operation. A general outline for operational phase performance assessment is listed in Figure 11-2. Figure 11-3 illustrates the basic relationships among these three steps. The objective of the strategy for assessing the safety of normal operations is to evaluate the performance of repository operation to ensure compliance with radiological exposure limits and the ALARA concept.

This strategy would apply to all operations related to waste handling in the facility, including transportation, retrieval, and decommissioning operations, as well as normal maintenance and construction activities. Doses

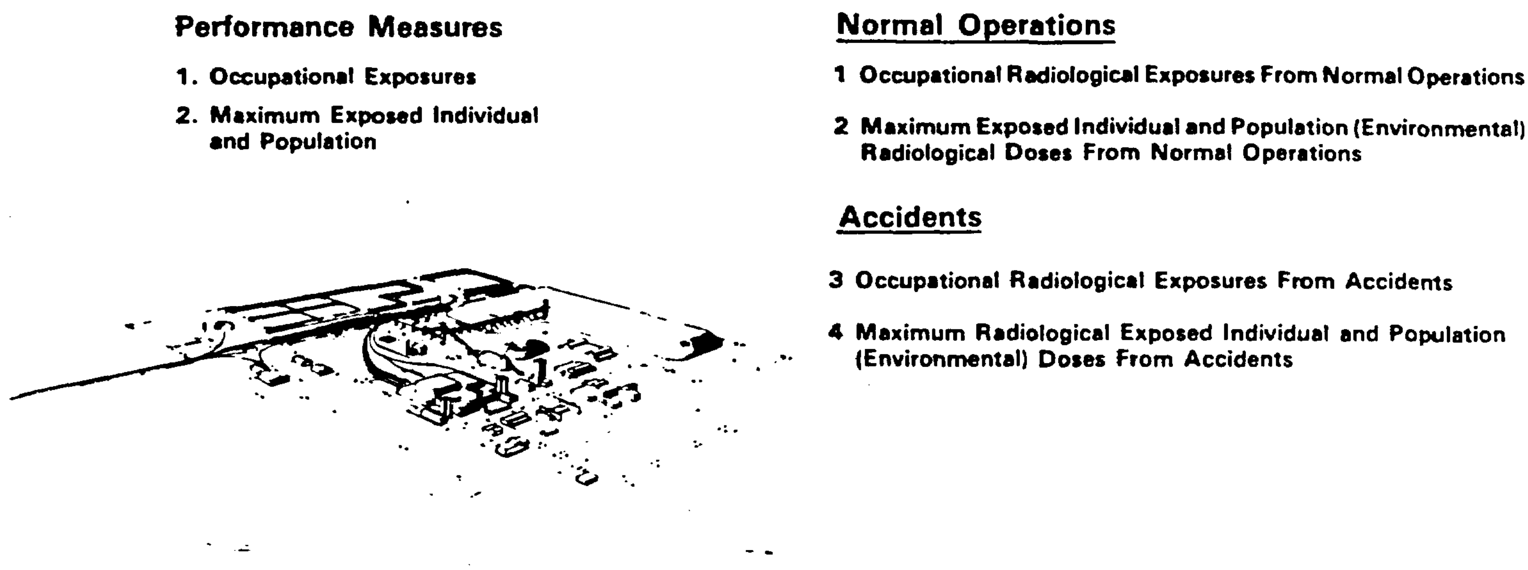
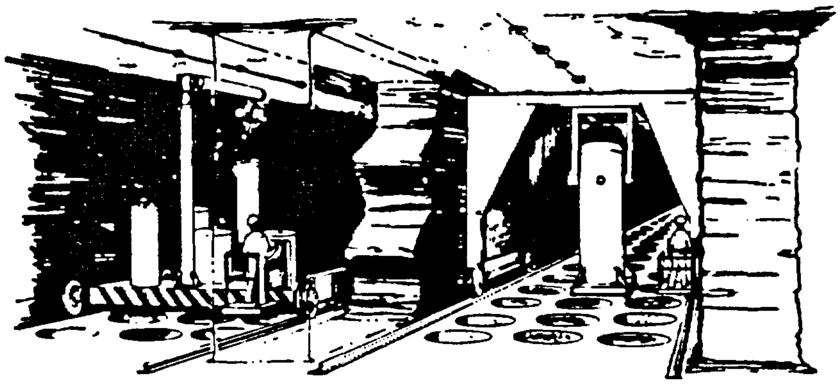


Figure 11-1. Operational Phase Radiological Safety Performance Assessment Plan



Normal Work Emplacement

Computer Codes

- Internal and External Dose Models

Input Data

- Detailed Task List and Descriptions
- Applicable ICRP Dose Assessment Models and Factors
- Task Screening Occupational Dose Limit
- ALARA Analysis Criterion
- Annual Limit for Occupational Exposure

Output

- Population Dose Estimates
- Determination of Level of Occupational Safety

Figure 11-2. Occupational Radiological Exposures From Normal Operations

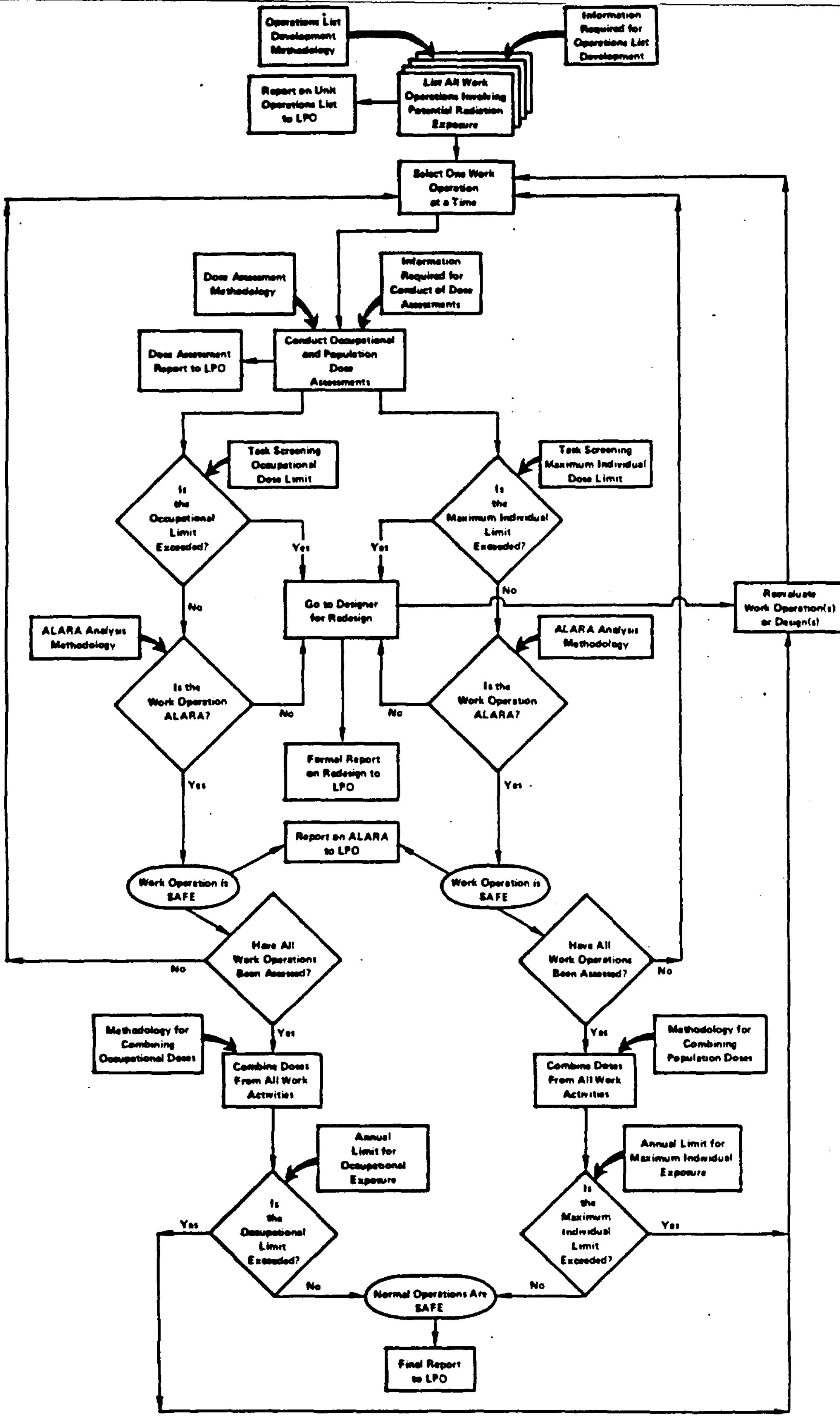


Figure 11-3. Strategy for Radiological Safety Assessment of Normal Operations Including Transportation and Retrievability

LPO denotes the regulatory component of the SRP to workers and to the public resulting from various unit operations will be determined and analyzed individually and collectively. Input data required at various steps in the assessment, methodologies to be utilized in the assessment, and appropriate limits will be specified explicitly. Mitigative feedback loops are provided for work operations found to be initially unacceptable.

11.1.1 Preparation of Unit Operations List

The first step in the safety assessment of normal operations will be the identification and classification of all operations into unit operations (UO) involving a potential hazard. When complete, this list should be documented by the facility design engineers in a report which describes each operation in detail and justifies its completeness.

The actual preparation of the unit operations list will be accomplished by means of a design review of operational procedures (including transportation, retrievability, and decommissioning operations) involving radiation or radioactivity. The documents required for this review are:

(1) Detailed facility design reports and operation procedures, primarily to aid in the preparation of the unit operations list for the operational phase

(2) Detailed retrievability operation report to supplement the design reports in preparing the unit operations list for the retrievability phase

(3) Detailed decommissioning report to supplement the design report in preparing a unit operations list for decommissioning activities.

The unit operations list so prepared should be of sufficient detail to permit an account of (1) all waste material transfers from receipt of the waste at the shippers facility to final emplacement, and (2) all other tasks recognized as involving radiation or radioactivity.

Each unit operation must have distinct boundary conditions; that is, each unit operation must have a unique radiological condition, a specific population or number of workers involved, a defined duration, and a defined physical boundary. This means that, at a minimum, a separate task must be identified and described every time there is a change in the number of workers involved or whenever the radiological conditions surrounding an operation vary. Most often, however, addition of a new task to the UO list will be considered necessary if the nature of the work at hand changes recognizably. Examples of a few unit operations are given in Table 11-1 and Figure 11-4.

11.1.2 Conducting Dose Assessments

The next step in safety assessment, following completion of the list of unit operations, will be to evaluate each UO and to conduct dose assessments for doses both to repository personnel and to the public.

The potential radiological hazards to repository personnel from normal operations are: (1) the presence of large quantities of radiation or radioactivity, and (2) work operations requiring long residence times in proximity to radiation sources. On the other hand, the potential public risk from normal operations generally is associated with (1) the accumulation of radionuclides continually released from the facility at low levels, and (2) recurring exposure to low-level radiation fields associated with transportation of waste. Dose assessments for these cases are described below.

11.1.2.1 Assessment of Doses to Workers

As stated previously, most occupational exposures during normal operations are external exposure from radiation fields. Internal exposures will be precluded in normal operations by measures such as the use of protective clothing and respiratory protection equipment. The methodology for the assessment of occupational exposures from normal operations for each UO is based on the quantification and multiplication of (1) the number (and classification) of workers involved in each task, (2) the duration of each task, and (3) the radiological conditions associated with each task. The total exposure is determined by forming the product of these three terms. Each is discussed below in greater detail.

Number and Classification of Workers. The first step in assessment of external occupational exposures will be the determination of the number and classifications of workers involved in a given UO. Experience has shown that facility construction and maintenance estimators can usually provide excellent

Table 11-1 Expected Exposure During Routine Canister Handling and Storage Operations

Operation Number and Source Locations	Personnel Location	Operation Performed
(1) Yard	Around shipping cask	Inspect and document cask on arrival
(2) Cask receiving and preparation area	Around shipping cask	Prepare cask for unloading washdown, and sampling
(3) Cask unloading area	Around shipping cask	Attach and seal cask to hot cell floor
(4) Canister transfer cell	Operating gallery	Remove floor plugs and cask cover and move canisters to holding station
(5) Transfer cask loading and transfer area	Around transfer cask	Move canister from holding station to transfer cask and to shaft-loading station
(6) - (7) - (8) Top and bottom of shaft	Around transfer cask	Load and unload waste cage at top and bottom of shaft and load transporter
(9) - (10) Mine level	In transporter cab	Transport cask to storage area, locate hole and spot transporter
(11) - (12) Mine level	Mostly in the cab but sometimes around cask	Remove plug, lower canister, replace plug

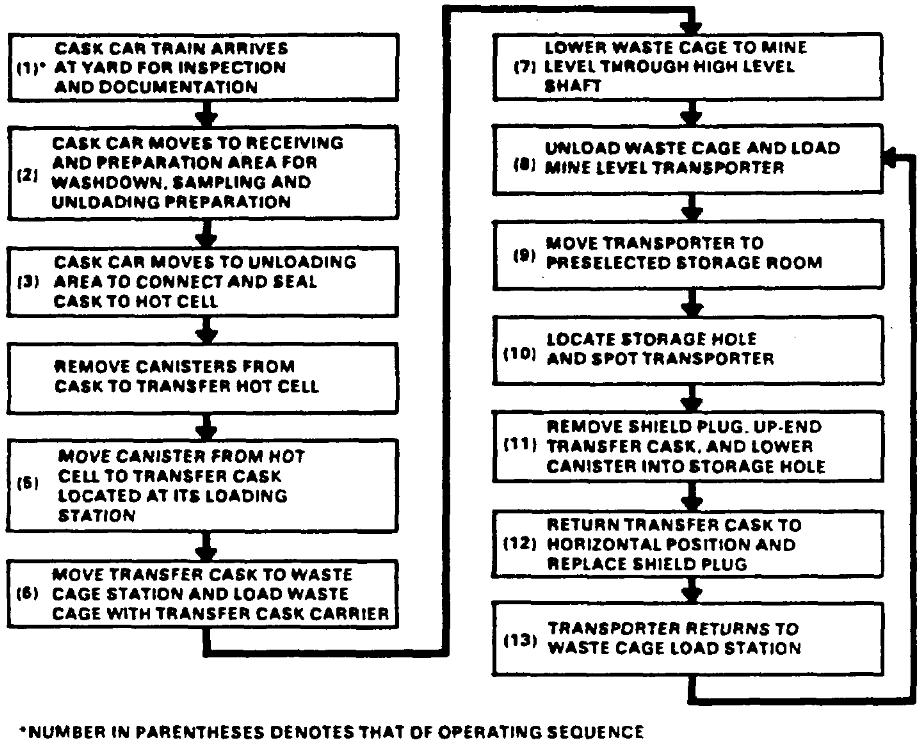


Figure 11-4. Simplified Canister Handling Sequence Diagram

predictions of these types of data. Some preliminary information for a repository is already available, but precise estimates will have to await more detailed designs. The recommended worker classification system is exemplified in the Stearns-Roger Engineering Company (1978) Conceptual Design Report, where repository personnel are classified into five worker categories, and one category, the operators, is classified into three subcategories, as follows:

(1) Operators
  - o Canistered waste
  - o Radwaste
  - o Low-level waste

(2) Maintenance and testing

(3) Health physics and chemistry

(4) Mining personnel

(5) Office personnel and security.

The complete description of each UO will require a determination of the number of workers, by worker classification, involved in the task. This will enable high-exposure groups to be identified and mitigative measures to be instituted at the earliest possible stage of facility planning.

Duration of Tasks. Like the estimates of number and classification of workers involved in various UOs, the duration of tasks must also be defined so that occupational doses can be calculated. Again, facility construction and maintenance estimators are the best sources for this information. Estimates of the duration of tasks will be based on information about qualifications and efficiency of workers. Lacking specific information on personnel training and qualifications, minimum requirements as reflected in 10 CFR 60 are assumed to be applicable. Determination of task duration will become better developed as specific plans become available from the Repository Task before a preliminary safety analysis report is prepared.

Radiological Conditions. The last parameter involved in dose calculations is the definition of radiological conditions for each UO. The intensity of radiation fields can be calculated from a knowledge of the types and quantities of radioactive materials present in various areas of the repository. Preliminary estimates of radiological conditions derived from quantities of radioactive materials, the geometry of the source and facility in which the materials are found, and the required shielding thicknesses are available in the Kaiser Engineers (1978) and Stearns-Roger Engineering Company (1978) Conceptual Design Reports. Updates and refinements may be necessary as designs and operational characteristics become more precisely defined.

Quantification of radiological conditions will be based on measurements under similar conditions in existing nuclear facilities where possible. Where this is not possible, the radionuclide mix should be calculated using the same fuel histories as were used in the "Reference Repository Conditions" documents, combined with application of the ORIGEN-2 computer code.

To make calculations possible, complex source configurations, as will occur in a repository, are simplified to point, area, or volume sources, or combinations thereof. The shielding, which is indicated in the facility or package design, must also be considered in the analyses of sources. Procedures for these analyses have been computer coded in the ISOSHLD code. This code is designed to calculate dose rates from any radiation source/shield/location combination. Example output parameters determined by this code are as follows:

- Nuclide mix
- Quantity of radioactivity
- Source geometry
- Shielding material(s)
- Shielding thickness
- Geometry of shield
- Distance from source to potential recipient.

Radiological Dose Assessment. The radiological conditions surrounding each UO discussed earlier are given in terms of expected maximum dose rate (mrem/hr). The total occupational exposure is determined by multiplying the number of workers involved in a task by the duration of the task and by the accompanying dose rate.

11.1.2.2 Assessment of Doses to Public

The methodology for the assessment of the potential for public exposure to radiation is based on an evaluation of the release of effluent materials from the repository during a given unit operation, and possible external exposures during transportation of radioactive wastes.

The effluents released routinely may be particulates, gases, or liquids; their quantities can be determined from operational aspects of the repository such as throughput rate. Following the identification of source terms, the critical pathways will be analyzed (as indicated below) to evaluate the proportion of the source terms which reaches a maximum individual exposure limit, and the radiological dose consequences will then be calculated. Figure 11-5 lists the general outline for performance assessment of environmental exposure from normal operations.

The data and information categories required for making a population exposure assessment are detailed in U.S. NRC (1977a) Regulatory Guide 1.109. This guide is designed to address any combination of environmental transport/biological uptake/radiological dosimetry. Examples of the parameters included in this guide are:

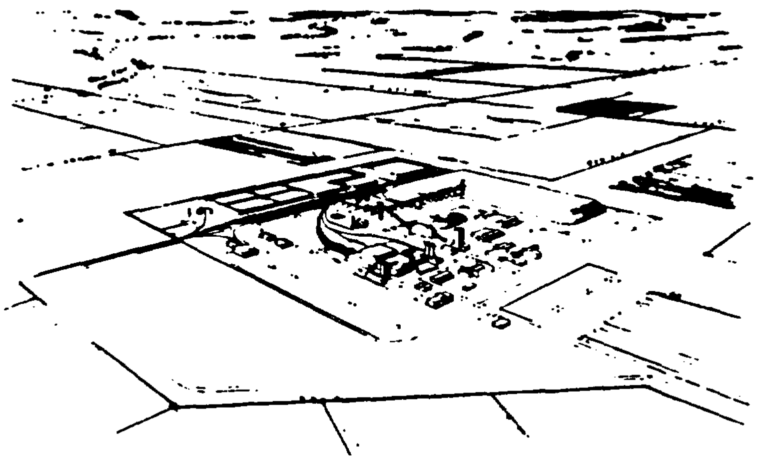
(1) Environmental transport
- o Meteorology
- o Radiological source release height
- o Duration of release

(2) Biological uptake
- o Concentration factors
- o Population consumption factors
- o Environmental characterization

(3) Dosimetry
- o Radionuclide physiology
- o Radiological charcteristics of source
- o Demography.

The assessment of transportation-related public exposure will be made on the basis of maximum dose rates allowed by U.S. Department of Transportation (1978) regulations (49 CFR). The methodology for assessing transportation-related exposures is given in NUREG-0170 (NRC, 1977b).

Critical Pathways. The methodology for identifying critical pathways includes consideration of (1) the pathways by which airborne and liquid radioactive effluents may be transported to individual receptors, (2) the location of these receptors, and (3) the maximum individual and population dose commitments within an 80-kilometer radius of the repository. The safety



Site Appearance During Normal Operations

Computer Codes

- PABLM
- DACRIN

Input Data

- Detailed Task List and Descriptions
- Source-Terms for Each Task
- Site Environmental and Demographic Characterization
- Task Screening Population Dose Limit
- ALARA Analysis Criteria
- Annual Limit for Environmental Exposures

Output

- Quantified Performance Assessment
- Determination of Level of Environmental Safety

Figure 11-5. Environmental Radiological Exposures Under Normal Operations assessment will include a determination of quantitative information on the production of major types of foods within 80 kilometers of the repository and the expected consumption of these foods by the projected population in the area during the operational life of the facility.

Radiological Dose Consequences. The radiological dose consequences are based on the quantities of radionuclides released to the environment and available for exposure of the public. A calculation of both the annual dose and the 50-year dose commitment will be made. The appropriate equations and models are available for all nuclides of interest. Codes reflecting ICRP-30 recommendations will be used. ICRP-30 (ICRP, 1978) contains specific physiological and radiological models for important human-organ systems. These include the respiratory, gastrointestinal, and skeletal systems. Recommendations on submersion in a radioactive cloud are also contained in ICRP-30. The data requirements necessary for input to the models for most radionuclides of interest are also tabulated in ICRP-30.

Many dose calculation codes exist for submersion, ingestion, or inhalation pathways. Because of their previous use in NRC-sponsored calculations and their proven applicability to the types of calculations anticipated to be needed for repositories, PABLM and DACRIN have been selected for use by the SRP. PABLM was selected to handle atmospheric releases to food pathways; DACRIN was selected for use in submersion and inhalation exposure calculations.

Once the occupational and public doses have been calculated for one iteration of each unit operation, they must be multiplied by the number of iterations per year before they can be compared with the appropriate limits which are given in terms of annual exposures.

These dose-assessment results, for both occupational and public exposure, will be documented in a report to support licensing efforts. This report will include complete and accurate specification of (1) all assumptions used in the calculations, (2) all information developed since preparation of the unit operations report, (3) dose models used, and (4) results. Input data drawn from standard sources or previous reports, such as detailed unit operations descriptions, nuclide mix, nuclide characteristics, reference environment, and population distribution and characteristics, will be referenced.

11.1.3 Development of Preventive and Mitigative Measures

As indicated in Figure 11-3, the results of each dose assessment will be screened for acceptability on the basis of radiological dose limits and ALARA (as low as reasonably achievable) concepts before being combined and compared with existing annual dose limits. These analyses of each unit operation will be used as the trigger mechanism for incorporation of necessary mitigative measures. In light of recent EPA occupational exposure-limit recommendations and the likely involvement of a single worker in several work operations, it is deemed prudent to compare calculated doses with a 0.3 rem/year or lower limit per unit operation, depending upon the detailed employee utilization plans of a particular project. For the maximum individual dose comparison which will be used to indicate public-exposure-limit conformance, EPA recommendations related to the nuclear fuel cycle indicate that a 25 mrem/yr whole body limit is appropriate for such comparison.

Should the appropriate limit be exceeded for any unit operation for either maximum individual exposure or occupational exposure, the operation must be referred to the facility or operation designer for redesign of the system components involved or reevaluation of the operation or other mitigative measures. The person making the radiological performance/dose limits comparison will be responsible for identifying the most logical means by which a dose reduction can be achieved. The two most appropriate alternatives are anticipated to be engineering and procedural modifications. Examples of specific modifications that might be required within each of these two categories are:

(1) Engineering
- Change in shielding thickness
- Change in radiological inventory involved during work operation
- Change in engineering layout of work operations
- Further mechanization of task

(2) Procedural
- Change of position of worker relative to source
- Streamline of procedure for executing task
- Increase in aptitude or skill qualifications of workers to be involved with task.

This process will be iterated until design and execution of the operation can be accomplished within the specified limits. This redesign and reevaluation activity will be documented in a formal report which covers the comparison of the results with limits, the identification and evaluation of mitigative alternatives, and the selection and impact of the preferred mitigative measure.

11.1.4 ALARA and Compliance With Limits

Should the 0.3 rem/year or lower limit recommended in Section 11.1.3 not be exceeded in the execution of a particular unit operation, that unit operation may be considered to have passed that phase of the screening process and therefore may progress in the assessment strategy to comparison with the ALARA concept. This will be done by conducting a modified or full-scale cost/benefit analysis on the basis of $1,000/person-rem. The details of this analysis are discussed in a report by R. L. Kathren (1980). This process should be documented in a formal report. Should the unit operation be in compliance with the ALARA concept in the context of both occupational and public exposures, the unit operation will be defined as safe, and the next work operation will be selected for the dose assessment process until all unit operations have been considered individually. If not compatible with ALARA, the same reevaluation procedures as described for "limit comparison" must be followed.

11.1.4.1 Combined Doses

As indicated in Figure 11-3, following the evaluation of each unit operation individually, the overall operation of the repository will be analyzed as a system. This will be accomplished by combining doses. Doses calculated for the complete list of unit operations will be combined for both occupational and public exposures. Where different critical organs have been identified as being at risk for different unit operations, the summation should be done as recommended in ICRP 26 and 30 (ICRP, 1977; ICRP, 1978), with weighting factors as advocated in EPA recommendations where there are EPA/ICRP conflicts.

Once the appropriate doses have been combined, the result should adequately reflect the annual doses that will arise from one year of repository operation. Where activities may be completely different from one year to the next, as would be expected for the construction/operation, operation/decommissioning, and possible operation/retrieval interfaces, selective combinations of unit operations which reflect the actual anticipated situation will be used for comparison with the limits. Where different worker categories are involved, the maximum individual dose within a work category should be used in this comparison.

11.1.4.2 Comparison of Combined Doses With Limits

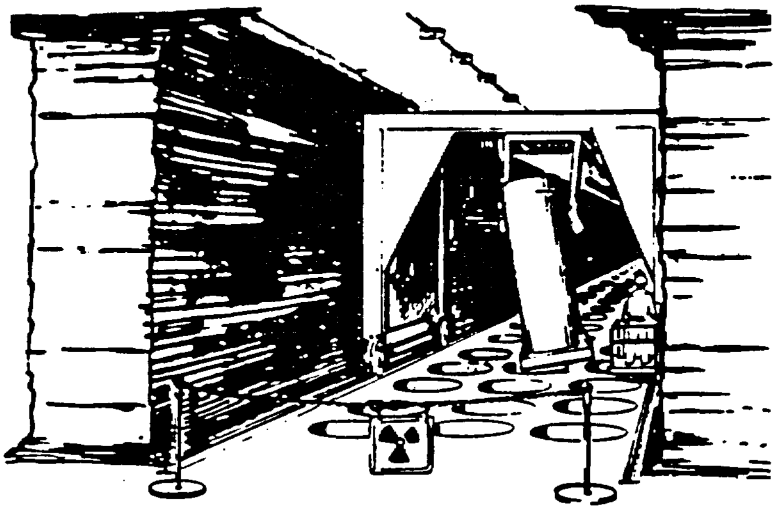
The appropriate limits for the comparison of annual system operation doses are 3 rem/yr for occupationally exposed individuals and 25 mrem/yr for average exposed individuals in the population. Should these limits be exceeded, the complete work package will be reevaluated on the basis of equipment and/or operation design, and appropriate modifications will be made to reduce cumulative doses to levels below the limits. Once this has been accomplished, the facility and its operations under normal conditions are defined as safe.

All assessment activities since the preparation of the ALARA comparison report will be documented in a formal report. In addition to presenting the final results of the assessment of normal operations, the report should summarize the highlights of the previously identified intermediate-step reports. In this way, the final report can be utilized to convey the highlights and final results of the total assessment, with intermediate-step reports being used as backup documentation.

11.2 SAFETY ASSESSMENT FOR ACCIDENTAL CONDITIONS

Figure 11-6 is the general outline for performance assessment of occupational exposures from accidents. The strategy for assessing the safety of accidental conditions is illustrated in Figure 11-7. The components of this strategy include: (1) identifying credible events which might initiate accidental conditions, (2) developing detailed scenarios for each event, (3) evaluating the consequences of each selected event scenario, and (4) examining in detail preventive or mitigative measures which will reduce the consequences or occurrence probability of each event.

Three event lists will be required: one for accidental events which are induced within the facilities, one for events related to transportation activities, and one for externally induced events. The intent of this division of discussion is to differentiate between events with consequences



Potential "Off Normal" Operations Condition

Computer Codes

- Internal and External Dose Models (See Tables 7-2 and 7-3)

Input Data

- Detailed Events Lists
- Detailed Events Scenarios
- Applicable ICRP Dose Assessment Models and Factors
- Event Screening Occupational Dose Limit

Assessment Output

- Quantified Performance Assessment
- Determination of Level of Occupational Safety

Figure 11-6. Occupational Radiological Exposures From Accidents

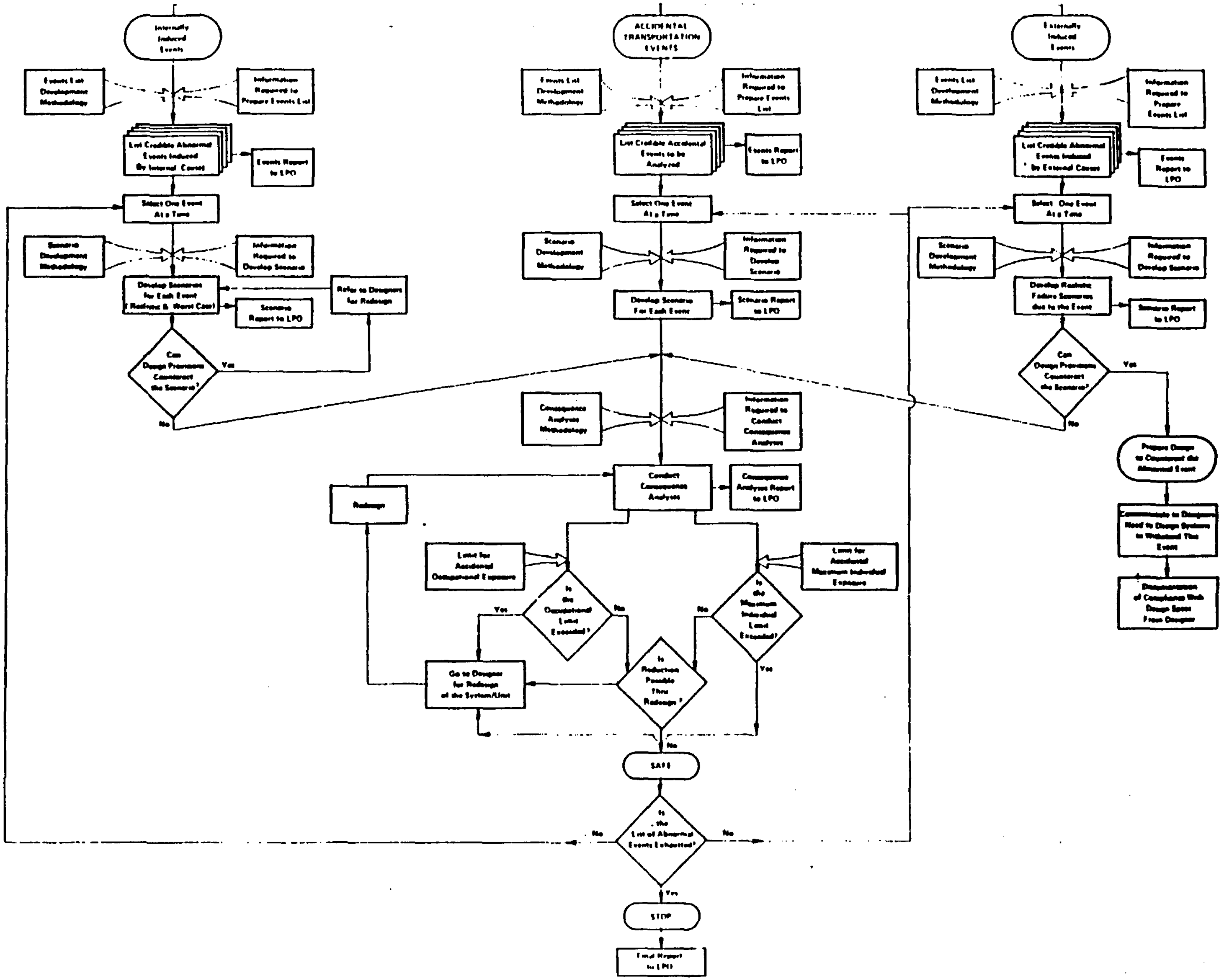


Figure 11-7.Strategy for Safety Assessment of Accidental Conditions (Preclosure)

affecting limited portions of the repository facilities (internally induced events such as mechanical failures and human error), events which may affect all or major portions of the repository (externally induced events such as natural phenomena), and those events which may not even occur at the repository site (related to transportation activities). These scenarios will be selected so that they span the range of potential consequences and occurrence probabilities, address all potential initiating mechanisms, and affect all components of the waste management and transportation systems. As indicated in Figure 11-7 doses to both workers and the public resulting from various accident scenarios will be determined and analyzed both individually and collectively. The results of the consequence analyses will be put in perspective by comparing the predicted performance with recommended radiological limits.

The input data required at various steps in the assessment, methodologies to be utilized in the assessment, and the appropriate limits will be specified explicitly. Mitigative feedback loops will be provided for redesign evaluation. Except for rare instances where the occurrence probabilities may indicate that it is inappropriate to do so, each event/scenario combination will be proven safe independently. That is, since every conceivable event consequence combination need not be analyzed completely, the summation of the annual doses from all events is meaningless and not necessary.

11.2.1 Preparation of Credible Events Lists

All postulated abnormal (internal, external, and transportation-induced) occurrences and accidents in the repository shall be listed and classified by type and by category of probability, indicating those that are not credible because of their low probability. Only credible occurrences and accidents will be analyzed, and only limiting events need be discussed in detail, but the selection of events will be justified on the basis that the scope and depth requirements of the completed lists are met; accidents and occurrences with a low probability and high consequence will be analyzed as well as those with high probability and low consequence. Evidence will be presented that no credible abnormal occurrences and accidents were omitted from consideration.

The approach outlined here is intended to:

(1) Ensure that a sufficiently broad spectrum of occurrences, accidents, and initiating events has been considered

(2) Categorize the initiating events by type and expected frequency so that only the limiting cases in each group need to be quantitatively analyzed.

To accomplish these goals, a number of malfunctions or failures of equipment, operator error, and intrusions by outside forces will be postulated. The postulated occurrences or accidents will be assigned to one of the types listed in Table 11-2.

Where appropriate and necessary, analyses will support the predictions of frequency, consequence, and risks resulting from abnormal occurrences and accidents. As indicated in Table 11-2, the Internally Induced List focuses on events such as mechanical failures and human-induced types of events. Identification of these types of events will be best made by close examination of comprehensive descriptions of facilities and related operations. Typical descriptions are to be found in the, Conceptual Design Reports (Kaiser Ergineers, 1978; Stearns-Roger Engineering Company, 1978), CRRD (Bechtel Group, Inc., 1981), and SARs (DOE, 1980a) for other similar facilities. The format and content of this list is indicated in the WIPP SAR outline (DOE, 1980a). This list should be documented in a report which describes each event in detail and justifies its completeness.

The events listed for external and transportation-induced accidents will tend to be much less facility-dependent than the internally induced events. Therefore, completeness of the external and transportation-induced events lists will be judged on the basis of comparison with accidents analyzed in SARs for power reactors and other major nuclear facilities as well as existing analyses of waste repositories.

Specific information for analyzing accidents in the retrieval or decommissioning phases of repository life are to be made available in formal reports on strategies for completing these operations. These reports will be used when they become available.

11.2.2 Scenario Development

Once a complete list of credible initiating events has been compiled, one event at a time will be selected for scenario development as indicated in

Table 11-2. Types of Accidents or Abnormal Occurrences to be Considered in the Operational Phase Accident Analysis

Internally Induced

- Explosion
- Fire
- Criticality
- Breaching of air locks
- Undetected or mishandled leaking fuel assembly
- Undetected "fresh" fuel assembly
- Events involving bare fuel in baskets
- Damage in weld-and-test cell (fuel assembly or canister)
- Events involving the transfer cask on the surface
- Events involving the waste shaft
- Events involving the underground transporter
- Failure of underground repository and surface ventilation systems
- Failure of pool cooling/cleanup system or liquid radwaste system
- Failure in gaseous radwaste system

Natural and Induced

- Earthquake
- Tornado
- Aircraft crash into surface facilities
- Flood
- Other severe natural phenomena

Transportation

- Traffic accident involving high-level waste shipment
- Waste transport cask fire
- Transportation cask malfunction

Figure 11-7. The event or sequence of events leading to the initiation of the accident will be described and a sufficiently detailed scenario to describe the accident uniquely will be developed. If necessary for complicated sequences, detailed event-tree analysis may be used to identify causes for internally induced events related to human error, equipment malfunction, or equipment failure. The following information will be included in all scenario developments:

(1) Starting conditions and assumptions, including the maximum number of fuel assemblies that can be affected by the occurrence, the postulated release fractions and transport pathways, mitigating devices and their operation, and frequency with which the operation is performed

(2) A step-by-step sequence of the cause of each accident, identifying all protection systems required to function at each step

(3) Any corrective actions necessary.

In summary, enough information will be provided to permit an independent evaluation of the adequacy of systems and equipment related to the event under study. Where possible, an appropriate scenario will be developed for each initiating event. The same sequence of activities described here for internally induced events will be employed to develop scenarios for externally induced and transportation-induced accidents as well. This compendium of scenarios will be documented in a report which describes each scenario in detail and justifies the completeness of its contents.

Once the scenarios have been developed, where appropriate, they will be referred to designers for analysis of design alternatives that might prevent or mitigate the consequences of a particular scenario. In the case of natural phenomena, the design bases for a facility at a particular site will be determined and documented by this method.

11.2.3 Consequence Analysis

When the appropriate accident scenarios have been developed and reviewed in the context of redesign, the consequences of scenarios will be analyzed. Historically, several methodologies have been applied to consequence analysis of accidental occurrences. Two methodologies commonly used are (1) the fault-tree approach and (2) the scenario approach. The fault-tree approach requires the availability of detailed design information and is most often focused on a calculation of risk (risk equals consequence multiplied by probability). Therefore, it will be appropriate to use the scenario approach (as previously described) in the repository safety assessment. The scenario approach uses the sequential application of known or postulated characteristics of the facility, site, and radioactive contamination. The sequence in which the characteristics are applied to the analysis is:

- Contaminant release characteristics (source term)
- Contaminant transport characteristics
- Deposition characteristics
- Radiological dose consequence.

11.2.3.1 Contaminant Release Characteristics

Based on the description of the initiating event and the inventory involved, the amount of contaminant released can be calculated. This quantity may be based on percentage of the inventory exposed to the initiating event, on the ability of moving air to keep particulates suspended, or on the rate of contaminant released and the duration of the incident.

These release fractions have been documented in regulatory guides for reactor accidents (NRC, 1972), some of which are applicable to waste repositories. In addition to regulatory guides, additional data are available from research and documented accident assessments for other fuel-cycle facilities (NRC, 1975; DOE, 1980b). These specific types of data are theoretical or laboratory-derived for the most part. It is not expected that estimates of this type will be modified significantly before a preliminary safety analysis report is prepared for a salt repository.

11.2.3.2 Contaminant Transport Characteristics

The result of applying the release fraction in the accident assessment sequence will be an estimate of the quantity of radionuclides available for transport either to the occupationally exposed person or to the public. How the contamination will be transported will depend upon the characteristics of the contaminant and the facility.

Important contaminant characteristics include physical characteristics (solid, liquid, gas), effect of association with an inert matrix, and chemical characteristics. Important facility characteristics include occurrence area air velocities, facility waste stream cleanup capabilities, facility air balance, and facility response to the detection of accident conditions. The mechanism by which the contamination was released (e.g., mechanical dispersion, explosion, or fire) could also have an appreciable effect on transport characteristics.

In the preliminary assessments, the operating characteristics for installed accident detection and response equipment will be consistent with requirements stated in the ERDA Emergency Instrumentation Preparedness Studies (Anderson, et al, 1974, 1976; Battelle Northwest Laboratories, 1971, 1972). This equipment includes area monitors for airborne particulates, radiation fields, or combustion products, and associated control circuitry designed to close or open dampers or otherwise modify ventilation as a result of abnormal area monitor readings. As more detailed designs become available and emergency response instrumentation is specified, the preliminary assumptions will be brought into agreement with the design features.

Enough preliminary design work is available to evaluate the methodology thoroughly and to determine what data needs remain. Reliance on conceptual design reports and the CRRD in the short term is anticipated.

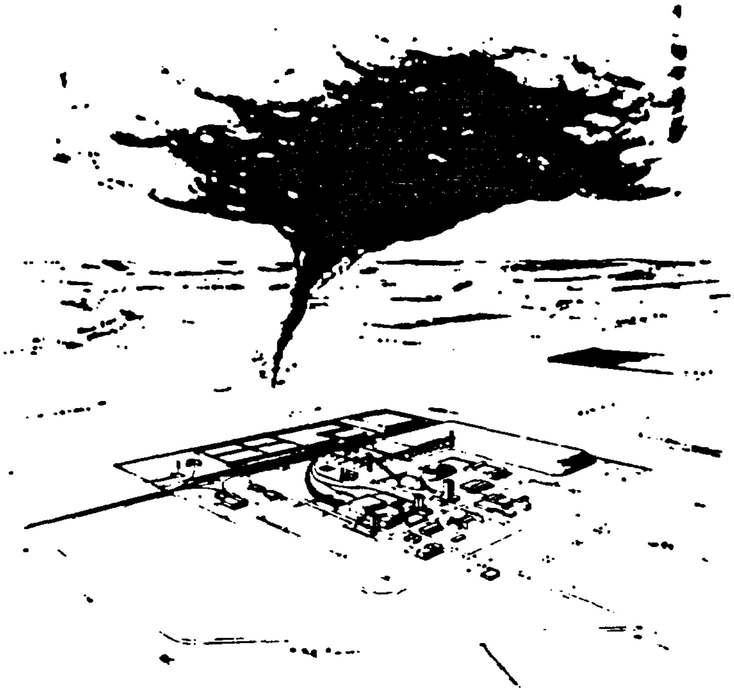
Release directly to the environment will be assessed for transportation accidents. The experimental evaluation of radionuclide releases as related to extraordinary environments (accidentally and intentionally produced) is reflected in two objectives of the Transportation System Safety Evaluation (TSSE) portion of the Transportation Technology Center program. These objectives are: (1) to obtain a data base of measured radiological source-term release from spent LWR fuel systems subjected to extraordinary environments, and (2) to obtain the response of radioactive material shipping systems to both extreme accident conditions and environments created by simulated intentional acts.

The tasks required to meet these objectives of the TSSE program will be divided into two major activities which will influence the schedule of the safety assessment. These activities are: (1) definition of extreme accident environments and (2) definition of intentional act environments. The extreme accident environments study will address the problem of radionuclide releases from radioactive material transportation systems subjected to extreme accident conditions. The tasks of the extreme accident environments study are: (1) an analytical program initially to determine and characterize spent fuel failure mechanisms and (2) an experimental program to determine and verify a radiological source-term data base. The study of the intentional act environments will address the problem of radioactive source term releases from radioactive material shipping systems subjected to a sabotage attack. The tasks of the study of the intentional act environments are: (1) an experimental program to determine package response to a range of credible attack modes; (2) an analytical program to improve and expand the radiological consequence model for handling experimental data; (3) an experimental program to determine and characterize the radiological source-term release from radioactive material shipping systems; and (4) using the data from items (1) and (3) and the improved model from (2), an evaluation of the radiological consequences to the exposed public.

11.2.3.3 Deposition Characteristics

In many analyses, the quantity of radioactive material deposited at any point in the facility or in the environment is treated as an end point. This approach is not appropriate for this assessment; here, the deposition characteristics will be the precursors of dose calculations, and deposition may be applied to occupational and public exposures. This case will include considerations such as personnel exposure time to the contaminant based on anticipated emergency response of employees. For release to the environment, parameters of importance in the determination of deposition include the critical environmental pathways for the nuclides released, the meteorological characteristics of the area, and other environmental characteristics. Figure 11-8 lists the performance assessment related to environmental accidents.

In the preliminary assessments, the operating characteristics of installed occurrence alarms will be consistent with requirements stated in ERDA's Emergency Instrumentation Studies (Anderson, et al, 1974, 1976; Battelle Northwest Laboratories, 1971, 1972). As more detailed designs evolve, these considerations will be further refined. The response of personnel in the area of an occurrence will have to be based on experience in other types of nuclear facilities. Considerations that can affect the assumptions made about personnel response include personnel training and the availability of emergency response plans. Both of these considerations will become better developed before a preliminary safety analysis report is prepared.



Computer Codes

- PABLM
- DACRIN

Input Data

- Detailed Events List
- Detailed Events Scenarios
- Site Environmental and Demographic Characterization
- Event Screening Environmental Dose Limit

Assessment Output

- Quantified Performance Assessment
- Determination of Level of Environmental Safety

Potential "Natural Phenomena" Environmental Accident

Figure 11-8. Environmental Radiological Exposure From Accidents

Because of the importance of site- and facility-specific data to the accident assessment, final input data will be gathered and evaluated when a site is selected. Many environmental transport computer codes exist for aquatic, terrestrial, and atmospheric pathways. Some have been widely used and have achieved a measure of acceptance. Documentation of these codes, regulatory guides, and code comparison reviews (Strenge et al, 1976; Hoffman et al, 1977; NRC, 1977b; Soldat et al, 1974) will be consulted during the preliminary assessments to help in the selection of the codes which best suit the needs of the SRP.

11.2.3.4 Radiological Dose Consequences

Computer programs for calculating radiological dose consequences to the public were described previously and will not be reiterated here. Several major differences in the application of these programs to accidents versus normal operation warrant discussion.

Because of the much shorter duration of the release during accidental conditions, the important exposure modes are those which have little or no time delay. That is, complex environmental pathways do not have time to operate because of the delays involved in the many compartment-to-compartment transfers. Therefore, the important pathways are those such as submersion in a contaminated cloud or acute inhalation exposures. Worst-case meteorology must be used because annual average values are not conservative enough for this type of evaluation. The similarity of these exposures to occupational exposures makes it possible to use the same assessment methodologies as those which have been previously discussed for personnel exposure assessments.

These consequence analyses results, for both occupational and public exposures, will be documented in a report, as indicated in Figure 11-3. This report will include complete and accurate specifications of (1) all assumptions used in the calculations, (2) all information developed since preparation of the events list report, (3) dose models used, and (4) results. Input data available in the open literature will be referenced so that each result can be duplicated by an independent analyst.

11.2.4 Development of Preventive and Mitigative Measures

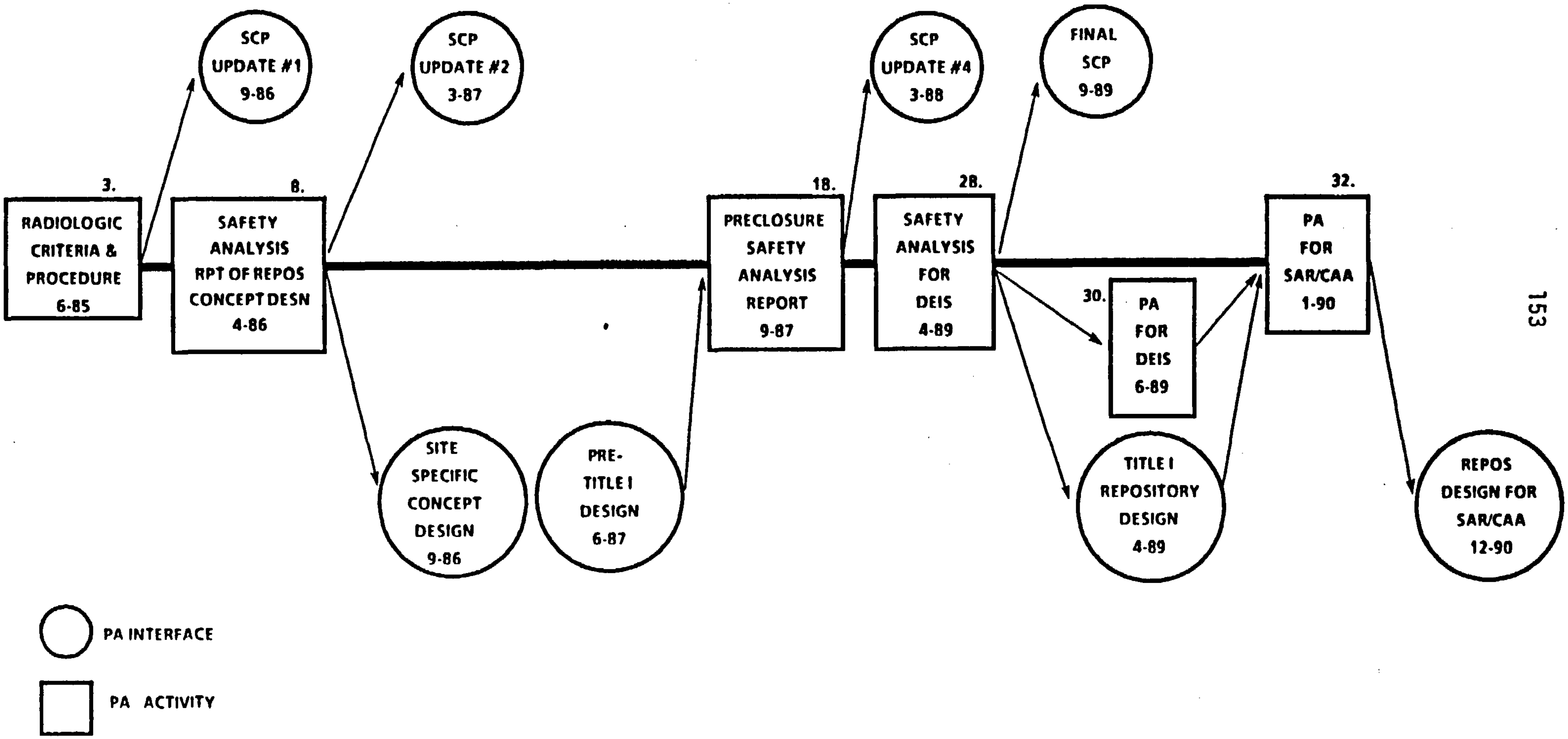
Even though no accepted standards exist for accidental doses to workers or the public, comparisons of the consequence analyses results and reasonable limits will be necessary to trigger necessary redesign mechanisms. It is thought that until more definitive guidance is available a 25 rem dose commitment limit should be used for occupational exposures from accidents and a 2.5 rem dose commitment limit for maximum exposure of a public individual.

Should the appropriate limit be exceeded for any scenarios for either occupational or public exposures, the scenario/systems description of the accident will be referred to the facility designer for redesign of the system components involved or reevaluation of mitigative measures originally incorporated into the scenario as indicated in Figure 11-7. This process is iterated until the systems design and mitigation of the accident consequences can be brought within the specified limits. Should the accident consequences be within the specified limits and not be amenable to further reduction in a cost-effective way, the facility or transportation operation will be defined as safe vis-a-vis that accident scenario; the next accident scenario will then be subjected to a consequence analysis, and this will continue until all selected event/scenario combinations have been analyzed.

All assessment activities since the preparation of the consequence assessment report will be documented in a formal report. In addition to presenting the final results of the analysis of accident conditions, this report will summarize the highlights of the previously identified intermediate reports. In this way, the final report can be utilized to convey the highlights and final results of the total assessment, with intermediate reports being used as backup documentation.

11.3 MILESTONES

To emphasize its relationship to this chapter, Figure 1-8 is repeated here as Figure 11-9. Its place in the SRP program is described in Section 1.4.



Figures 1-8 and 11.9. Preclosure Performance Assessment Logic
(Completion Milestones)

12 ANALYSIS CREDIBILITY

This chapter describes the activities undertaken to enhance the credibility of performance assessments within the Salt Repository Project. Included in this discussion are code documentation, and code testing using analytical solutions and benchmark problems. All of these activities are accompanied by appropriate technical and peer reviews, and are designed to meet NRC requirements. The total process employed to enhance credibility of analyses done using computer codes is termed 'validation and verification' (V&V). Validation is defined in 10 CFR 60 (NRC, 1983) as: "assurance that a model as embodied in a computer code is a correct representation of the process or sytem for which it is intended." Verification provides: "assurance that a computer code correctly performs the operations specified in a numerical model" (NRC, 1983).

The primary emphasis of verification and validation of the performance assessment technology is the identification of activities which determine that the computer code and data base used in performance assessment are an adequate representation of the physical system. The V&V of mathematical models is needed to provide acceptance in scientific and engineering communities. The documented and reviewed analytical solution and the salt site-specific benchmark problems will provide systematic testing of the computer codes. The verification and validation activities will be documented to provide a sequential, traceable, and auditable process for licensing acceptability.

This chapter defines and describes the current status and plan of activities required to verify and validate the mathematical models and computer codes used in SRP performance assessments. V&V activities, through software development, testing, and application will enhance the quality (appropriate accuracy and precision) and confidence in the codes and their results.

To achieve these overall objectives, this plan addresses the following:

1. Documentation of mathematical models used in performance assessment, their current verification and validation status, and the level of their acceptance by the scientific and engineering communities.
2. Verification with analytical solutions of idealized problems which have been or are proposed to be used for verification of different options provided in the computer codes.

3. Verification with salt site-specific benchmark problems which will provide means for verifying the performance assessment computer codes over the expected site-specific parameter ranges.
4. Documentation of the current V&V status of the codes selected or considered for performance assessment.
5. Preliminary reviews of the selected codes and details of V&V activities for individual codes.
6. V&V activities identified by the above procedures.
7. Baselining of the computer codes and the appropriate data base
8. Validation of the performance assessment technology with site specific data collected during site characterization, as well as appropriate laboratory tests and possible natural analogs.

At this stage, no standard formats are proposed for the V&V documents to be developed for specific codes and models. Testing, verification, and validation of software are difficult tasks which must be tailored to each individual model. The proposed verification and validation activities include various major components which must be considered, viz., mathematical models, analytical solutions and benchmark problems for code testing, appropriate data bases, current V&V status of each code and implementation of additional activities, and site specific validations. In addition to the above, independent peer review, wide distribution of documents, and repeated applications of salt geologic repository system assessments will assure the technical quality of the analyses and will meet the regulatory requirements.

12.1 DOCUMENTATION OF CODES

All performance assessment codes must be completely documented. Documentation requirements are given by the NRC in NUREG-0856 (Silling, 1983). This documentation includes descriptions of the mathematical and numerical models, user's manual for the codes, accounts of verification and validation tests performed, and information and listings for revisions as they occur after code acceptance. This documentation will be prepared according to procedures officially adopted as part of SRP quality assurance. Revisions to codes will be documented as well.

12.2 VALIDATION AND VERIFICATION DURING CODE DEVELOPMENT

V&V activities are performed at different stages of code development. To illustrate the role of these activities, the overview in this chapter includes V&V activities during the definition, development, documentation, and operation stages. A generic software development process is conceptualized in Figure 12.1 with identification of verification and validation at different stages.

Frequently, in scientific and engineering programs, significant effort is put forth to define the requirements and specifications adequately. This effort is associated with derivation of models, definition of key phenomena to be analyzed, identification and assimilation of data, and so forth. These activities are shown in Figure 12.1 as prerequirement analyses.

The software development process involves a sequential set of segmented activities. The identification of errors or problems at each stage of a code is less costly and makes problems easier to solve than during subsequent stages, and it enhances the quality of the code. Also, if a systematic set of activities is followed, it is easier and more cost-effective to correct conceptualization and formulation errors.

As shown in Figure 12.1, the four stages of a given software development process are (1) definition, (2) development, (3) documentation, and (4) operation and maintenance. The V&V activities in each of these stages are briefly described in the following subsections.

12.2.1 Definition Stage

Performance Specification. The definition of code requirements leads to development of the performance specifications for the software. In V&V literature, the term "requirements" is used synonymously with "performance specifications." Both terms (requirements and performance specifications) are used in this report. Performance specifications are a detailed statement of what is expected from a code or a system of integrated codes. The performance specifications verification review includes (1) analyses to be conducted, (2) adequacy of mathematical models and computer codes for the analyses proposed, (3) criteria for mathematical model and computer code acceptance, and (4) input and output parameters.

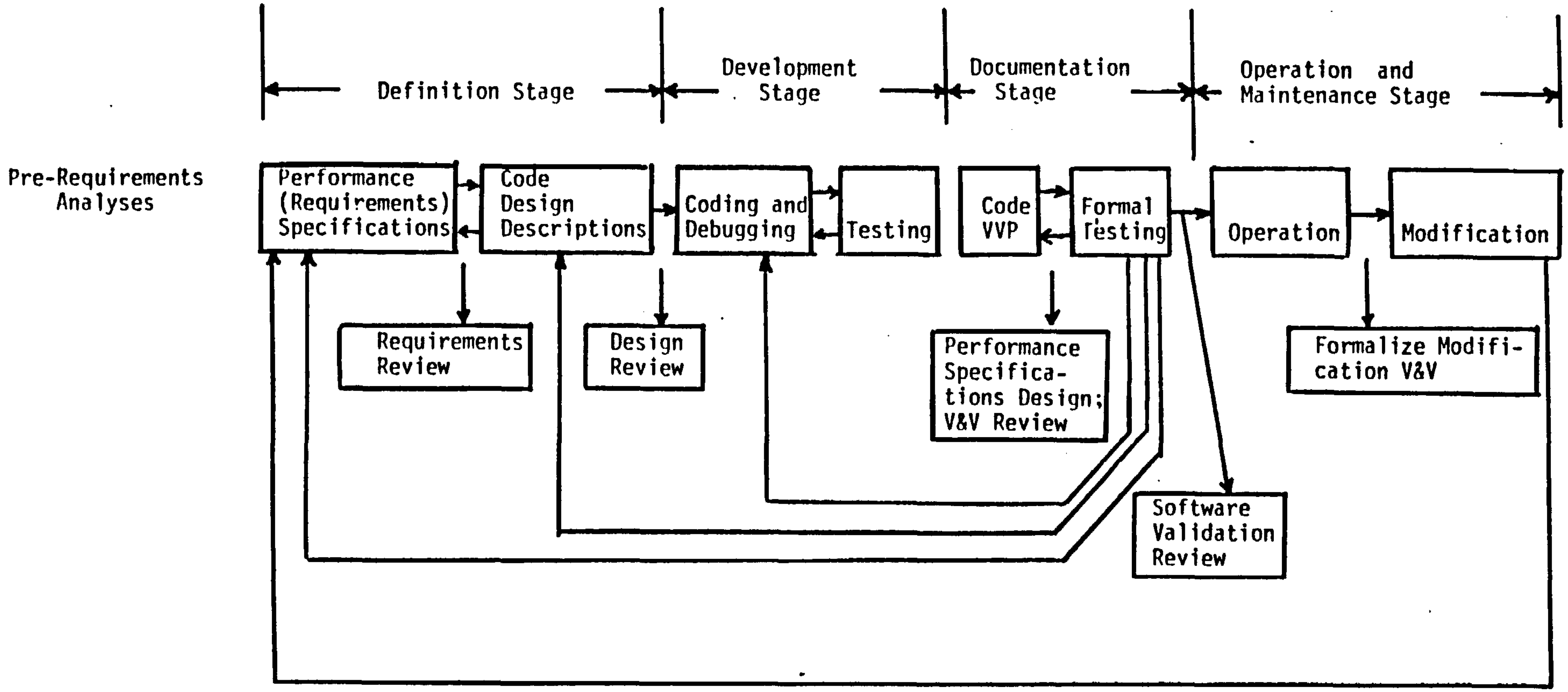


Figure 12.1 Generic Computer Code Stages

The performance specifications review is done to assure completeness; whenever required, a physical description of the system to be modeled will also be included.

Code Design Description. The code design description activity defines the design specifications of a computer program for implementation of the mathematical model or the set of models described in the performance specifications. The design description verification includes review of (1) analytical or numerical techniques for solution of the mathematical equations, (2) structure and organization of the computer program, (3) program storage and handling, (4) program language and coding standards, (5) model/system interfaces including implementation plan, (6) data input/output layout, (7) operating environment, (8) required support software, and (9) input parameter range applicability.

A formal design review prior to initiation of coding is conducted to assure consistency between the proposed design and the performance specifications.

12.2.2 Development Stage

The V&V activities during the development stage are grouped into (1) coding and debugging, and (2) testing.

Coding and Debugging. The development stage consists of converting the code design into a tested, completed computer program (a machine-readable set of instructions). The design decisions made during the coding activity are documented, reviewed, and incorporated into the design documentation.

Debugging consists of using compilers or other automated software tools to process the coding and to check for correct use of the language, interface and variable type correctness, data structures, and so forth, as well as to execute test problems to identify any module interface problems and errors in model implementation. The code documentation includes descriptions of the actual implementation of the design and defines the variables, data, and logic. The V&V activities at the development stage verify the code against the performance specifications and code design documentation.

Testing. Testing during the development stage consists of verification that the program solves the equations it is designed to solve, and that the information obtained from the solution is valid for the physical system being modeled. The testing (using analytical solutions of idealized problems, and site-specific benchmark problems using the expected range of parameters and laboratory/field measurements) conducted during software development is included in the code documentation to describe the test specifications and results. The test specifications include (1) purpose and limitation of each test, (2) criteria for a successful test, (3) applicable equations (e.g., analytical solution), (4) specified test data covering a realistic range, and (5) a demonstration that all elements of the program are exercised. The results show how the criteria are met, what kind of conclusions can be drawn relative to applicability and limitation of the model and the code, and whether any revisions are required in the performance or design specifications. Some of the tools mentioned in the next section are also applicable to the development stage.

12.2.3 Post-Development Stage

The V&V activities of the documented code involve review by the code developer and other persons of the performance specifications, code design, verifications and validations conducted during code development. The review identifies the needs, specifications, tools and other details for V&V within the available resources and develops a detailed check list of activities. The V&V activities of documented codes include manual techniques and automated tools. The manual techniques include inspections, code reading, formal reviews, and walk-through of the source list. The automated tools include static tools (cross-reference generator, data flow analyzer, control structure analyzer, interface checker, physical limits checker, code auditor, comparator, test data generator) and dynamic tools (cause-effect graphing equipment, interactive test aids, execution time estimator, software monitor, statement coverage equipment, and symbolic evaluator). The use of automated tools depends on their availability and on the importance of each code.

The operations and maintenance stage does not require V&V activities, except for baselining the codes and the appropriate data base. During operations or use, however, required modifications are frequently identified. To implement modifications, it is necessary to formalize the process. If the modifications are significant, i.e., require an overall change through modification, deletion, or addition, then they will be implemented as though a new scientific or engineering program were being developed. If the requirements do not need to be changed considerably, then modifications are implemented through procedures that identify only design changes, coding modification, and retesting. The extent of retesting depends upon the extent of the modification. Verification of design and coding changes and validation of the modified part of the program are required, and the new version of the code has to be baselined.

12.3 VALIDATION AND VERIFICATION MANAGEMENT

A well-documented and workable schedule, documentation requirements, management with configuration control, and a quality assurance system have well-delineated roles in the verification and validation of computer codes.

Assignment of responsibility for code development, documentation requirements review, design, coding, testing, verification and validation, code custodianship, quality assurance audits, users documentation, and standards are some of the items to be considered for schedules, documentation, and management of the V&V activities. Depending on the size of the effort and budgetary constraints, the details for a given V&V activity vary significantly. Therefore, this plan will be updated as necessary, which is currently anticipated to be on an annual basis.

12.3.1 Configuration Control

It is imperative to implement a configuration control system that can identify and track completed documentation and software. This system ensures that only authorized changes are implemented and defines responsibility for the official version of the documentation and software. Some of these activities are also referred to as baselining of the computer codes.

All forms and reports completed during V&V activities on a scientific and engineering computer program will be maintained by a code custodian as part of the SRP Configuration Control System (CCS), along with the code and the code documents. The main function of the CCS is to identify and track completed documentation and software. These forms and reports contain such information as the adequacy of models, their range of applicability, the definition of acceptance criteria, analysis of data and logical structures, model implementation, input and output, data requirements, the ability to meet performance requirements, range of model validity, the operating environment, and code documentation verification. Requests for modifications will also be kept by the CCS, stating purpose and scope. The V&V activities which are affected by the modification will be repeated, and required documentation will be completed and maintained by the CCS.

12.3.2 Quality Assurance

The quality assurance (QA) requirements of V&V activities include all efforts needed to assess, enhance, and maintain the quality of the computer codes. This will specify procedures and personnel to perform quality assurance functions, maintenance of QA records, audits, management reviews, and similar activities. This will be done under the SRP QA plan which provides for aggressive implementation of corrective actions as necessary and assures corrective action followup. QA procedures for (1) code documentation, (2) code revision, and (3) code transfer have been placed in effect.

12.3.3 Technical and Peer Review

Technical and peer reviews will enhance technical quality and technical acceptability by the regulatory bodies. In addition to peer review by the SRP, NRC is provided with the code documents for additional independent review and testing of the codes. The code documentation will be published and distributed to the technical community for their evaluation and use. Section 12.4.6 discusses technical and peer review further.

12.4 DETAILS OF VERIFICATION AND VALIDATION ACTIVITIES

An overview of the different stages in code development and associated V&V activities were identified. Most SRP performance assessment codes have been partially verified, documented, and, where possible, validated. In this chapter, brief details of the V&V activities and tools are included.

12.4.1 Performance Specification Review

The performance specifications form the foundation of the computer program to be developed. It is recognized that the quality of software is strongly related to the effort spent to ensure that the requirements are complete, correct, unambiguous, and testable. For scientific and engineering programs, the adequacy of models, the range of applicability, the definition of acceptance criteria, and so forth, are key items to be defined in the specifications. The verification activity constitutes an independent review of the specifications. This review consists of an analysis of each specification as well as its overall correctness and completeness. Performance specification review should cover the following:

1. Analyses to be Conducted. The description of the analyses to be conducted is an integral part of the conceptual design and mathematical model and, therefore, it is reviewed for technical soundness and completeness.
2. Conceptual Design. The conceptual design consists of two parts -- a physical system description, and the process or phenomenon to be modeled. As an example, if the performance specifications define a two-dimensional model, the adequacy of the system description in two dimensions will be reviewed at this stage. If required, scoping analyses will be done at this stage. The conceptual design of the process will involve definition of appropriate processes to be included.
3. Adequacy of Mathematical Model and Equations. The review focuses on appropriateness of the mathematical model and equations for the processes and phenomena to be modeled. Review of the mathematical models proposed for code design are required to ensure that the mathematical equations are adequately adopted from the published literature and generally accepted by the scientific and engineering communities. It may include derivation of differential equations from first principles and scoping analyses to judge the adequacy of the assumptions and simplifications. For some of the processes, empirical equations have to be used. These empirical equations need to be supported using available laboratory and field data. If the empirical equations do not describe the processes completely, the conservatism of the equations has to be established.

4. Criteria for Mathematical Model and Computer Code Acceptance. A criterion or a set of criteria is established that defines how the intended application needs of the model are met.
5. Range of Applicability. Performance specifications identify the anticipated ranges in key parameters for the intended applications and the adequacy of the mathematical formulations over those ranges.
6. Input and Output. The data requirements and output data are clearly stated.

12.4.2 Design Review

Design specifications describe numerical implementation of the performance specifications. The review assures that the code design is a correct representation of the requirements. The design specifications should be technically sound, complete, and practically feasible. Design review is the first step in code verification. The review comments are documented and baselined within the quality assurance system. The configuration control and the quality assurance systems assure that if any deficiencies are found in the design specifications, they are resolved before the computer program coding stage. Design specifications review covers the following:

1. Mathematical Equations. Governing equations are part of the performance specifications, but derivation of the numerical model equations are part of the design specifications. The review of these equations consists of the derivations and and evaluation of the assumptions and simplifications made. This may involve judging the adequacy of finite-difference approximations, finite-element approximations, boundary condition representations, or other simplifications such as decoupling coupled equations or linearizing a nonlinear equation.
2. Numerical Technique. A number of numerical solution methods are available. There is no single method which is the best for all types of equations over all parameter ranges. The most appropriate method is the one that meets computer storage and processing time constraints, minimizes numerical truncation error, and is numerically stable.

3. System Interface. Interrelationships between various models used in performance assessment are defined by scientific considerations. Practical considerations dictate that the complete waste isolation system cannot be adequately modeled by one code. Therefore, the system must be divided into a number of models, and coded independently. Interfacing among various codes must satisfy scientific adequacy considerations described in performance specifications and must be feasible and practical.
4. Input and Output Structure. The code design must provide for entering the code input in an efficient and understandable manner, and provide flexibility to control different levels of printouts. Visual display techniques for input parameters and output results may be used. They assist program users in verification of input data, and make it easier to see relationships between input parameters and results.

12.4.3 Code Design Verification

The purpose of code design verification is to ensure that the program design is a correct representation of the performance specifications and code design. The code design verification is performed to check the:

- o Principal data structures, including physical units
- o Functions, algorithms, or special techniques used for processing
- o Basic program organization including subdivided or modularized as well as internal and external interfaces.

The testing must be performed in an organized and systematic manner (Adrion, Brandstad, and Cherniavsky, 1982). The testing is dated, annotated, and at least the most recent updated test is saved. Testing performed in a random manner is slow and effective. The systematic code design verification will help to produce an adequate and reliable code design verification. A check list to help programmers to organize efforts to test a code or module is developed. The code design verification tests also identify valid functional domain inputs that are not in the domain.

12.4.3.1 Manual Design Verification

The person responsible for design verification must be knowledgeable in the scientific or engineering field for which the software is being reviewed. The reviewer must also have adequate knowledge of software design, development, and testing.

There are a number of review techniques which fall under manual review, such as code reading, round robin reviews, walk-throughs, and inspection. Properly conducted manual reviews provide a very effective verification of code design. The details of manual verifications are described in Section 12.4.6. These activities differ in formalities, participants' roles, and responsibilities according to size and importance of the code being reviewed. Independent manual checks by (persons other than the code designer) are very effective for:

1. Determining completeness and consistency of the code with the design
2. Discerning unreasonable routing using logical switches and inappropriate physical units
3. Examining module interfaces to assure that calling routines provide the information and environment required by called routines and are in the form, formats, and units assumed
4. Examining data structures for inconsistencies and awkwardness
5. Evaluating input/output handling
6. Checking performance specifications to assure that
   - Requirements are satisfied
   - Constraints specified in the requirements have been met
   - The design assumes the same form, format, and units for input and output as stated in the requirements
   - Functions listed in the requirements are included.

For manual checks, the list of alphabetized keywords used in the code (most of the compilers provide alphabetically arranged lists) with brief descriptions are provided by the code developer. Automated structured listings also will be generated to assist in manual design verification.

12.4.3.2 Automated Design Verification

NBS - Special Publication 500-93 (Powell, 1982) lists various automated tools for static and dynamic analysis of code design. Use of specific tools depends on the availability of the tools and the need for the specific code. Most compilers normally have options for assisting in discovering syntax errors and providing information for verification of code design. The SRP has available VAX, IBM, and CDC computers. In addition to common compiler features, each of these widely used systems has unique supportive software to assist in verification of code design. The tools for automated verification are mostly used in the development stage and during debugging. Most of the SRP performance assessment codes are already documented and may need only formal verification. However, depending on need and availability, these additional tools can be used for code design verification.

12.4.4 Verification with Analytical Solutions

Analytical solutions of idealized problems provide means to check that the formulation is coded properly. These solutions also assist in checking the simulative ability after formulation and provide means for sensitivity analyses of grid size and time steps. For numerical solutions, the grid size and time steps used have important effects on round-off errors. For idealized problems, modelers usually adjust the grid size and time steps to match the analytical solution. Along with the "best" matched results, the sensitivity results provide an indication of the effect of grid or time step changes.

For various processes simulated by a computer code, the appropriate analytical solutions are used to check various options provided in the code. The input and output data from such test analyses are saved on a magnetic tape by the code custodian to check the code whenever substantial modifications are implemented.

12.4.5 Verification with Benchmark Problems

Analytical solutions of idealized problems normally provide a limited but confidence-building verification exercise. Site specific problems (size, geometry, parameter and stress ranges) generally need more than the analytical solution capabilities. Comparison of results from two computer codes for a given problem specification is another effective verification activity.

A benchmark problem set is being developed by the SRP using the site specific data and proposed engineering design. The dimensionality, size, range of parameters, and boundary condition stress ranges will be those normally involved in the site performance assessment. Code to code comparison will use this set of problems. After effective code to code comparison, sensitivity analyses will be conducted. The NRC has developed a set of standard benchmark problems (Ross et al, 1982; Wart et al, 1984; Mills et al, 1983) which will also be used as appropriate.

12.4.6 Technical and Peer Review

Technical and peer reviews of a given code provide independent and objective evaluation by the scientific and engineering communities (Powell, 1982). In addition to the review described here, the code documents are provided to NRC for its independent review and testing.

DOE/NWTS-33(1) (DOE, 1982a) identifies review as one of the important aspects of safety assessment processes. Properly conducted, peer review of models is a very cost-effective verification and validation activity. Some models are difficult to validate; for them peer review and acceptance will be the principal means to assure their adequacy for licensing.

The qualitative benefits of peer reviews (Powell, 1982) include:

- Higher visibility
- Decreased debugging time
- Early detection of design and analysis error which would be more costly to correct in later development phases
- Identification of design or code inefficiencies
- Assurance of adherence to standards
- Increased program readability
- Increased user satisfaction
- Communication of new ideas or technology
- Increased maintainability.

For effective review, familiarity with the concept and methodology is required. Peer reviews are most successful when the individual with responsibility for the review is knowledgeable about the process being modeled and its intended results.

Proposed V&V Related Peer Review

As discussed above, peer review has an important role in performance assessment technology development and implementation. The following procedures will be used.

- o The major codes which are used for licensing related performance assessments will be identified.
- o The status report of each of these codes will be prepared.
- o The required material for peer review will be prepared.
- o A detailed check list will be developed.
- o Internal SRP peer reviews of the code will be conducted.
- o For each code, individual peer reviewer(s) will be identified.
- o The internal preliminary pre-review comments will be evaluated and the checklist will be updated before detailed peer review is authorized.
- o The review coordinator and code custodian will complete the documentation of the review process and results.

12.4.7 Site-Specific Validation

Site-specific validation will be used to provide real world comparisons of model predictions with physical measurements wherever possible. While experimental time is short compared to the times over which a repository must be modeled, successfully predicting the results for in situ experiments carried out over several years in the area of the actual repository site will provide a basis for confidence that the models which were based on physical principles are sufficiently accurate for long term predictions. In addition, scale model experiments offer the possibility of scaling time such that a few years of experiment time might be equivalent to hundreds or thousands of years of repository time. For example, in heat transfer, an appropriate experiment would consist of an array of small (1-ft long) resistance heaters with a programmed output, where the size, heat output, and array dimensions are determined by use of Fourier's and Poisson's Laws. Normalized time would be at/L**2, where a is the thermal diffusivity, t is time, and L is the length of the heater sources. Thus, for example, if the experimental heaters and array spacings are made 1/10 the active length of the waste packages and planned repository spacings, one year of experiment time would simulate 100 years of repository time because of the square power of L. Opportunities for similar scaling of other phenomena will be examined.

Specific validations are planned in conjunction with the exploratory shaft. Model validation studies are planned for rock mechanics and thermal studies. In addition, results for near-field permeability studies can be correlated with flow models. Further validation studies, including nuclide transport studies, may be conducted if a salt site is selected for a repository.

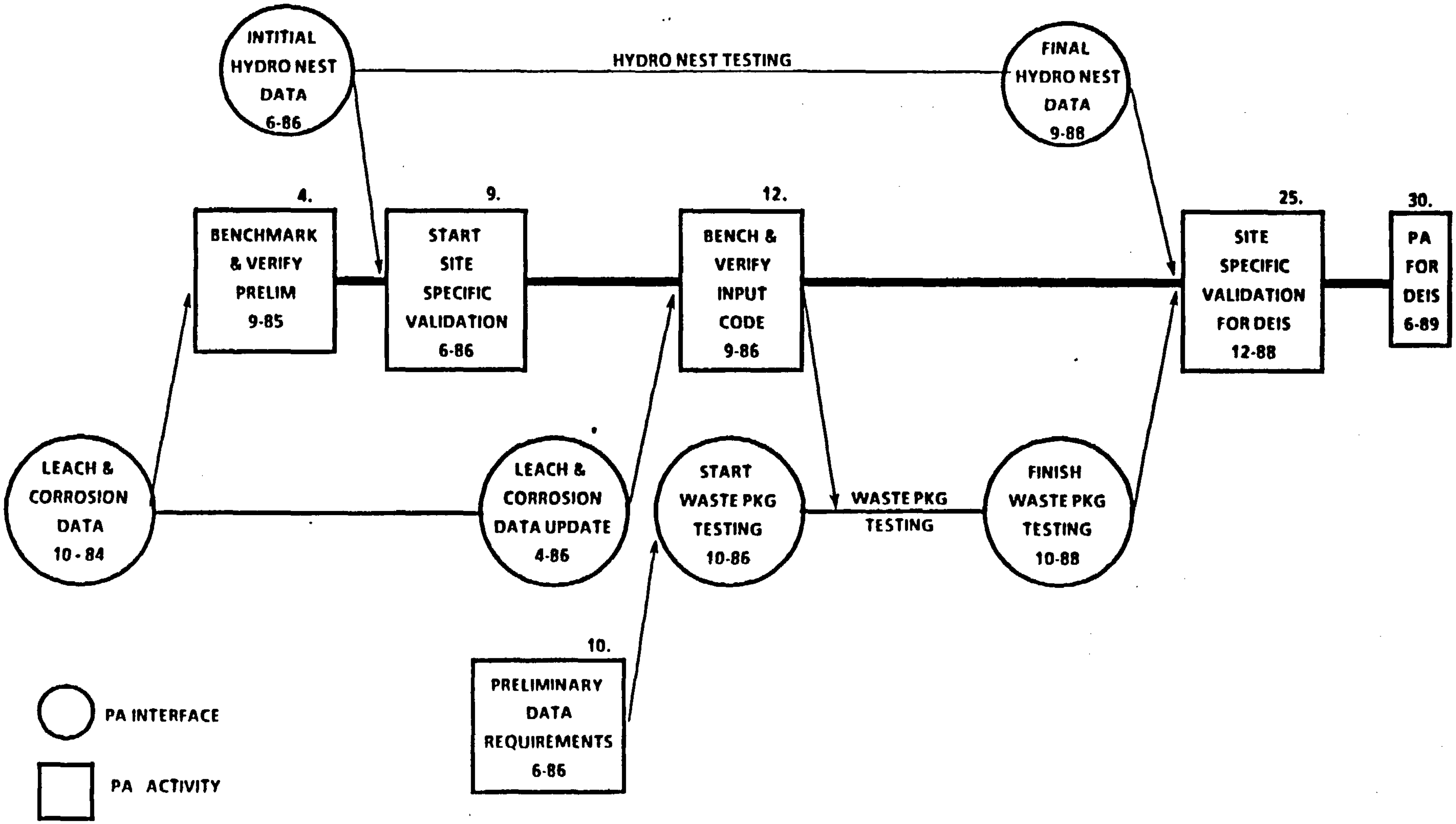
Laboratory studies can also be used for site-specific validation using samples collected from the prime salt site area. These studies can be used to validate nuclide transport models using ground-water and stratigraphic samples from the site area. Flow experiments with tracers of iodine, strontium, cesium, americium, and technetium may be conducted. A priori predictions of sorption and nuclide transport can thus be made and confirmed.

Site specific validation also includes acquisition of appropriate data by laboratory analyses of core and water samples taken from the site area. These analyses include:

1. Ground water characterization
2. Brine analysis
3. Brine inclusion migration
4. Waste form leaching with brine and ground water
5. Corrosion studies with brine and ground water
6. Sorption
7. Characterization of host rock and adjacent formations for:
    a. Thermal properties
    b. Chemical composition
    c. Porosity
    d. Surface area

12.5 MILESTONES

To emphasize its relationship to this chapter, Figure 1-9 is repeated here as Figure 12-2. Its place in the SRP program is described in Section 1.4.



Figures 1-9 and 12-2. Performance Assessment Verification/Validation Logic

(Completion Milestones)

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Appendix A. SUMMARIES OF MODEL CODES

The summaries of model codes that are candidates for performance assessment application given in this section focus on three main areas: (1) description of the code's purpose, capabilities, and limitations; (2) status of the elements of documentation and review essential for code verification and validation; and (3) proposed application of the model for performance assessment in the context of salt repository systems. The summaries are written in sufficient detail so that a reader unfamiliar with individual model codes can gain an understanding of their capabilities, methods of approach, limitations, and utility. The status of verification and validation activities has been reported in terms of presently available documented reports, not in terms of future plans. Particular attention has been paid to the results of verification and validation activities with regard to their impact on model applicability to the specific problems of waste disposal in salt. Also included in the summaries are discussions of the important relationships among different codes. Areas covered in each model code summary are:

1. Code Name. SRP identifier.
2. Code Description. A general description of the purpose and approach of the model is given in terms of what the model provides for given inputs. The assumptions about the governing processes are outlined, and the method of calculation and/or solution is discussed. Limitations of both the approach and solution technique are indicated. Computing machine and software requirements are included.
3. Development Stage. Stage of model development refers to distinctions between recently coded models and well-established models in later versions. References to the original and/or antecedent models and codes are provided.
4. Documentation. The primary measure of adequacy of documentation is NUREG-0856 (Silling, 1983). The specific guidelines for document content, not just format, have been compared with available model code documentation. Exceptions to NUREG-0856 guidance and gaps in important documentation are noted.
5. Performance Specification Review. The performance specification review includes examination of conceptual design of the model,

scoping analysis, adequacy of the mathematical model and derivations, range of model applicability, and input/output requirements. While the developers of model codes often address such issues, the reference to performance specification review in the appendix focuses on external review of these items, independent of any reviews that may have been conducted by model code developers and independent of the context of nuclear waste disposal in a salt environment.

6. Code Design Review. Code design review includes examination of equations of the numerical model, numerical solution technique, computational error and solution stability, system interfaces, and input/output structures. The appendix focuses on external, independent reviews of these items within the SRP context.
7. Verification. Verification studies are tests and evaluations conducted to assure that a computer code correctly performs the operations specified in a mathematical model. As such studies rarely cover the entire range of possible applications of a model code, the summary identifies specifically those verification studies that have been conducted and the results. The purpose of this approach is to inform the reader of the extent to which the code has been exercised to aid in the planning of additional testing and potential application.
8. Validation. Validation studies are tests and evaluations conducted to assure that a model as embodied in a computer code is a correct representation of the process or system for which it is intended. This appendix, as in the case of verification, seeks to identify and distinguish among various existing validation studies to assist in planning model application and evaluating suitability.
9. Proposed SRP Application. On the basis of SRP documents, the proposed use of the model code is noted. The type(s) of performance assessment (waste-package, repository, and site) for which application is planned are identified, as well as the particular problems specifically addressed by the code. The use of other similar codes for this application may be noted as well, with distinctions among codes discussed.

10. Relationship of Model to Other Codes. The primary issue addressed here is whether the code stands alone or requires input from other codes. Links to other codes in terms of output of the subject code are indicated. Constraints on input and output data resulting from such linkage are noted.
11. Application of Code to Other Problems. Documented applications of the code to other (nonsalt and/or nonrepository) situations are listed here. The relevance of these applications to the SRP is noted.
12. Suitability of the Model for SRP Application. Limitations of the model that may make it unsuitable for application in performance assessment for various aspects of the SRP are given. Codes and models may be applicable only to parts of the disposal system in salt.
13. Peer Review. Documented independent peer reviews of model code specifications, design, and/or performance by recognized experts and peer groups are cited.
14. References. References cited in the appendix are listed.

A.1 BRINEMIG: A ONE-DIMENSIONAL FINITE DIFFERENCE CODE FOR BRINE MIGRATION MODELING

A.1.1 Code Description

BRINEMIG is a one-dimensional, explicit time-marching finite difference code which models brine migration by assuming that the migration rate may be expressed by the Jenks equation (Jenks and Claiborne, 1981):

$$\text{Log } (V/G) = 0.00656T - 0.6036$$

V = velocity of brine migration, cm/y

G = thermal gradient, degrees C/cm

T = temperature, degrees C.

The Jenks equation is empirical and models intracrystalline migration conservatively. To use the code requires the assumption that intercrystalline migration conservatively. To use the code requires the assumption that intercrystalline migration occurs at the same velocity as intracrystalline migration. The salt is assumed to be homogeneous and isotropic.

Three types of data are required by the code: 1) an initial moisture content of the salt, 2) a value for the threshold gradient, and 3) a talbe of temperatures at various distances from the waste package center line and times. The first radius at which temperatures are reported must be the package radius.

A.1.2 Development Stage

BRINEMIG is a fully operational code.

A.1.3 Documentation

No documentation of the code exists.

A.1.4 Performance Specification Review

No internal or external performance specification is documented.

A.1.5 Code Design Review

No internal or external code design review is documented.

A.1.6 Verification

No verification is documented.

A.1.7 Validation

No validation is documented.

A.1.8 Proposed ONWI Application

BRINEMIG will potentially be used to model brine migration to individual waste packages in a salt repository.

A.1.9 Relationship of Model to Other Codes

BRINEMIG is a stand-alone model. For application to salt repository problems, salt temperatures as a function of location around the waste package and time are required. These may be generated by TEMP. Results of brine migration calculations are used as input to WAPPA waste package analyses.

A.1.10 Suitability of Model for Salt Repository Applications

The model was designed expressly for salt repository applications.

A.1.11 Peer Review

No documentation of peer reviews exists.

A.1.12 References

Jenks, G. H. and H. C. Claiborne, 1981. Brine Migration in Salt and Its Implications in the Geologic Disposal of Nuclear Waste, ORNL-5818, Oak Ridge National Laboratory, Oak Ridge, TN.

A.2 CFEST: A MULTIDIMENSIONAL FINITE-ELEMENT CODE FOR THE ANALYSIS OF COUPLED FLUID, ENERGY, AND SOLUTE TRANSPORT (PNL-4260)

A.2.1 Code Description

CFEST is a coupled fluid, energy, and solute transport code that simulates seasonal energy storage in underground confined aquifers in three dimensions. It treats single-phase Darcy flows in a horizontal or vertical plane, or in fully three-dimensional space under nonisothermal conditions. A special case of axial symmetry in a vertical cross section can also be treated. Both steady state and transient simulations are possible. The code is designed to operate in an interactive mode to aid in understanding complex aquifer systems. It can also be used to help design field experiments and to interpret sparse field data.

Input requirements include fluid and hydrogeologic properties, which can be dependent or independent of head, temperature, solute concentration, and fluid density. Fluid properties include compressibility, thermal coefficient of expansion, solute concentration (only one species is allowed), heat capacity, internal energy, and viscosity. Aspects of the overall geologic region and the constituent geologic units must be specified. The isotropic or anisotropic properties of each confining rock unit that must be entered include permeability, porosity, compressibility, specific storage, dispersivity length, thermal conductivity, heat capacity, and thermal properties.

The model is based on three governing partial differential equations, namely, conservation of total liquid mass, conservation of energy, and conservation of mass of dissolved contaminant. They are coupled through fluid density (ρ), which is expressed as a function of pressure head (h), temperature (T), and solute concentration (C). The dependent variables h, T, and C are functions of space and time. Fluid viscosity is a function of T and C. Flow is transient and laminar (Darcian). Aquifer properties (porosity, permeability, and thickness) may be space-dependent. Hydrodynamic dispersion is a function of fluid velocity. Boundary conditions permit heat losses or gains to adjacent formations, natural movement of water in the aquifer, and arbitrary location of wells. The fluid and the porous media are compressible, whereas rock density and heat capacity are treated as constants. The energy balance ignores viscous dissipation.

The code employs a staged execution structure and can be operated in an interactive mode. It uses a right-hand Cartesian coordinate system throughout. The two- or three-dimensional modeled domain is assumed to be bounded by piecewise smooth boundaries. In addition to the three basic conservation equations, the model also specifies fluid density and porosity relations. Density is expressed as a function of the solute concentration, temperature, and pressure head using only the zeroth and first order terms of a Taylor series. Porosity is expressed in terms of compressibility. These relations are substituted into the three basic conservation equations, which are then solved using the Galerkin finite-element method. Gaussian quadrature is used to integrate the finite-element equations numerically. The following processes are not considered: adsorption into a porous media substrate, chemical reactions in solution, and radioactive decay chains.

Source language and machine requirements are not mentioned in PNL-4260 (Gupta, et al., 1982).

A.2.2 Development Stage

CFEST is a fully operational code that is an extension of the finite-element three-dimensional groundwater code (FE3DGW) developed by Gupta, et al. (1979). CFEST has been technically documented and tested, but no user's manual is available.

A.2.3 Documentation

Current documentation is limited to PNL-4260 and a revised draft document, compatible with NUREG-0856 (Silling, 1983) requirements, is in preparation.

A.2.4 Performance Specification Review

Internal review was conducted by Pacific Northwest Laboratories and DOE-Richland for publication as PNL-4260.

A.2.5 Code Design Review

Internal review was conducted by Pacific Northwest Laboratories and DOE-Richland for publication as PNL-4260.

A.2.6 Verification

Several tests conducted by the code authors to check the correctness of the coding and to test the sensitivity of the results to grid and time-step size are discussed in PNL-4260. Results of these tests are summarized below.

1. Steady drawdown from flow to a well in a confined aquifer. CFEST results were compared with published analytical results that assumed axial symmetry. Results showed excellent agreement for a fine, axisymmetric grid system. Results were slightly sensitive to choice of grid (i.e., Cartesian versus cylindrical coordinates) and grid spacing.

2. Unsteady drawdown from flow to a well pumped at a constant rate in a vertically confined but horizontally infinite and isotropic aquifer. CFEST results were compared with published analytical results that assumed axial symmetry. Results showed excellent agreement for long time periods but somewhat poorer agreement for short time periods.
3. Unsteady drawdown from flow to a steadily pumped well draining an elastic artesian aquifer confined by semi-pervious (leaky), elastic strata. The flow is vertical through the confining formations and horizontal through the aquifer. The flow region is occupied by five layers. CFEST results were compared with published analytical results, showing good agreement for several radii and all except the shortest dimensionless times.
4. Uniform regional flow with sources and sinks. CFEST results were compared with published analytical results. Results on a two-dimensional plane showed good agreement, with accuracy somewhat dependent on grid structure.
5. Dirichlet upstream boundary condition test; linear, one-dimensional geometry. CFEST results were compared with published results, with good agreement evident.
6. Mixed upstream boundary condition test, one-dimensional geometry. CFEST results were compared with published results. Results showed good agreement, with absolute errors somewhat dependent on time-step size.
7. Single well problem, with radially varying velocity and dispersion. CFEST results were compared with an approximate analytical solution. This is the first test with nonconstant velocity and dispersion. Results compared reasonably well; discrepancies were attributed to the approximate nature of the analytical solution.
8. Energy transport including cap and bedrock conduction. This is the first test involving energy loss to the confining media. CFEST results were compared with two published analytical solutions. Results verified CFEST's capability to simulate conductive heat loss in conductive cap rock and bedrock.

A.2.7 Validation

In the document being prepared, field applications of the code for seasonal thermal storage, remedial measures for the LaBounty landfill site, volatile chlorinated hydrocarbon and phenol transport, and migration and fate of selenium in a waste disposal facility of a coal fired power plant are included as partial validation of the code.

A.2.8 Proposed SRP Application

CFEST, along with DOT, HEATING6/5, and SWENT, are listed by SRP as potentially useful in analyzing waste package thermal boundaries. It is similarly listed as suitable for temperature analyses within the waste package for repository subsystem thermal environment and fluid assessment, and for groundwater flow and hydrologic budget analyses.

These applications all require CFEST's multidimensional flow and energy transport simulation capabilities. The inputs required for such simulations include specification of the various geologic units making up the flow system as well as various fluid and media properties.

A.2.9 Relationship of Model to Other Codes

CFEST is a stand-alone, general-purpose, complex-aquifer simulation model. For application to salt repository problems, in the current version (being documented) salt dissolution and heat flow through the solid state are included. Enhancement of code capabilities for radionuclide transport is in progress. Flow through fractured media will be also considered in future updates. Source codes like WAPPA will be used to provide input data on leachates and thermal conditions.

A.2.10 Suitability of Model for Salt Repository Applications

The suitability of the model for salt repository applications has not been addressed in SRP documents or in PNL-4260. CFEST was developed at Pacific Northwest Laboratories for use in their seasonal thermal storage program. Outside of the salt deposit, that is, for far-field or regional applications, CFEST appears to be well suited to the problem of transport of contaminated groundwater through a complex of unfractured geological formations, provided that chemical reactions, adsorption, and radioactive decay and formation are not important. Because of its ability to treat a wide variety of hydrogeologic problems, it could be used for analyses supplemented by other codes that treat these other aspects in detail but place less emphasis on the hydrological aspects of the problem. The same may be said for the waste package environment after resaturation of the salt deposit and backfill has occurred. However, limitations of applicable ranges of temperature and pressure are not documented.

A.2.11 Peer Review

Any peer review should address, among other things, the role that CFEST could play in salt repository performance assessment. No documentation on peer reviews is available.

A.2.12 References

Gupta, S.K., et al., A Multidimensional Finite-Element Code for the Analysis of Coupled Fluid, Energy, and Solute Transport (CFEST), Battelle Pacific Northwest Laboratories, Richland, Wash., PNL-4260 (Aug. 1982).

Gupta, S.K., C.R. Cole, and F.W. Bond, Methodology for Release Consequences Analysis, Part III: Finite-Element Three-Dimensional Ground-Water (FE3DWG) Flow Model, Battelle Pacific Northwest Laboratories, Richland, Wash., PNL-2939 (Sept. 1979).

Silling, S.A., Final Technical Position on Documentation of Computer Codes for High-Level Waste Management, U.S. Nuclear Regulatory Comm. Report NUREG-0856 (June 1983).

A.3 DACRIN: A COMPUTER PROGRAM FOR CALCULATING ORGAN DOSE FROM ACUTE OR CHRONIC RADIONUCLIDE INHALATION (ONWI-431)

A.3.1 Code Description

DACRIN rapidly calculates consistent estimates of the effective radiation dose to the human respiratory tract and other organs resulting from inhalation of radioactive aerosols. The code is an outgrowth of the development of a mathematical model for organ dose that follows the basic precepts of the International Commission on Radiological Protection task group on lung dynamics (ICRP, 1959). Mathematical models describing atmospheric dispersion have also been included as part of the code's evaluation of doses resulting from either accidental or chronic atmospheric releases of radionuclides.

For each case, the code calculates the effective radiation dose to any of 18 organs and tissues from inhalation of any one or a combination of no more than 10 of the over 600 radionuclides considered by ICRP. Organ doses are calculated by specifying either the quantity of radionuclide inhaled or the quantity released to the atmosphere. In the latter case, duration of release, release height, wind speed, atmospheric dispersion parameters, and downwind distance at which the dose is to be calculated must also be specified. As many as 10 distances may be specified for each use.

Required input consists of a few program control variables, the duration of inhalation exposure, the ventilation rate, the time interval within which the dose is delivered, the organs of interest, the quantity of radionuclide inhaled, its solubility class and particle size and, when an atmospheric dispersion model is involved, the additional parameters required for the model selected. Output consists of the effective radiation doses to the specified organs at selected time intervals for each radionuclide inhaled.

DACRIN is based on the precepts of the ICRP task group and a simple exponential model for retention by an organ of interest. The model divides the respiratory tract into three regions: nasopharyngeal, tracheobronchial, and pulmonary. Deposition is assumed to vary with the aerodynamic properties of the aerosol distribution. Atmospheric dispersion is described by a bivariate normal distribution model incorporated into the code; however, normalized air concentrations at specific distances as calculated by any other atmospheric dispersion model can be used as input. All atmospheric dispersion and dose equations directly depend on the values of input parameters and are solved analytically. There may be no more than 10 downwind distances at which dose is calculated, 10 organs of interest, 10 time inter-vals measured from the most recent intake, and 5 multiple intake intervals.

The complexity of the model, or programming class, is designated in ONWI-78 (SAI, 1981) as B/C, indicating a program of 250-1000 lines of instruction that requires a minimum configuration of a minicomputer to a super minicomputer, with an approximate set-up time of 30 minutes to one hour and an approximate execution time of two hours. The programing language is FORTRAN (FORTRAN V for the SCEPTER version of DACRIN), and the computers for which the program is designed are the UNIVAC 1100 and CDC CYBER 176. Fifty-six thousand words of memory are needed to execute the code. Compiling the DACRIN source and executing a sample problem required 100 seconds of central processing unit (CPU) time on a UNIVAC 1100/44.

A.3.2 Development Stage

CDC and UNIVAC versions of DACRIN are available and operational(SAI, 1981;NESC, 1981). DACRIN was originally developed for use on UNIVAC machines by Battelle Pacific Northwest Laboratories (Houston, et al, 1974). It was adapted for CDC machines and modified and revised in ONWI-431 (INTERA, 1983) in order to include it in the SCEPTER project. The changes made include (1) conversion for use with a CDC computer; (2) removal of defunct print options; and (3) insertion of a unique code identification number that must be matched to allow execution.

A.3.3 Documentation

The CDC version is documented in ONWI-431 in accordance with NUREG-0856 including the federal information processing standard software summary, user's manual, and other required features. The UNIVAC version is fully documented in BNWL-B-389 (Strange, 1975) and further documented by National Energy Software Center (NESC, 1981, Houston et al., 1974). Additional documentation, including summary documentation, is available in SAI (1981, Shriner and Peck (1978), and Miller (1978).

A.3.4 Performance Specifications Review

The UNIVAC version has been accepted by the nuclear industry and NRC, and has been used extensively in the licensing of nuclear projects. No documented additional review has been performed for performance assessment purposes.

A.3.5 Code Design Review

The UNIVAC version has been accepted by the nuclear industry and NRC, and has been used extensively in the licensing of nuclear projects. No documented additional review has been performed for performance assessment purposes.

A.3.6 Verification

Verification tests have been conducted on the original DACRIN code (Houston et al., 1974) and the DACRIN code as modified for the SCEPTER project (INTERA, 1983). The same two sample problems were run in each case.

Verification problem 1 demonstrated the chronic dose calculation. It used the direct inhalation option and consisted of a calculation of the dose to 10 different organs or tissues from chronic inhalation of a mixture of fission products for five dose times following termination of uptake.

Verification problem 2 was an acute dose problem. It made use of the atmospheric diffusion model built into the program that uses the Simpson-Fuquay stable atmospheric diffusion model option to calculate the dose to four organs at two dose times following passage of a cloud produced by short-term release to the atmosphere of a mixture of transuranic nuclides.

Calculated dose results for these two problems using both in the modified for SCEPTER and unmodified DACRIN codes are reported to have matched exactly when identical organ data libraries were used.

A.3.7 Validation

Although DACRIN is based on the respiratory tract model adopted by the ICRP task group on lung dynamics and has been applied to CRWM-type situations, no formal validation of the model has yet been documented.

A.3.8 Proposed SRP Application

DACRIN will be used to estimate environmental radiological exposures under normal operation of a nuclear waste repository in salt and also for environmental radiological exposures from repository accidents.

Because DACRIN calculates atmospheric dispersion and radiological doses via inhalation, it is appropriate for analyzing scenarios in which radioactive wastes are transported from the repository system into the atmosphere. Envisioned events that may allow for such transport include drilling into or mining of the waste or waste package, tectonic or volcanic events that would bring waste to the surface, transport of aerosols associated with contaminated irrigation water, and windblown erosion of contaminated soils.

DACRIN does not directly estimate the releases that would occur in situations such as those mentioned above. These releases must be estimated by other codes and supplied as input to DACRIN. Such input might include the likelihood and degree of geologic or human intrusion events, waste composition, waste release concentrations, waste particle sizes, meteorological conditions, and human population information, such as population distribution and cultural practices that could affect inhalation exposure.

Once such information is provided, DACRIN can be used to evaluate, in part, the impacts of the radionuclide releases in terms of dose to particular organs or tissues. DACRIN does not estimate the dose associated with ingestion or external exposure; this information can be obtained from PABLM. These two dose assessment codes can then be used to determine the relative importance of radionuclide releases and thereby provide more complete repository system assessments.

DACRIN can be most useful for safety calculations associated with the operational phase. However, certain special scenarios associated with assessment of long-term isolation performance also may require the capabilities of this code. Examples of long-term scenarios that could result in atmospheric releases are direct drilling through a canister or solution mining, with related surface release of insolubles.

An example of a problem for which an acute dose calculation using DACRIN would be appropriate would be a situation in which a waste canister is ruptured, resulting in the sudden release of material in the presence of humans. A chronic dose calculation using DACRIN would be appropriate when nuclear waste material is inadvertently brought to the surface by mining or some other method and is allowed to remain exposed to the elements for a period of time in the vicinity of humans.

A.3.9 Relationship of Model to Other Codes

Many other biosphere transport and radiological dose codes exist; a tabulation of a subset of these codes used in nuclear waste isolation applications is found in SAI (1981). Other programs that calculate organ dose include SUBDOSA, which calculates external doses from atmospheric releases of radionuclides; AERIN, which calculates organ and tissue burdens resulting from acute exposure to a radioactive aerosol; and ARRRG, FOOD, and PABLM, which calculate radiation doses to humans from radionuclides in the environment. The two data libraries used by DACRIN are RMDLIB, the radionuclide decay data library, and ORGLIB, the organ data library.

More than one version of DACRIN is extant. The version documented in ONWI-431 incorporates the minor changes made to provide consistency with the SCEPTER technology package.

A.3.10 Application of the Code to Other Problems

This code has been extensively used in the licensing of nuclear projects.

A.3.11 Suitability of Model for Salt Repository Application

Because the dosimetry model is independent of the origin of the radionuclides, DACRIN is applicable for salt repositories. There are no unique aspects to its application for a nuclear waste repository in salt.

A.3.12 Peer Review

ONWI has no special plans for peer review.

A.3.13 References

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A.4 EQ3/EQ6: A GEOCHEMICAL SPECIATION AND REACTION PATH CODE PACKAGE SUITABLE FOR NUCLEAR WASTE PERFORMANCE ASSESSMENT (ONWI-472)

A.4.1 Code Description

EQ3/EQ6 (Wolery, 1979; INTERA, 1983a; Thomas et al., 1982) is a software package consisting of two separate codes. EQ3 is a geochemical code that computes solution speciation, that is, the distribution of ions, ion complexes, and neutral species in an aqueous solution given user- specified reactions, elements, and compounds. EQ6 is a geochemical transport code that simulates reaction paths, that is, the sequence of steps going from equilibrium state to equilibrium state. It calculates changes in phase equilibria at each intermediate equilibrium step and determines the mass of each constituent transported from one phase to another. Gas, solution, and solid phases are included.

In contrast to PHREEQE (INTERA, 1983b), a combined speciation/transport code that calculates only the final state from user-specified initial conditions, EQ6 starts with the solution model calculated by EQ3 and simulates small progressive changes, keeping track of interphase transport in each step as the final state is approached. Hence, it is a more detailed and more powerful simulation tool than PHREEQE, but requires more core memory and computer time. It is also easier to use than PHREEQE, since the reaction path simulation is carried out automatically in a single run without the careful hand operations required for a reaction-path simulation with PHREEQE. Because of its computational power and ability to handle intermediate steps in a reaction-path simulation, EQ3/EQ6 is more suited than PHREEQE to applications in the near-field environment (waste package and wasteform) and has replaced PHREEQE for SRP applications. Perturbations from equilibrium resulting in significant interphase transport are more likely to occur there than in the far field.

Although any temperature in the range of 0-300C can be handled, simulation pressures are limited to either a fixed value of 500 bars or 1 atm for temperatures between 0C and 100C or values along the saturated steam curve for temperatures greater than 100C.

The input data set required to run EQ3/EQ6 includes equilibrium constants for each reaction described by mass action equations and for each dissolution/precipitation reaction at specified temperatures. These are internally corrected for the specific simulation temperature. The data set also includes coefficients used to compute the activity of water as a function of electrolyte concentration and temperature, and the activities of neutral and ionized species as functions of total ionic strength and temperature. Debye-Hückel constants at various temperatures are also included in the data set and are used to compute the activity coefficients of ionized species. The user can choose from several alternative formulae for computing these coefficients. EQ3/EQ6 is currently being revised to deal with aqueous solutions with ionic strengths greater than 1 molal.

A.4.2 Development Stage

Because the EQ3 and EQ6 codes are relatively new, they have not been widely used. Most of the work on these codes was done at the Department of Geological Sciences, Northwestern University, with subsequent work done at Lawrence Livermore Laboratory (Thomas et al, 1982). The codes are based on earlier work by Garrels and Mackenzie (1967), Helgelson et al. (1970), Wolery (1979) and others.

A.4.3 Documentation

The code as documented in ONWI-472 generally conforms to NUREG-0856, except that the discussions of the theory and solution methods are relegated to an appendix written by one of the code authors rather than by one of the documentation authors. This appendix gives a concise but good general review of geochemical modeling and associated numerical methods, thus providing the reader with some perspective on EQ3 and EQ6.

A.4.4 Performance Specification Review

With regard to requirements for application to repository performance assessment, ONWI-472 makes the comment that "only PHREEQE and EQ3/EQ6 meet certain of the SCEPTER performance requirements (INTERA, 1982b). The particular qualifying requirements were: 1) incorporation of a general algorithm with aqueous species and solid phase identities set by user input,

2) ability to handle temperature variations, and 3) readily available source code and adequate user manual documentation." No documentation of external performance specifications review is available.

A.4.5 Code Design Review

An internal review conducted by INTERA served as the basis for Sec. 3 of ONWI-472. Comparison of the geochemical codes PHREEQE and EQ3/EQ6 suggests that, while the former is designed for relatively fast operation for scoping-type calculations, the latter is a more powerful, if costlier to run, computational tool and is more suited to near-field waste package assessment problems. EQ3/EQ6 was also designed for easier use. EQ3/EQ6 has now completely supplanted PHREEQE for SRP licensing-directed simulations.

To solve the system of simultaneous, nonlinear, algebraic mass balance and mass action equations in EQ3, an iterative solution method is used. EQ6 employs a variation of the differential equation method of solving a system of nonlinear algebraic equations first used by Helgeson et al (1970). The present method avoids some of the difficulties of an earlier implementation of Helgeson by correcting the predicted values using a Newton-Raphson method to satisfy the original algebraic equations instead of the difference equations that represent the corresponding differential equations (Wolery, 1979). The total software package includes the main codes EQ3 and EQ6, a set of supporting data files, two utility routines for data-file management, and sample input files for EQ3 and EQ6. It has been written for operation on CDC equipment. Both EQ3 and EQ6 require the IMSL subroutine package. The entire package comprises over 30,000 card images.

No external code design review has been documented.

A.4.6 Verification

EQ3/EQ6, with its own thermodynamic data set and with the data set provided with PHREEQE, has been applied to several test problems for code verification, intercode comparison, and illustrative purposes. Three tests are reported in the verification section of ONWI-472; two others that are basically illustrative in nature are reported in the user's manual as example problems.

1. Speciate Major Ions of Seawater. The purpose of problem 1 was to verify EQ3 coding by comparing computed concentrations of free and complexed ions (combinations of four cations and five anions) with those resulting from hand calculations. This was not an adequate verification of EQ3 because the thermodynamic data sets used for EQ3 and the hand calculations were different. The lack of agreement in the results was probably due to the input data differences.
2. Speciate Full Seawater Analysis. The purpose of problem 2 was to compare EQ3 to PHREEQE and WATEQF/WATEQ (INTERA, 1983a; Plummer et al, 1976), and to test the sensitivity of the thermodynamic data sets. The effect of entering carbon species via "total inorganic" versus "total alkalinity" was on the order of 5% or less. The effect of the two different thermodynamic data sets (one developed for EQ3 and one for PHREEQE) was 10% or less on minor and major ionic species concentrations but was much larger on mineral saturation indices, indicating that the input thermodynamic data are a major source of uncertainty for such calculations. Code-to-code differences using as close to the same input data as feasible showed generally smaller differences than those obtained from using different data sets with the same code.
3. Dissolve Microcline in Dilute Hydrochloric Acid. The purpose of problem 3 was to illustrate the reaction-path-simulation and phase-boundary-finding capabilities of EQ3/EQ6, and to compare these with those of PHREEQE. An additional purpose was to compare computed phase boundaries with those obtained from hand calculations. Location of phase boundaries was found to be a sensitive function of the thermodynamic input data set. The data sets that came with EQ3/EQ6 and PHREEQE gave substantially different results. Reaction paths were also found to change substantially when the two data sets were used in the same codes. Code-to-code differences when using the same data sets were quite small.
4. Reduce an Oxygenated Calcite and Hematite Saturated Solution by Adding Methane. The purpose of problem 4 was to illustrate how EQ3 and EQ6 are used to simulate reaction paths that include redox reactions and to compare results with those calculated using PHREEQE. Comparisons were close when using the same input data.

5. Carbonate Aquifer Dedolomitization by Gypsum Solution with Increasing Temperatures. The purpose of problem 5 was to illustrate the temperature-changing capabilities of EQ6.

Note that PHREEQE does not treat temperature as a dependent variable. It must be provided by the user.

A.4.7 Validation

Although no validation efforts have been reported, some comparisons have been made between observations and calculations of a few of the equations used in EQ3 to calculate activity coefficients. Such comparisons suggest that these calculations are a major source of uncertainty in general and pose great difficulties in the case of strong electrolyte solutions and for solutions containing radionuclide-bearing compounds for which few data are available. SRP has tentatively suggested the following candidate validation exercises.

1. Calculating radionuclide solubilities in site-specific far-field brine groundwaters and comparison with laboratory measurements.
2. Predicting the pH of far-field groundwaters in equilibrium with the limestones both in situ and after sampling (outgassing of carbon dioxide with consequent pH change) and comparison with field data.
3. Predicting the composition of waste-glass leachate or corrosion solutions and comparison with laboratory results, assuming that the necessary code capabilities and input data are available at the time.

A.4.8 Proposed SRP Application

In the near field, EQ3/EQ6 will be used to assess geochemical reactions affecting the waste package barriers and near-field transport. The results will be used as input to corrosion and hydrological mass transport codes. In the far field, the code will be used to assess geochemical reactions affecting radionuclide transport in the repository regime. The results will provide inputs to hydrological mass transport codes. Information required as input to mass transport codes includes distribution of radionuclide species in dissolute and solid phases as a function of temperature, pressure, and solution composition. To provide such information, the geochemical codes must be able to handle concentrated brine solutions and must have input data on solution reactions involving radionuclide-bearing compounds. These are difficult requirements to satisfy. EQ3/EQ6 is being adapted to include the necessary algorithms or input data sets required.

A.4.9 Relationship of Model to Other Codes

To perform calculations within the framework of repository assessment, the model will have to be operated in conjunction with codes that provide information about thermodynamic variables and chemical constituents. In the near field, WAPPA and ORIGEN2 can provide informa tion on rates of heat generation and radionuclide inventories. EQ3/EQ6 can provide input to WAPPA for computation of leaching and corrosion. It can also be used to provide concentrations of radionuclide-bearing compounds to mass transport codes like SWENT and CFEST.

A.4.10 Application of Code to Other Problems

Applications to several problems are discussed in by Wolery (1979) and Secs. 4 and 13 of ONWI-472 (INTERA, 1983a).

A.4.11 Suitability of Model for Salt Repository Application

For both near- and far-field applications, the code should be able to handle concentrated brine solutions and to predict radionuclide distributions in solution and solid phases as a function of temperature, pressure, and solution composition. Whereas thermodynamic equilibrium is probably acceptable for the far field, it may not be adequate for near-field phenomena, where temperature, pressure, and available solid constituents will change as successive waste package barriers are breached and kinetic effects become more important. The necessary thermodynamic data sets shall be available in FY 1985.

A.4.12 Peer Review

No documented peer review is available.

A.4.13 References

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A.5 FE3DGW: FINITE-ELEMENT THREE-DIMENSIONAL GROUND-WATER FLOW MODEL (PNL-2939)

A.5.1 Code Description

The FE3DGW code simulates three-dimensional, time-dependent water flow in fully saturated porous media. The code can represent single-layered systems having variable thickness or multilayered systems in which the number of layers (up to 20) and the thickness of each layer can be varied. Hydrologic conductivity can be anisotropic and inhomogeneous. The groundwater and the porous media it saturates are both taken to be compressible. It is assumed that the porous matrix material does not dissolve in water.

Input consists of the geometry of the finite-element network at surface level; well log data at each node; descriptions of layer depths and thick nesses, and of the geologic properties within each layer (hydraulic conductiv ity tensor, porosity, and compressibilities); boundary conditions; and time steps. Output consists of flows and the hydraulic head as functions of time and of position in the region being simulated. The output is obtained by solving an equation proposed by Jacob (1950) for three-dimensional transient flow. This equation is solved by a finite-element approach, which can accommodate the irregular boundaries that often occur in geologic systems. FE3DGW is limited to simulating saturated media. The code is written in FORTRAN IV-Plus.

A.5.2 Development Stage

FE3DGW can be used on a mini computer (such as the VAX 11/20) or a large frame computer (such as the CRAY) is ready for use on a PDP 11/45 computer.

A.5.3 Documentation

FE3DGW is documented in PNL-2939 (Gupta, et al., 1979) which includes a user's manual and a program listing. Revised documentation in the NUREG-0856 format is being prepared.

A.5.4 Performance Specification Review

Performance specification review was conducted by Pacific Northwest Laboratory, Richland and DOE-Richland for publication as PNL 2939.

A.5.5 Code Design Review

Performance specification review was conducted by Pacific Northwest Laboratory, Richland and DOE-Richland for publication as PNL 2939.

A.5.6 Verification

FE3DGW has been verified by comparing its solutions to analytic solutions in three cases: (1) time-dependent radial flow to a well pumping at a constant rate in an infinite, homogeneous, and isotropic aquifer; (2) steady state, two-dimensional flow through a rectangular aquifer with a reservoir having a head 25 feet above the water table; and (3) time-dependent, radial flow to a well pumping at a constant rate from an elastic aquifer confined by semipervious elastic strata.

Agreement between the FE3DGW-generated solutions and the analytic solutions was close in the first two cases and generally close in the third. In the first case, the values of drawdown as a function of time obtained from the code are consistently slightly less than those obtained from the analytic solution. In the second case, agreement was excellent. In the third, agreement was very close, except at early times in the subcase of a radius of 7.389 m. There, the discrepancy was about 10%.

The revised draft has additional verification (steady flow in a well bounded by a fully penetrating stream, stream-aquifer interaction, decay of a ground-water mound, and a partially penetrating well),benchmarking and other field applications.

A.5.7 Validation

Use of FE3DGW for steady-state and historical potential measurements of a ground-water reservoir are published as a Water Resource Research paper (Gupta, et al., 1984).

A.5.8 Proposed SRP Application

The FE3DGW code will be used by SRP to simulate the flow of ground water to and away from the waste repository. Hence, FE3DGW is a site assessment code.

A.5.9 Relationship of FE3DGW to Other Codes

FE3DGW is used for regional and local groundwater flow. The FE3DGW package includes supporting programs to verify input data. The pathline and travel time estimates from FE3DGW could be used as input to radionuclide transport codes like SCOPE.

A.5.10 Application of FE3DGW to Other Problems

FE3DGW has been used to simulate water flow through aquifers in the Sutter Basin in California (Gupta and Tanji, 1976), and flows under Long Island in New York. (Gupta and Pinder, 1977; Gupta et al, 1984).

A.5.11 Suitability of FE3DGW for Salt Repository Application

FE3DGW has been applied for the following problems related to the CRWM program: INFCE Salt Repository (Cole, 1983a, pp 57-63; INFCE Hard Rock (Granite) Repository (Cole, 1983b, pp 83-107); Hypothetical Repository in Basalt (Dove et al., 1982, pp 106); Drawdown and Pumping Requirements from a Generic Mine (Carlsson and Carlstedt, 1980); Near-Dome Hydrologic Simulation of a Hypothetical Repository (Harwell, et al., 1982).The code FE3DGW is suitable for simulating the flow of regional and local groundwater. Flow through a salt formation is simulated as Darcian flow. Because the code simulates only flow, the temperature and salinity gradient have to be explicitly specified. FE3DGW can be used for analysing flow to address sensitivity and uncertainties in the hydrogeologic data. To accouont for time variant temperature and concentration its upgraded version CFEST, can be used.

A.5.12 Peer Review

The first version of FE3DGW was developed at the University of California, Davis (Gupta, Tanji, and Luthin, 1975). It was upgraded at Princeton University (Gupta and Pinder 1977). PNL-2939 was its third stage of documentation. A revised document in NUREG-0856 format is in progress. Several journal papers have been published on the FE3DGW mathematical model (Gupta and Tanji, 1976), code structure (Gupta and Tanji, 1977a), equation solver Gupta and Tanji (1977b) and its application to the Long Island, New York groundwater reservoir (Gupta et al., 1984). All the above and the various field applications have had an internal and external peer review. A formal peer review of the revised document will be conducted.

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A.6 SALT GSM - SALT-GEOLOGIC SIMULATION MODEL

Salt GSM (currently under development and documentation) is a code to analyze the approximate geologic and climatic state of a salt nuclear waste repository site over geologic times. Within a probabilistic framework, salt GSM attempts to represent quantitatively a number of geologic and climatic conditions for a given repository and to treat natural and man-induced changes in these conditions. It accounts for cumulative and interactive effects of multiple phenomena. Sub-models of this model predict the occurrence of, or simulate the effects of, climatic change, tectonics, regional deformation, geomorphic processes, and dissolution fronts on the hydrologic behavior of a site.

Salt GSM handles this problem by defining probability density functions (pdf's) for the parameters. Other inputs are inherently probabilistic, such as the probability of occurrence of a certain kind of event. Thus, the output parameters of Salt GSM simulations would be expected to be random variables with their own pdf's. Because of the large number of probabilistic input parameters, Salt GSM uses a Monte Carlo simulation (instead of mathematical or analytic calculation0 approach to model long-term changes in the site or the probability of occurrence of specific conditions. In such an approach, the selection of random numbers with certain statistical properties is lused as an analog to select specific parameters, and by repeated simulations one makes inferences about the overall behavior of the system.

The following kinds of information are required for input to the GSM: 1) program control options, 2) site geometry, and 3) submodel input parameters.

Program control options cover mainly the length of time over which simulation is to take place, the number of simulations, and types of output desired. Site geometry covers specification of structures, stratigraphy, repository location, and river points. Submodel input parameters will include both some with particular values and some in the form of pdf's necessary for running submodels. Some may be site specific, others more universal or reflective of hypotheses.

The Salt GSM may be operated in two modes: 1) the Monte Carlo mode, in which the results of multiple simulations are analyzed statistically, and 2) the single-run mode, in which one or a small number of runs are carried out to trace particular kinds of effects. In the Monte Carlo mode, there are two major contributions to the stochastic nature of the output. The first is the probabilistic nature of certain events, whose actual occurrences are simulated; the second is the probabilistic description of many model parameters, which are characterized by probability density functions. All stochastic aspects can be fully simulated by random numbers, or an operator can assign certain values to some parameters or force specific events to occur and then simulate over the remainder.

Validation of initial results will be "by peer review", a process by which the most knowledgeable experts on each submodel will pass judgment on the reasonableness of the results as no true validation is possible because of the extremely long time scales involved.

The following are the three additional limitations of the GSM:

1. The probabilistic data of each submodel are necessary to carry out a simulation for a specific site.
2. A large number of simulations are necessary to gain useful information concerning all but the most likely occurrences or perturbations at a particular site.
3. The code will need to be modified and upgraded for application to specific salt sites.

The Salt GSM code is based on Pacific Northwest Laboratories' Geologic Simulation Model (PNL-2892, PNL-3542) and Far Field State Model-FFSM (ONWI 436). As compared to earlier versions of GSM, the Salt GSM includes only important features associated with salt sites. Salt GSM is being developed and documented at Pacific Northwest Laboratories. The documentation will include example applications to a Palo Duro repository site.

A.6 References

Foley, M. G., et al., Geologic Simulation Model for a Hypothetical Site in the Columbia Plateau, Volume 2: Results, Battelle Pacific Northwest Laboratories, Richland, Wash., PNL-3542-2 (1982).

INTERA Environmental Consultants, FFSM: Far Field State Model, ONWI-436 (1983).

Petrie, G. M., et al., Geologic Simulation Model for a Hypothetical Site in the Columbia Plateau, Battelle Pacific Northwest Laboratories, Richland, Wash., PNL-3542 (1981).

A.7 GRESS: GRADIENT-ENHANCED SOFTWARE SYSTEM (ORNL/TM-8339)

A.7.1 Code Description

GRESS is not a computer code for a model specifically designed for waste-package-, repository-, or site-performance assessment. It is a general software package that could be used as a tool to facilitate sensitivity studies with model codes. However, the user's guide for GRESS (Oblow, ORNL/TM-8339) simply describes the general package and does not discuss sensitivity studies for model codes as part of performance assessment. Thus, apart from the following brief summary of the package, no code summary is provided in this appendix.

GRESS is a FORTRAN compiler language that enhances conventional FORTRAN programs with analytic differentiation of arithmetic statements. It handles any standard FORTRAN code that contains arithmetic text material as part of the source program. The GRESS compiler reads the FORTRAN source code text, redefines the variables and their storage locations, searches for arithmetic statements, translates the latter for gradient calculations, and then generates a new source program that now includes gradient capabilities in all arithmetic statements. GRESS allows any standard FORTRAN code to be upgraded to calculate any derivatives required, whether they be for internal use in a calculation (e.g., for iteration) or for external use (e.g., sensitivity studies).

A.7.2 References

Oblow, E.B., GRESS: Gradient-Enhanced Software System, Version B, User's Manual, Oak Ridge National Laboratory Report ORNL/TM-8339 (no date).

A.8 HEATING6/5: A MULTIDIMENSIONAL HEAT CONDUCTION ANALYSIS WITH THE FINITE DIFFERENCE FORMULATION

A.8.1 Code Description

HEATING6/5 is the most recent version of the HEATING (heat engineering and transfer in nine geometries) program. HEATING6/5 was developed from HEATING5 by (1) adding a free-form input package, (2) inserting more diagnostic messages, (3) putting in a thin surface boundary condition capability, and (4) refining the implicit numerical techniques used to solve the heat balance equation.

HEATING6/5 solves steady state and transient heat conduction problems in one-, two-, or three-dimensional Cartesian coordinates; in one-, two-, or three-dimensional cylindrical coordinates; or in one-dimensional (radial) spherical coordinates. Thermal conductivity can be anistropic and can depend on both spatial coordinates and temperature. Density and specific heat can, likewise, depend on both spatial coordinates and temperature. The heat generation rate per unit volume can be a function of time, position, and temperature. Materials can experience a change of phase. HEATING6/5 can treat problems whose boundary conditions depend on time and position. Boundary conditions can be in the form of specified temperatures or any combination of specified heat flux, forced or natural convection, and radiation. Also, it is possible to specify radiative heat transfer across regions embedded in the physical system being simulated.

Input to HEATING6/5 consists of system geometry, materials, a heat source function, initial temperatures, and boundary conditions. Output includes predicted temperatures. Output is obtained from input by solving a finite-difference formulation of the heat balance equation. Steady state problems are solved by the point successive overrelaxation iterative method plus a modification of the "Aitken w extrapolation process," with the direct solution technique being an alternative method when the problems are one- or two-dimensional.

Transient thermal transport problems can be solved by the implicit technique, by an explicit method that is stable for a time step of any size, or by the stability-limited classical explicit procedure. Of these three alternatives, the generally recommended method is the implicit technique, which ranges from the Crank-Nicolson procedure to the classical implicit procedure. The equations used in the implicit technique are solved by point successive overrelaxation iteration.

HEATING6/5 is quite generally formulated and appears to have only three limitations. First, when spherical coordinates are used, only the radial dimension is available. In contrast, with both Cartesian and cylindrical coordinates, all three dimensions are available. Second, HEATING6/5 includes only conductive heat transfer, not convective or radiative. This limitation could be overcome in the case of conductive and radiative transfer by using an effective thermal conductivity that includes the radiative contribution, provided the radiative absorption length is small compared to other scales of the system. Third, boundaries must be parallel to coordinate planes.

In the case of steady state problems, the user of HEATING6/5 should vary the mesh spacing and change the convergence criterion in order to develop confidence in the solution. These same things should also be done in the case of transient problems, but the user should also vary the time increment to be sure that the numerical solution has converged to the true solution.

HEATING6/5 is written in FORTRAN-IV (enhanced) for use on an IBM 3033 or 36-195 computer.

A.8.2 Development Stage

HEATING6/5 is complete and ready for use.

A.8.3 Documentation

HEATING6 is well documented in NUREG/CR-0200.1 However, the documentation departs from the NUREG-08562 format in the following respects:

1. A standard software summary is not included.
2. A section explicitly devoted to the presentation and discussion of the assumptions and limitations of the code is missing.
3. Model review is not discussed.
4. Code verification and model validation are not discussed.
5. A description of the maintenance and quality assurance programs for the code are not provided.
6. NUREG-0856 requires a "user's manual," but NUREG/CR-0200 does not contain a separate section with that title. However, the information that should be presented in the user's manual is, in fact, thoroughly presented in NUREG/CR-0200.

A.8.4 Performance Specification Review

Performance specification review has only been done internally by ORNL.

A.8.5 Code Design Review

Code design review has only been done internally by ORNL.

A.8.6 Verification

Verification tests of HEATING6/5 are not described in NUREG/CR-0200 or in any other known document.

A.8.7 Validation

Validation tests of HEATING6/5 are not described in NUREG/CR-0200 or in any other known document.

A.8.8 Proposed SRP Application

HEATING6/5 can be used for waste package and repository assessment. In repository assessment, HEATING6/5 has far more general capabilities than TEMP.

A.8.9 Relationship of Model to Other Codes

With respect to the other SRP codes, HEATING6/5 is a stand-alone code. However, within the ORNL SCALE (standardized analyses for licensing evaluation of nuclear systems) system, it is an interactive code. HEATING is very similar, but not identical, to the code THAC-SIP-3D as documented in K/CSD/TM-24 (Turner, 1978).

A.8.10 Application of Code to Other Problems

HEATING6 was designed to solve heat flow problems arising in nuclear licensing applications.

A.8.11 Suitability of Code for Salt Repository Application

If there were significant convective heat transport in salt due to, say, water, then HEATING6/5 would not yield accurate results. If the radiative transfer in salt (salt is transparent in the infrared) were significant and if the radiative heat flow were not combined into an "effective" (conductive plus radiative) conductivity, then, again, HEATING6/5 would be inaccurate.

A.8.12 Peer Review

HEATING6/5 has not been peer reviewed.

A.8.13 References

Elrod, D.C., G.E. Giles, and W.D. Turner, HEATING6: A Multidimensional Heat Conduction Analysis with the Finite Difference Formulation, U.S. Nuclear Regulatory Commission Report NUREG/CR-0200, Oak Ridge National Laboratory Report ORNL/NUREG/SCD-2/V2, Vol. 2, Sec. F10 (Oct. 1981).

Turner, W.D., THAC-SIP-3D: A Three-Dimensional, Transient Heat Analysis Code Using the Strongly Implicit Procedure, Oak Ridge Gaseous Diffusion Plant, Oak Ridge, Tenn., K/CSD/TM-24 (Sept. 1978).

A.9 LAYFLO: A ONE-DIMENSIONAL SEMIANALYTICAL MODEL FOR THE MIGRATION OF A THREE-MEMBER DECAY CHAIN IN A MULTILAYERED GEOLOGIC MEDIUM (ONWI-466)

A.9.1 Code Description

LAYFLO calculates the transport of radionuclides in groundwater for site subsystem assessments where a layered geologic medium is present. The model output of concentration of radionuclides in groundwater (activity per unit volume) at some distance from a source can be used as input to biosphere dose codes for site assessment.

LAYFLO solves a one-dimensional equation for the transport, dispersion, decay, and sorption-desorption of radionuclides in a multilayered geologic medium. For the fully dispersive case, up to six layers, each with a different constant value for bulk soil density, porosity, and dispersion coefficient, are permitted. For the nondispersive case (zero longitudinal dispersion coefficient), any number of layers can be employed. Sorption-desorption of radionuclides is represented by linear relationships as the products of radionuclide concentrations and distribution coefficients, that may take on different constant values for each layer. Consequently, retardation factors (distribution coefficients combined with soil density and porosity) may have different constant values in each layer.

First-order radioactive decay is specified for three-membered decay chains. The source of radionuclides can take one of two forms: a continuous source at the beginning of the flow path that changes with time in accord with radioactive decay or a band release at the beginning of the flow path for which concentrations become zero after some given finite time interval.

The model is applied in the following manner. A multilayered geologic medium of distinct layers is subjected to fully saturated groundwater flow. The results of another model or analysis of this flow system delineate streamtubes (streamlines in two dimensions) through which flows a constant rate of groundwater. The one-dimensional model LAYFLO is assumed to apply through such a streamtube, which contains distinct layers, with each one having different, but constant, velocities, hydraulic properties, and sorptive properties. Given these properties, the source type and concentration, and the radionuclide decay constants for the three-member chain, LAYFLO predicts the concentration (activity per unit volume) of each radionuclide as a function of time and distance from the source.

The solution technique for LAYFLO is semianalytical in that the governing equations, source terms, and boundary conditions, including those between adjacent layers, are subjected to Laplace transforms, and the convolution theorems used to obtain inverse Laplace transforms result in expressions requiring numerical solution. In particular, summations and integrals involving exponential and complimentary error functions are required. Gauss-Legendre quadrature and various approximations and asymptotic expansions are employed. Complications in the evaluation of some terms require iteration and, if the complications are not resolved successfully after two iterations for the dispersive case, the nondispersive solution is sought.

The code has been run on the CDC CYBER 74 using FORTRAN IV. There are 3280 source program statements, and the storage requirements are 133,200 octal words (Gureghian and Jansen, 1983). The graphics package used with LAYFLO is DISSPLA.

There are several underlying assumptions and limitations that need to be considered in applying LAYFLO. Groundwater flow must be fully saturated and steady. Transverse dispersion of the contaminant is neglected by the one-dimensional nature of the model. The assumption of distinct layers and uniformity within each layer usually represents a simplification of actual geologic structures. Implicit in the model formulation is the assumption that the flow field is not modified by heat generation (temperature) or by the chemical composition of the water as it might affect viscosity and density. Dissolution of salt might, for example, violate this assumption.

A.9.2 Development Stage

The model as described in ONWI-466 was developed recently and has undergone some testing by the developers. It has apparently been made available to the National Energy Software Center. It is not fully documented in ONWI-466; documentation of use by others is not available.

A.9.3 Documentation Stage

LAYFLO is not documented in ONWI-466 as suggested in NUREG-0856.While a theoretical basis for the model, along with the governing equations, is given and several verification tests are described very briefly, the actual numerical solution technique and computer code are not discussed in any detail. There is neither a user's manual nor a listing of the code in ONWI-466. The single-solution flow chart and two appendixes related to numerical evaluations of portions of the equations are inadequate for detailed understanding of the solution procedure. The discussions of model assumptions, limitations, solution stability and accuracy, and code support and maintenance procedures are insufficient to satisfy NUREG-0856 requirements.

A.9.4 Performance Specification Review

There is no documented record of performance specification review other than what has been conducted by the code developers.

A.9.5 Code Design Review

The only evidence of any code design review is the statement that the National Energy Software Center has tested the code. However, the results of those tests are not presented in ONWI-466.

A.9.6 Verification

Several verification tests of parts of the model and the entire model are reported briefly. The verification tests and the results were as follows:

1. Two- and Three-Layered Medium, No Sorption, No Decay. Predictions were made to investigate the response of (and in a sense to validate) the transport and dispersion portions of the solution without sorption or decay. The predictions were for two-and three-layered systems in sand, for which Shamir and Harleman (1966) had laboratory experimental data. The agreement with the results of these short-time experiments is relatively good, with some deviations between predictions and data in the later part of the breakthrough curves.

2. Homogeneous (one layer) Medium, Nondispersive. The case of $^{234}U \rightarrow {}^{230}Th \rightarrow {}^{226}Ra$ was examined for the radionuclide and hydrologic conditions set forth in case 1.3 INTRACOIN (Grundfelt and Anderson, 1983) and compared with the results of code UCB-NE-25. Excellent agreement was found. Comparisons of two slightly dispersive (large Peclet numbers -- 5 v 103 and 5 v 104) runs showed close agreement with each other for ^{230}Th. However, the large Peclet number cases produced ^{230}Th concentrations almost double those of the nondispersive solution.
3. Homogeneous (one layer) Medium, Dispersive. The case of $^{234}U \rightarrow {}^{230}Th \rightarrow {}^{226}Ra$ was examined for the radionuclide and hydrologic conditions set forth in case 1.33 INTRACOIN which is the same as case 1.3 except for higher dispersion. The results were compared with those resulting from using code UCB-NE-10.2. Excellent agreement was found. The Peclet number for this dispersive case was 10 (relatively high dispersion). The results for ^{230}Th concentrations in this case are almost identical to those of the nondispersive case. This unexpected result, that is, almost no dispersion effect, has not been explained or discussed.
4. Two-Layer Medium, Nondispersive. The cases of $^{234}U \rightarrow {}^{230}Th \rightarrow {}^{226}Ra$ and $^{245}Cm \rightarrow {}^{237}Np \rightarrow {}^{233}U$ were examined for the conditions of cases 2.1 and 2.3 INTRACOIN respectively. The results of LAYFLO and code UCB-NE-30 agreed exactly for these cases.
5. Three-Layer Medium, Dispersive. Three cases were investigated using the decay chains used in the two-layer case, a dispersive Peclet number of 10, and two different sets of retardation coefficients. The results of LAYFLO were compared with several INTRACOIN results, and fair agreement was noted in the majority of solutions.

A.9.7 Validation

With the exception of the no sorption and no decay case comparisons mentioned in ONWI-466, no validation studies have been reported.

A.9.8 Proposed SRP Application

The proposed application of LAYFLO appears to be for performance assessment at site scale in cases where a layered medium exists. The area of application would need to be sufficiently far from the repository so that heat generation would not be an important process. The groundwater flow pattern through the layered medium would have to be determined prior to application of LAYFLO, as would the source terms.

While the code SWENT might, in theory, handle the case of a multi-layered geologic medium in its prediction of groundwater flow, energy transfer, and radionuclide transport, LAYFLO is simpler to operate as it predicts only radionuclide transport.

A.9.9 Relationship of model to Other Codes

LAYFLO does not require direct input from other codes. However, the groundwater flow field parameter input for LAYFLO could be derived from groundwater flow models. Specification of the radionuclide source terms could come from a repository assessment model, or they could be specified indepen dently. The output of LAYFLO nuclide concentrations in a given groundwater flow provides the release rates required as input to the biosphere transport and dose assessment codes, PABLM and DACRIN.

A.9.10 Application of Code to Other Problems

None are documented.

A.9.11 Suitability of Model for Salt Repository Application

Dissolution of salt in domes or bedded formations could result in violation of important assumptions underlying LAYFLO. Concentrations of solutes are not permitted to modify flow properties like viscosity or density, which could in turn modify the flow field. Also, sorption characteristics might vary substantially through the medium in the case of significant dissolution.

A.9.12 Peer Review

No peer or independent review of LAYFLO is documented.

A.9.13 References

Gureghian, A.B., and G. Jansen, LAYFLO: A One-Dimensional Semianalytical Model for the Migration of a Three-Member Decay Chain in a Multilayered Geologic Medium, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-466 (1983).

Shamir, U.Y., and D.R.F. Harleman, Numerical and Analytical Solutions of Dispersion Problems in Homogeneous and Layered Aquifers, MIT Report No. 89, Massachusetts Institute of Technology, Cambridge, Mass. (1966).

Grundfelt, B., and K. Anderson, INTRACOIN -- Report of Final Results of Level 1 (1983).

A.10 MMT: A RANDOM-WALK ONE-DIMENSIONAL MULTICOMPONENT MASS TRANSPORT CODE (ONWI-432)

A.10.1 Code Description

MMT calculates the transport of radionuclides in ground-water. Its output of radionuclide release rates as a function of time at the end of the specified flow path is appropriate input to biosphere dose codes for site assessment (INTERA, 1983).

MMT solves a one-dimensional equation for the transport, dispersion decay, and sorption-desorption of radionuclides in a simplified groundwater system. The groundwater system is characterized by constant (spatially uniform and steady) velocity, constant porosity, constant bulk density, and constant longitudinal dispersion coefficient. The sorption-desorption of radionuclides is represented in the model by a linear relationship as the products of radionuclide concentrations and spatially uniform distribution coefficients. The distribution coefficients and related retardation coefficients depend on bulk rock properties and average geochemical data and must be specified as input to the model.

Radioactive decay of up to ten different radionuclides can be accommodated. First-order radioactive decay can be included as can linear or branched decay chains (with daughter products) with an arbitrary number of members. Specification of the source of radionuclides for the one-dimensional framework is relatively general -- it can have a general time dependence, that is, it is not restricted to an impulse or band release. For example, the release can be leach-limited, with an arbitrary form of leach rate, or it can be solubility-limited, with a constant concentration but variable mass.

A simplified summary of the input to the code follows. The groundwater system is characterized by its transport velocity, dispersion coefficient, bulk density, and porosity. The height, width, and length of the "one-dimensional" transport pathway are specified. Each radionuclide contaminant is identified by a code number relating it to an external library of half-life data, is assigned a distribution coefficient for sorption-desorption, and is given an initial inventory in curies. Radioactive decay is specified as no chain, linear chain, or branched chain, and decay constants must be inputted. The source of radionuclides is described both spatially and in time in terms of (1) the center of the release position along the direction of flow, (2) the length of the initial release position, (3) the time of leaching start, (4) the fraction of inventory remaining versus time function, and (5) the total time of leaching.

Given these input data, the code accounts for transport, dispersion, sorption-desorption, and radioactive decay as the contaminants are carried away from the source region. The release rate in curies per year is calculated for each individual contaminant at the end of the specified flow path as a function of time.

The numerical solution of the governing equation follows a discrete-parcel-random-walk (DPRW) approach in contrast to a finite-difference approach. The DPRW approach is inherently stable and minimizes computational errors associated with finite-differencing of problems with a convective transport component. Such errors are often manifested by difficulties in conserving mass. While there is some numerical dispersion in the DPRW approach resulting from generation of members of a decay chain with different retarded transport velocities, the dispersive error does not accumulate to frustrate mass conservation.

The DPRW simulation traces the behavior of a finite number of discrete parcels through the system. There is no means of determining the number of parcels and the accuracy of the results other than experience and solution comparisons. The DPRW solution usually takes more computational time than comparable finite-difference solutions for which stability and accuracy are acceptable, but, for many problems, the inherent stability and accuracy of DPRW offset the increased time requirements. Solution accuracy increases as the square root of the number of parcels used and, in the case of linear source terms, solutions from independent computations can be averaged to increase accuracy. A certain amount of statistical noise in the solutions results from the random-walk aspect of the simulation. Postprocessing with a variable-window, moving-average filtering method is available to deal with this problem.

The computer program compiles on a FTN5 compiler for CDC systems, particularly the CYBER 176. The compiler is compatible with the FORTRAN V language. The program is set up for mixed batch and interactive usage. The interactive aspect facilitates setting up the problem to be run, whereas the production of raw nuclide release rates is done in batch mode. A plotting routine compatible with CALCOMP software is used. The core storage requirement is largest for the main release rate computation, which requires approximately 77,000 decimal words.

There are several general assumptions and limitations of MMT that should be considered before application. The groundwater transport system is highly simplified: fully saturated flow and temporal and spatial uniformity are assumed. Consideration of dispersion is limited to the longitudinal direction because of the one-dimensionality, which means that transverse dispersion is neglected. The flow field is assumed to be independent of the temperature and chemical composition of the groundwater. Thus, flow fields affected by heat sources can not be handled by this approach. Also, significant dissolution of the porous medium (particularly salt) would invalidate the MMT approach.

A.10.2 Development Stage

The version of MMT described in ONWI-4321 was modified by INTERA in 1983 for use on CDC computer systems. The theoretical and numerical approaches for MMT were established earlier at Battelle's Pacific Northwest Laboratories

(Ahlstron et al., 1977; Washbuirn et al., 1980). INTERA has also initiated verification of MMT.

A.10.3 Documentation

MMT is documented in ONWI-432 in accordance with the guidelines of NUREG-0856,4 including a complete user's manual and program listing.

A.10.4 Performance Specification Review

The only documented performance specification review is the one in ONWI-432. No peer review or other outside review of MMT has been documented.

A.10.5 Code Design Review

Preparation of ONWI-432 by INTERA constitutes the only documented code design review. While a "reader's comments" card is provided in ONWI-432 for comments on code performance, no outside code design reviews have been documented.

A.10.6 Verification

Comparisons of the results of MMT and existing analytical solutions for two different cases with the same hydrologic parameters are described. One case considers the fate of a single radionuclide, ^{129}I, and the other of a two-member decay chain of ^{248}Cm and ^{244}Pu. The analytical solutions were from Lester et al. (1975). The hydrologic data were: (1) groundwater velocity = 100 m/yr, (2) length of flow path = 10,000 m, (3) bulk density of soil to porosity ratio = 5 g/ml, and (4) longitudinal dispersion coefficient = 1 m^2/yr. The nuclides were apparently released (leached) linearly from the source for 1000 years. The data on the nuclides for both cases are shown in Table A-1.

Numerical solutions for MMT were found for a base case for ^{129}I, ^{248}Cm, and ^{244} Pu using parcel densities of 6500, 3250, and 7500, respectively. Then, for each nuclide, the corresponding particle densities were doubled,

Table A-1. Nuclide Data Use in Comparing MMT and Existing Analytical Solution Results

Nuclide	Inventory (curies)	Half-Life[a] (yr)	Distribution Coefficient (ml/g)	Retardation Coefficient
^{129}I	1.0	1.72×10^7	0.0	1
^{248}Cm	0.5	4.7×10^5	333	1666
^{244}Pu	5.36×10^7	7.6×10^7	1000	5001

[a]These half-life values are incorrect but were used consistently in both the MMT and analytical solutions.

Source: INTERA, 1983.

increased fourfold, and increased eightfold. For ^{129}I, increased parcel density resulted in increased agreement between numerical and analytical results, primarily in the timing of peak release rates. The same result was true for ^{248}Cm. The release rate histories for the daughters of ^{248}Cm and ^{244}Pu showed shifts in peak locations with increasing parcel density. In all cases, agreement between MMT results and the analytical solutions was quite good, with deviations in release rates being less than 10%. INTERA felt that deviations from analytical results would be attributed to the statistical nature of MMT results and the smoothing filter. Also, the finite length of the path for MMT, in contrast to the infinite boundary conditions for the analytical solution, may have affected the comparisons.

A.10.7 Validation

According to ONWI-432, no formal validation has yet been performed.

A.10.8 Proposed SRP Application

The proposed application of MMT is for performance assessment in the far field. It is anticipated that MMT can be used where the one-dimensional simplification of the groundwater system can be justified (perhaps as the result of more detailed groundwater system study) and where the distance from the repository will permit neglect of temperature influences on the flow field. The generalized form of the radionuclide source terms and the flexibility of handling several nuclides with branched decay chains makes MMT attractive for screening the relative merits of various proposed or hypothetical waste disposal systems. The simplified nature of the hydrologic environment representation may mean that MMT will have greater value for such comparisons than it will for detailed analysis of a specific site.

Two other codes address generally similar problems. SWENT evaluates hydrologic flow and energy transfer, as well as radionuclide transport. Because it handles coupling among these processes, it is much more sophisticated. Because SWENT has a finite-difference solution, numerical dispersion does present a problem. Because MMT has the flow field specified and uncoupled from energy and radionuclide transport, it is far simpler to apply than SWENT. GETOUT is similar to MMT in that it is one-dimensional, with constant transport properties. GETOUT has a Laplace transform solution approach that limits the application to three-member decay chains and to impulse or fixed band source terms. Being less limited, MMT is more versatile than GETOUT.

A.10.9 Relationship of Model to Other Codes

MMT does not require direct input from other codes. However, the groundwater flow field required as input could be derived from groundwater flow models. Radionuclide source terms could be specified using results from repository assessment models or could be specified independently. MMT doesrequire input on radionuclide half-lives from the data library SWNUCLB, a radionuclide library that is part of the INTERA SCEPTER program.

The output of MMT -- radionuclide release rates as a function of time at the end of the flow path -- can be used directly as input to a biosphere transport and dose assessment code such as PABLM.

A.10.10 Application of Code to Other Problems

As stated in ONWI-432, MMT has been applied to a number of problems. However, no documented applications have been cited.

A.10.11 Suitability of Model for Salt Repository Application

The major difficulty in applying MMT to sites in salt domes or bedded salt formations is the assumption that concentrations of solutes in the groundwater are so low that they do not to affect the viscosity or density of the solution significantly. Violation of this assumption with regard to either parameter could result in serious modifications to the transport flow field. Also, if dissolution is significant, there is the possibility of major changes in the sorption-desorption characteristics of the medium.

A.10.12 Peer Review

Apart from ONWI-432, no independent review of MMT has been documented.

A.10.13 References

INTERA Environmental Consultants, Inc., MMT: A Random-Walk One-Dimensional Multicomponent Mass Transport Code, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-432 (April 1983).

Ahlstron, S.W., et al., Multicomponent Mass Transport Model: Theory and Numerical Implementation (Discrete-Parcel-Random-Walk Version), Battelle Pacific Northwest Laboratories Report BNWL-2127 (1977).

Washburn, J.F., et al., Multicomponent Mass Transport Model: A Model for Simulating Migration of Radionuclides in Ground Water, Battelle Pacific Northwest Laboratories Report PNL-3179 (1980).

Lester, D.H., G. Jansen, and H.C. Burkholder, Migration of Radionuclide Chains through an Adsorbing Medium, Adsorption and Ion Exchange, American Institute of Chemical Engineers Symp. Ser. 152, Vol. 72 (1975).

A.11 ORIGEN2: A REVISED AND UPDATED VERSION OF THE OAK RIDGE ISOTOPE GENERATION AND DEPLETION CODE (ORNL-4628)

A.11.1 Code Description

ORIGEN2 is a point depletion and decay computer code for use in simulating nuclear fuel cycles and calculating the nuclide compositions of nuclear fuel cycle materials (Roff, 1980). The code is an updated version of the ORIGEN code that was distributed by Oak Ridge National Laboratory (ORNL) in the early 1970s (Bell, 1973). It can be applied to a wide variety of fuel cycle flowsheets and fuel/reactor-type combinations. The code generates, as a function of time after irradiation, spent fuel and waste characteristics, including nuclide inventory, radioactivity, and thermal power. This information is needed for design of fuel reprocessing plants, spent fuel and waste shipping casks, and waste treatment and disposal facilities. Outputs also include radioactive ingestion and inhalation toxicity, and chemical ingestion toxicity. In other works, the code calculates the amount of air or water required to dilute substances to acceptable levels.

The buildup and depletion of nuclides in materials during irradiation is calculated using point geometry and quasi-one-group neutron cross sections. The model does not account for spatial or resonance self-shielding effects or changes in the neutron spectrum other than those encoded initially. However, provision has been made to incorporate appropriate cross sections from more sophisticated reactor physics codes. This option requires calculations using separate codes supplied by the user.

The buildup and depletion processes are represented by a system of first-order ordinary differential equations with constant coefficients. This system is solved using a matrix exponential numerical method that is so memory intensive that a recursion relation is used to reduce the memory requirements. To maintain numerical accuracy and keep computing time down, only the long-lived isotopes are treated with the matrix exponential method. Alternative techniques are used for the short-lived isotopes.

ORIGEN2 requires three data libraries that can be prepared from three master libraries at ORNL by ORNL staff. User-supplied input data are also required. Cross sections from other, more sophisticated reactor physics codes may also be required if the point-geometry assumptions used in ORIGEN2 are inadequate.

The code is composed of some 60 subroutines. An overlay procedure is used to conserve core memory space. Written entirely in FORTRAN, the code is composed of some 7300 source statements. Versions are available through the ORNL Radiation Shielding Information Center for both IBM and CDC machines. Core requirements range from 175K to 600K, depending on the problem size.

A.11.2 Development Stage

ORIGEN2 is a substantially revised version of the ORIGEN code that has been in use since the late 1960s and early 1970s.

A.11.3 Documentation

The documentation does not conform to NUREG-0856. It includes a brief description of ORIGEN2, a technical description of the original ORIGEN code, and a user's manual for ORIGEN2 (Croff, 1980b). The documentation of ORIGEN2 in ORNL-4628 provides a brief description of the differences between ORIGEN2 and ORIGEN, but ORNL-4628 is not a stand-alone documentation of the ORIGEN2 code. Furthermore, a standard software summary is not included.

A.11.4 Performance Specification Review

No performance specification review has been documented.

A.11.5 Code Design Review

No code design review has been documented.

A.11.6 Verification

Code verification has not been discussed in the available code documentation.

A.11.7 Validation

Validation exercises have not been documented.

A.11.8 Proposed SRP Application

SRP has not indicated what specific problems require the use of ORIGEN2, except to say that it can be used for "waste package subsystem analyses." Because several other models have been selected for specific roles in the waste package assessment plan, it appears that ORIGEN2 could serve as the source-term generator for those other models. If so, it would be worth while to look into how well that role could be satisfied by ORIGEN2 and, in particular, what modifications, if any, would be required to satisfy that role.

A.11.9 Relationship of Model to Other Codes

ORIGEN2 provides source-term information on wasteform element and isotope inventory, radiation levels, and heat generation as a function of time. This information is required by the process models contained in the WAPPA package, as well as by other codes used in performance assessment of the waste package and its immediate surroundings. However, the detailed links between ORIGEN2 and WAPPA, for example, are not discussed in the documenta tion, and it is not known if any additional data processing is required.

A.11.10 Application of Code to Other Problems

ORIGEN2 is a revision of ORIGEN, a code that has been widely distributed since the early 1970s. Although it has been used by ORNL for license application calculations, specific applications of ORIGEN2 are not cited in the documentation.

A.11.11 Suitability of Model for Salt Repository Application

Since ORIGEN2 is a source-term code, its application to a specific type of repository is not at issue, so long as the wasteform can be handled by the code. Details regarding the specific wasteform and the ability of ORIGEN2 to handle such a wasteform have not been documented.

A.11.12 Peer Review

The documentation does not indicate that ORIGEN2 has been peer reviewed.

A.11.13 References

Croff, A.G., ORIGEN2 -- A Revised and Updated Version of the Oak Ridge Isotope Generation and Depletion Code, Oak Ridge National Laboratory Report ORNL-4628 (July 1980a).

Bell, M.J., ORIGEN -- The ORNL Isotope Generation and Depletion Code, Oak Ridge National Laboratory Report ORNL-4628 (May 1973).

Croff, A.G., A User's Manual for the ORIGEN2 Computer Code, Oak Ridge National Laboratory Report ORNL/TM-7175 (1980b).

A.12 PABLM: A COMPUTER PROGRAM TO CALCULATE ACCUMULATED RADIATION DOSES FROM RADIONUCLIDES TRANSPORTED TO AQUATIC AND TERRESTRIAL PATHWAYS IN THE BIOSPHERE (ONWI-446)

A.12.1 Code Description

PABLM is a biosphere transport and dose code that calculates internal radiation doses to humans from ingestion of food and water contaminated with radionuclides and from external radiation doses from radionuclides in the environment, for both acute and chronic exposures (Napier, et al., 1980). Radiation doses from radionuclides in the environment may be calculated from deposition on the soil or plants during an atmospheric or liquid release, or from exposure to residual radionuclides after the releases have ended. Radioactive decay is considered during the release, after deposition, and during storage of food after harvest. The radiation dose models consider exposure to radionuclides (1) deposited on the ground or crops from contaminated air or irrigation water, (2) in contaminated drinking water and in aquatic foods raised in contaminated water, and (3) in bodies of water and sediments where people might fish, boat, or swim. For vegetation, the radiation dose model considers both direct deposition and uptake through roots. Doses can be calculated for either a maximum-exposed individual or for a population group. The program can also calculate accumulated radiation doses from chronic ingestion of food products that contain radionuclides and from chronic external exposure to radionuclides in the environment. A first-year committed dose is calculated as well as an integrated dose for a selected number of years.

A chain decay scheme including branching for transitions to and from isomeric states is used for radioactive decay. The equations for calculating internal radiation doses are derived from those given by the International Commission on Radiological Protection (ICRP, 1959) for body burdens and the maximum permissible concentration (MPC) for each radionuclide. These doses are calculated as a function of radionuclide concentration in food products, ingestion rates, and a radionuclide-specific dose-commitment factor. Radiation doses from external exposure to contaminated water and soil are calculated using the basic assumption that the contaminated medium is large enough to be considered an "infinite" volume or plane relative to the range of emitted radiation. The equations for calculating the radiation dose from external exposure to shoreline sediments include a correction for the finite width of the contaminated beach.

The code can accommodate no more than 23 possible body organs or tissues, 19 ingestion pathways, five organs and 100 radionuclides in a mixture, and four external exposure pathways.

The programming language is FORTRAN V. The computer for which the program was designed and other available machine version packages are the UNIVAC 1100 and CDC systems. Eighty thousand words of memory are required to execute the PABLM program. The National Energy Software Center (NESC, 1981) reports executing sample problems in two minutes of central processing unit (CPU) time on a UNIVAC 1100/44.

A.12.2 Development Stage

PABLM is ready for use. It is available in an operational UNIVAC as well as in an operational CDC version.

A.12.3 Documentation

The CDC version of PABLM is documented in NUREG-0856 format in ONWI-446 (INTERA, 1983), which contains a federal information processing standard summary, a user's manual, and a sample case. The UNIVAC version is fully documented in PNL-3209 (Napier et al., 1980) and is further documented by the National Energy Software Center (NESC, 1981). Additional summary documentation of PABLM is available in SAI, 1981; Shriner and Peck, 1978. The documentation summary of PABLM in ONWI-78 is erroneous with respect to purpose, description, and keywords, in that it incorrectly identifies PABLM as a code dealing with ingestion of radionuclides from the air pathway.

A.12.4 Performance Specification Review

The UNIVAC version of PABLM has been accepted by the nuclear industry and NRC, and has been used extensively in the licensing of nuclear projects (USDOE, 1980). No performance specification review has been carried out specifically for nuclear waste isolation applications.

A.12.5 Code Design Review

The UNIVAC version of PABLM has been accepted by the nuclear industry and NRC, and has been used extensively in the licensing of nuclear projects. No performance specification review has been carried out specifically for nuclear waste isolation applications.

A.12.6 Verification

The version of the PABLM code incorporated into the SCEPTER (Brecher and Pearson, 1983) package is reported in ONWI-446 as having been thoroughly checked to ensure that it produces results that are substantially the same as those from the earlier version of the code (Napier et al., 1980). These efforts were made to ensure that the modifications of the code made to generalize its application to CDC and other computer systems, and to provide integration with other codes in the SCEPTER package did not lead to errors.

The checks included, as a verification test, an aquatic release sample problem described in the documentation of the original code. The sample problem calculates the dose to a maximally exposed individual living down stream from a groundwater discharge point. The groundwater is assumed to be contaminated with radionuclides and to be seeping into a river. In the original application, this problem included a tank leaking radionuclides into a river. While it would be unlikely that this description would apply to a repository system, it was used for the sample case.

The biosphere pathways in the above sample problem assume that the individual uses the contaminated river for irrigation water, fishing, and drinking water. Chronic exposure is assumed to occur over a 70-year period. Five radionuclides, ^{3}H, ^{14}C, ^{90}Sr, ^{137}Cs, and ^{239}Pu, are released to the river at time equals 1000 years, with initial release rates of 50, 5, 0.5, 1.0, and 0.1 Ci/year, respectively. The PABLM code automatically includes the important daughter products of the selected radionuclides in the evaluation. The results of running this sample problem with the new PABLM code were found to agree very well with those using the earlier version of PABLM.[5]

A.12.7 Validation

PABLM is based on the well-known ICRP-2 methodology, which has been used for many years. It provides predictions of dose based on idealized discharges of radionuclides from the repository system to the biosphere. The individual models used to determine the dose conversion factors are each based on empirical data. The factors are then related to the phenomenology for biosphere transport and uptake by plants, animals, and human beings.

Thus, the code is tied closely to existing data and is based on methodology that has been considered satisfactory for a number of years. Because of the simplicity of the discharge model of radionuclides, use of the code should provide a conservative upper bound estimate of the dose (INTERA, 1983). However, in this case, the code is intrinsically not susceptible to validation. Examples are not available in nature with which dose predictions with the code can be compared. In other words, it is not feasible to compare a predicted dose to the "real" dose received by a person. It is in this sense, then, that dose assessment models cannot, strictly speaking, be validated.

PABLM appears to have been accepted as valid for use by NRC and the nuclear industry, and has been used extensively in the licensing of nuclear projects (USDOE, 1980).

The use of ICRP-2 methodology is defended in Sec. 2.4 "Advantages and Limitations of the Approach" of ONWI-446. Because PABLM is well documented and well understood, and represents a rather large investment, arguments can be made to use this code until ICRP-30 codes are developed to a comparable level of trust.

A.12.8 Proposed SRP Application

PABLM is to be used as a site assessment code for biosphere radionuclide transport and radiation dose. In particular, it is to be used as a human dose model for ingestion and external exposure through different pathways, both for environmental radiological exposures under normal operations and for environmental radiological exposure after accidents. The code could be used to assess the performance of a geologic radioactive waste repository system both during operation and after post-closure releases. Because the dosimetry model is independent of the origin of the radionuclides, PABLM and related codes are applicable to a nuclear waste repository in salt.

A.12.9 Relationship of Model to Other Codes

Many models and codes for biosphere transport and for radiological dose to humans are available; relevant tabulations are found in (SAI, 1981). ARRRG,FOOD performs related calculations restricted to a one-year dose and a committed dose from one year of exposure. Other programs that compute organ dose factors include AERIN, which calculates organ and tissue burdens resulting from acute exposure to a radioactive aerosol; DACRIN, which calculates organ dose from acute or chronic radionuclide inhalation; and SUBDOSA, which calculates external dose from atmospheric release of radionuclides.

PABLM requires the following data libraries: master radionuclide and radiological decay data library RDMLIB, organ data library ORGLIB, aquatic bioaccumulation factor library BIOAC, external radiation dose factor library GRDFLIB, and food transfer coefficient library FTRANSLIB.

The PABLM code can be coupled with the DACRIN code for radiation dose from inhaled materials. It can be used in conjunction with solute transport codes like SWENT, LAYFLO, MMT, GETOUT, and DPCT (Thomas et al., 1982). PABLM is incorporated as part of the SCEPTER technology package (Brecher and Pearson, 1983). It can be used in conjunction with site subsystem groundwater flow and radionuclide transport codes to assess site subsystem performance. This same approach can be applied to the other subsystems (waste package and repository), although care must be taken in specifying the pathway from the subsystem to the biosphere and the model for discharge to the biosphere itself. The version of PABLM used in SCEPTER does not evaluate inhalation dose; this calculation can be performed by the code DACRIN, which is also in the SCEPTER package and, together, these codes can be used to evaluate the total dose commitment associated with predicted radionuclide release rates.

A.12.10 Application of Code to Other Problems

PABLM has been used extensively in the licensing of nuclear projects. The original version of the PABLM code was written to calculate internal and external radiation doses from radionuclides released to the biosphere from a nuclear facility (Napier et al., 1980).

A.12.11 Suitability of Model for Salt Repository Application

Because the dosimetry model is independent of the origin of the radionuclides, PABLM is suitable for salt repository applications. There are no unique aspects to its application for a nuclear waste repository in salt.

However, there are some limitations in the use of this code in the assessment of such a situation. PABLM is designed to evaluate the dose that occurs within one generation, for example, during the lifetime of an individual. There may be situations where multigenerational effects may be important for long-term releases(Smith et al., 1982). For example, although the present version of PABLM considers the accumulation of radionuclides in farmland as a result of continued irrigation with contaminated water, this accumulation is not considered for more than the time of exposure.

Another limitation is in the dose models themselves. The models in PABLM are all based on the formulation of the models in ICRP-2 More recent developments suggest that some of these models may need to be reviewed (ICRP, 1979).

PABLM can be used in conjunction with the site subsystem groundwater flow and radionuclide transport codes to assess site subsystem performance. This same approach can be applied to the other subsystems (waste package and repository); however, care must be taken in specifying the pathway from the subsystem to the biosphere and the model for discharge to the biosphere itself.

A.12.12 Peer Review

No peer review has been documented.

A.12.13 References

International Commission on Radiological Protection, Report of ICRP Committee II on Permissible Dose for Internal Radiation, ICRP Pub. 2, Pergamon Press, New York, N.Y. (1959).

National Energy Software Center, PABLM, NESC No. 926.1100, PABLM Tape Description and Documentation of Changes Made Subsequent to PNL-3209 Publication, NESC-926, Note 81-72 (April 3, 1981).

INTERA Environmental Consultants, Inc., PABLM -- A Computer Program to Calculate Accumulated Radiation Doses from Radionuclides Transported to Aquatic and Terrestrial Pathways in the Biosphere, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-446 (1983).

Napier, B.A., et al., PABLM -- A Computer Program to Calculate Accumulated Radiation Doses from Radionuclides in the Environment, Battelle Pacific Northwest Laboratories, Richland, Wash., PNL-3209 (March 1980).

Science Applications, Inc., Tabulation of Waste Isolation Computer Models, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-78 (Aug. 1981).

Shriner, C.R., and L.J. Peck, Inventory of Data Bases, Graphics Packages, and Models in Department of Energy Laboratories, Oak Ridge National Laboratory Report ORNL/EIS-144 (Nov. 1978).

U.S. Department of Energy, Final Environmental Impact Statement -- Management of Commercially Generated Radioactive Waste, U.S. Dept. of Energy Report DOE/EIS-0046F (Oct. 1980).

Brecher, A., and F.J. Pearson, Jr., The SCEPTER Waste Package Subsystem Computer Model for Performance Assessment, in Scientific Basis for Nuclear Waste Management VI, D.G. Brookins, ed., Elsevier Science Publishing Co., New York, N.Y. (1983).

Thomas, S.D., B. Ross, and J.W. Mercer, A Summary of Repository Siting Models, U.S. Nuclear Regulatory Comm. Report NUREG/CR-2782 (July 1982).

Smith, C.B., et al., Population Risks from Disposal of High-Level Radioactive Wastes in Geologic Repositories, U.S. Environmental Protection Agency Report EPA-520/3-80-006, unpublished manuscript (Dec. 1982).

International Commission on Radiological Protection, Report of the ICRP Committee II on Permissible Dose for Internal Radiation, ICRP Pub. 30, Pergamon Press, New York, N.Y. (1979).

A.13 SPECTROM-58: A SENSITIVITY STUDY OF BRINE TRANSPORT INTO A BOREHOLE CONTAINING A COMMERCIAL HIGH-LEVEL WASTE CANISTER (ONWI-384)

The SPECTROM series of codes has been developed by RE/SPEC to analyze a wide range of rock mechanical, thermal, thermomechanical and hydrologic problems. The SPECTROM-58 code is addressed in this appendix.

A.13.1 Code Description

SPECTROM-58 is a two-dimensional (Cartesian) finite-element code for predicting brine transport in natural rock salt as a function of time. The model on which the code is based views the rock salt as consisting of individual crystals, with some of the pore space between the crystals being hydraulically connected and the rest unconnected.

A rock salt crystal typically contains small inclusions of liquid brine. In the presence of a temperature gradient, these inclusions migrate up the gradient to the hotter region. (Dissolution of salt at the hot end of the inclusion and its precipitation at the cool end have been invoked to account for this migration.) This thermally driven transport of brine within salt crystals is one of two brine transport mechanisms in the SPECTROM-58 model. The other is the pressure-driven transport of brine through the connected pore space. When migrating brine inclusions reach the boundary surface of an individual crystal, the model assumes that the inclusion-brine passes through that surface into the pore space and never reenters the same, or any other, crystal.

Inclusion-brine that thus enters connected pore space contributes to the brine flow through that space. In the conceptual SPECTROM-58 model (i.e., the model on which the code SPECTROM-58 is based), the very discontinuous salt crystal matrix is replaced by a continuous volume of salt, and an equation expressing conservation of inclusions in that continuous volume is formulated. This equation contains a term that represents the loss of inclusions at crystal boundaries. The derivation of this equation assumes that all brine inclusions are of uniform size and shape and remain as such.

A second equation is derived by (1) considering the connected pore space to be fully saturated with brine, (2) assuming the connected-pore-space brine flows according to Darcy's equation, (3) assuming that flow is driven only by pressure gradients, and (4) writing down a mass conservation equation for the connected-pore-space brine. This conservation equation contains a source term that takes into account the flux of inclusion-brine into the connected pore space. Permeability can be anisotroptic, and the salt matrix and the brine are both taken to be compressible. A third model equation is the empirical equation that expresses the inclusion velocity within crystalline salt as a function of the temperature and temperature gradient.

The three model equations constitute the basis for the SPECTROM-58 code. Input to the code consists of system geometry, temperature field, properties of the brine and salt, and initial and boundary conditions. Output includes pressures, values of inclusion density, and the components of the two-dimensional inclusion velocities. The Galerkin finite-element method is used to obtain output from input.

Limitations of SPECTROM-58 include those arising from the above-noted assumptions. Other, and probably very significant, limitations are that the SPECTROM-58 model does not take into account absorption of water molecules by the salt crystals or dissolution of salt into the connected-pore-space brine. Even if the brine has an equilibrium concentration of salt at one temperature, when it convects to a warmer (or cooler) location, it will no longer be in equilibrium.

The code SPECTROM-58 is presumably written in FORTRAN. The code documentation specifies neither the language nor the type of computer on which the code has been run.

A.13.2 Development Stage

SPECTROM-58 is complete and operational.

A.13.3 Documentation

SPECTROM-58 is documented in ONWI-384 (Ratigan, 1983a), and in two additional documents by Ratigan (1983a,c). These documents do not, and clearly were not intended to, follow the NUREG-0856 format. Nevertheless, they contain many of the elements required by that format, including a reasonably complete derivation of the mathematical model, a thorough description of the finite-element solution to the model equations, a report of a verification test, and parts of a user's manual.

The following points pertain to the derivation of the mathematical model as presented in ONWI-384.

1. The assumption that all brine inclusions have the same size and shape is probably weak. It may not be necessary to make this assumption. Instead, it may be possible to base the theory on average properties (volume and velocity) of the inclusions.
2. It appears that the mechanism that makes the inclusions migrate to a region of higher temperature should also make the connected-pore-space brine move to the higher temperature region. But the SPECTROM-58 model excludes all transport except that caused by pressure gradients.
3. Equation 2-3 in ONWI-384 is

$$Q = \frac{|\tilde{V}|}{D} \rho$$

where:

Q = flux of brine inclusion density across a crystal surface per unit volume of crystal.

$|\tilde{V}|$ = magnitude of inclusion velocity $\tilde{V}$

D = ratio of crystal volume to crystal surface area, and

ρ = brine inclusion density.

As it appears, Ea. 2-3 is incorrect. The correct equation, found by averaging over the entire crystal, is

$$Q = \frac{|\tilde{V}|}{D} \, \rho\tilde{n} \cdot \frac{\tilde{V}}{|\tilde{V}|}$$

where $\rho\tilde{n} \cdot \frac{\tilde{V}}{|\tilde{V}|}$ denotes the average values of $\rho n \cdot \frac{\tilde{V}}{|\tilde{V}|}$ ($\tilde{n}$ = outward normal to the crystal surface) over the crystal surface.

This average value will always be nonnegative and could be zero, For example, it would be zero for a crystal that is infinitely long and whose axis is in the direction of the temperature gradient.

4. The model's assumption that the connected pore space is fully saturated seems highly unlikely to be realized in a salt formation selected for its dryness.

A.13.4

Performance Specification Review

No performance specification review is known to have taken place.

A.13.5 Code Design

No code design review is known to have taken place.

A.13.6 Verification

One verification test, for a very simple geometry, has been made. As the number of mesh elements increased and the size of the time steps decreased, the finite-element solution approximated the analytic solution much better. The number of elements was increased to eight and no higher; for this number, the discrepancy between the SPECTROM-58 solution and the analytic solution was good for the pressure curves (for which the analytic solution was continuous) but not so good for the inclusion density curves (for which the analytic solution was discontinuous).

A.13.7 Validation

SPECTROM-58 has not been validated.

A.13.8 Proposed SRP Application

SPECTROM-58 could be used for repository assessment. In fact, it has already been used to estimate the rate at which inclusion brine is transported to the waste package (Ratigan, 1983a). SPECTROM-58 might also be used to study the flow of water through the salt formation in which the repository is embedded.

A.13.9 Relationship of Model to Other Codes

SPECTROM-58 needs to obtain input temperatures from a thermal transport code like HEATING6/5, DOT, TEMP. The code MIGRAIN (Rickertsen, 1980) like SPECTROM-58, simulates the migration of brine inclusions but, unlike SPECTROM-58, it has no capability for simulating the flow of brine through the connected pore space of a salt formation.

A.13.10 Application of Code to Other Problems

No other application is currently envisaged.

A.13.11 Suitability of the Model for Salt Repository Application

SPECTROM-58 is intended to simulate the transport of brine in natural rock salt in the presence of temperature and pressure gradients. However, the code's neglect of water absorption by the salt and of dissolution of the salt into the brine may cause significant inaccuracies.

A.13.12 Peer Review

SPECTROM-58 has not been peer reviewed.

A.13.13 References

Ratigan, J.L., A Sensitivity Study of Brine Transport into a Borehole Containing a Commercial High-Level Waste Canister, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, Topical Report RSI-0185, ONWI-384 (Feb. 1983a).

Ratigan, J.L., A Finite Element Formulation for Brine Transport in Natural Rock Salt, submitted to Int. J. for Analytical and Numerical Methods in Geomechanics (1983b).

Ratigan, J.L., Input Guide for SPECTROM-58, Technical Letter Memorandum RSI-0090, RE/SPEC, Inc., Rapid City, S.D. (1983c).

Rickertsen, L.R., Brine Migration in a Bedded Salt Nuclear Waste Repository, Proc. Heat Transfer in Nuclear Waste Disposal, Annual Winter Meeting of ASME, HTD, Vol. II, p. 101 (Nov. 16-21, 1980).

A.14 STEALTH-2D HYDROLOGICAL MODEL (ONWI-256)

A.14.1 Code Description

STEALTH is a package of explicit finite-difference codes developed to solve time-dependent, nonlinear problems in continuum mechanics and time-dependent problems in fluid flow. STEALTH-2D is a two-dimensional planar or axisymmetric thermomechanical code (Hofmann, 1976). The STEALTH-2D HYDROLOGICAL MODEL is a two-dimensional planar or axisymmetric code that solves the equations of fluid flow in a porous medium (Hofmann and Hart, 1979). When STEALTH-2D predicts thermally induced rock fracturing, the STEALTH-2D HYDROLOGICAL MODEL can be coupled with it to predict water flow through the fractures. Input to STEALTH-2D HYDROLOGICAL MODEL consists of the geometry of the flow region; values of liquid viscosity, compressibility, and density; values of the permeability and porosity of the porous medium; boundary conditions; and the initial pressure as a function of position. Output is fluid pressure and flow as a function of position and time. The equations solved by the STEALTH-2D HYDROLOGICAL MODEL are the Darcy equation, the mass conservation equation, and the equations for fluid potential piezometric head and fluid compressibility.

In addition to being restricted to two-dimensional geometries, the STEALTH-2D HYDROLOGICAL MODEL code has the following limitations: (1) dimensions must be such that Darcy flow is legitimate; (2) the spatial region modeled must be homogeneous, although the permeability can be anisotropic; (3) it is assumed that the porous medium does not dissolve into the fluid; and (4) the product of the fluid compressibility and the pressure is assumed to be much less than one. ONWI-256 specifies neither the language in which STEALTH-2D HYDROLOGICAL MODEL is written nor the type of computer on which the code has been run.

A.14.2 Development Stage

STEALTH-2D HYDROLOGICAL MODEL is ready for use within the constraints imposed by the Proprietary nature of STEALTH-2D.

A.14.3 Documentation

The documentation in ONWI-256 is generally good, but incomplete (Hofmann and Hart, 1979). Because ONWI-256 was written prior to issuance of NUREG-0856, it does not follow those guidelines. In particular, ONWI-256 uses the term "validation" to mean what NUREG-0856 defines as "verification," and the document does not include a user's manual.

Aside from the NUREG-0856 guidelines, the ONWI-256 documentation is deficient in three respects. First, it is incomplete in that the reader is referred to Ref. 5 of ONWI-256, a proprietary document, for important explanatory material. Second, the types of boundary conditions required for the solution of Eq. 2.10 should be discussed. Third, ONWI-256 assumes that the fluid density is constant while the fluid compressibility is nonzero. It is possible to have both constant fluid density and nonzero compressibility only if the pressure is constant as a function of position and time. In any problem of practical interest, this condition will not be realized. Actually, it is not necessary to assume both constant density and nonzero compressi bility to derive Eq. 2.10 of ONWI-256, the basic equation of the model. One should instead assume nonzero compressibility and compressibility constant with respect to pressure, and that the product (dimensionless) of pressure, p, and compressibility, β is small compared to one. Then Eq. 2.6 can be solved to obtain the following solution:

$$\rho = \rho_o \exp \quad \beta p \quad = \rho_o \quad 1 = \beta p + \ldots$$

where the subscripts have been dropped. According to this solution, the fluid density ρ is nearly, but not strictly, constant. Using this solution, Eq. 2.10 can be derived by dropping terms of order βp. As written, the derivation of Eq. 2.10 is quite confusing, since the text states that ρ is constant but the zonzero β requires that it not be constant. In fact, it is not constant, but varies with p as indicated in the above solution.

A.14.4 Performance Specification Review

Performance specification review is not known to have been carried out.

A.14.5 Code Design Review

Code design review is not known to have been carried out.

A.14.6 Verification

Three verification tests were applied to the model: a potential boundary condition test, a fluid-flow boundary condition test, and a pressurized well-bore simulation test, all of which involved comparisons with analytical solutions. All tests assumed isotropic hydraulic conductivity, porosity and hydraulic conductivity that are constant in space, a slightly compressible fluid, and an incompressible porous matrix. In the second test, a discrepancy between the code solution and the analytic solution arises at later times. This discrepancy is accounted for by the fact that the code solution assumed a compressible fluid while the analytic solution assumed an incompressible fluid. In the first and third tests, there was very close agreement between the code and analytic solutions. Taken together these tests provide significant verification of STEALTH-2D HYDROLOGICAL MODEL code. However, many more verification tests should be made, particularly some involving two dimensions.

A.14.7 Validation

No validation tests were reported in ONWI-256.

A.14.8 Proposed SRP Application

STEALTH-2D HYDROLOGICAL MODEL will be used in repository assessment. It is suitable for predicting water flow through fractured rock that had low permeability before fracturing. Because of the considerations noted in Sec. A.14.11, it is not suitable for use in the salt bed itself.

A.14.9 Relationship of the Model to Other Codes

The extent of rock fracturing predicted by STEALTH-2D can be converted into input data for STEALTH-2D HYDROLOGICAL MODEL.

A.14.10 Applicability of the Model to Other Problems

In its two-dimensional axisymetric mode, this model could be useful in modeling the behavior of an aquifer in contact with a gas or oil reservoir.

A.14.11 Suitability of Model to Salt Repository Application

STEALTH-2D HYDROLOGICAL MODEL should not be applied to water seeping through salt. Salt goes into and out of solution readily, and this phenomenon is not taken into account in the model. However, as noted in Sec. A.14.8, the model is suited for modeling water flow in insoluble fractured rocks lying below or above a repository.

A.14.12 Peer Review

No formal peer review of STEALTH-2D HYDROLOGICAL MODEL has been carried out.

A.14.13 References

Hofmann, R., STEALTH, A Lagrange Explicit Finite-Difference Code for Solids, Structural, and Thermohydraulic Analysis, Vol. 1: User's Manual, prepared for Electric Power Research Institute, Palo Alto, Calif., by Science Applications, Inc., San Leandro, Calif., EPRI NP-260 (1976).

Hofmann, R., and Hart, R., Hydrological Model in STEALTH 2D Code, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, by Science Applications, Inc., ONWI-256 (Oct. 1979).

A.15 SWENT: A THREE-DIMENSIONAL FINITE-DIFFERENCE CODE FOR THE SIMULATION OF FLUID, ENERGY, AND SOLUTE RADIONUCLIDE TRANSPORT (ONWI-457)

A.15.1 Code Description

SWENT uses a finite-difference technique to simulate steady state and transient, three-dimensional transport processes, including fluid flow, heat flow, chemically inert contaminant transport, and radionuclide transport in heterogeneous geologic media. The first three processes are modeled by three nonlinear partial differential equations that are coupled by the fluid properties. Simultaneous solution of these equations yields a velocity field that serves as input to the radionuclide transport equation, which does not influence the solution of the first three equations because the radionuclides are assumed to be present in trace quantities. The main algorithm is based on a linearization of the coupled equations.

The code is generally applicable to local and regional flow conditions, with or without thermal and salinity effects coupled to the heat and radio nuclide transport expressions. Major assumptions include a single liquid phase, laminar (Darcy) flow, first-order salt dissolution reaction, linear equilibrium adsorption, and linearly velocity-dependent hydrodynamic dispersion coefficients.

Several useful options are provided to users, along with a wide choice of boundary conditions, which permit inclusion of radionuclide sources, heat losses to over- and underburden, recharge due to rainfall, natural flow in the aquifer, and well conditions at the wellhead or well bottom. A leach submodel is also provided. The submodel can be used to compute source rates based on user inputs, or SWENT will accept source rate input supplied directly by the user. Such rates might be obtainable from codes like WAPPA. Another option useful for repository assessment provides for steady state flow of fluid and transient movement of radionuclides.

Input data include system geometry, formation and fluid properties, wellbore parameters, radionuclide chain data, nuclide inventories, and waste properties. Output data include Darcy velocities, pressure, temperature, and solute and nuclide concentrations at all grid blocks. The code was written in FORTRAN IV for use on a CDC CYBER 176 machine and consists of about 15,000 source statements.

SWENT comprises three aquifer-model, nonlinear partial differential equations coupled by fluid density and viscosity. A fourth differential equation for radionuclide transport is independent of the first three, except that it uses the velocity field generated as part of its solution.

The aquifer-model equations include (1) the pressure equations, which are a combination of the continuity equations and Darcy's law in three dimensions; (2) the solute concentration equation, which includes terms for production, injection, and salt dissolution; (3) the energy equation, which provides for heat input from radioactive decay; and (4) the radionuclide transport equation, which includes terms for direct source input, production, and radioactive formation and decay. The radionuclide source term can be entered directly or computed by the leach model that is incorporated into SWENT. The leach model assigns each nuclide to either the "unleached from waste matrix," "leached but undissolved," or "dissolved" states. Phases 1 and 2 are coupled by a constant leach rate, whereas phases 2 and 3 are coupled by their solubilities. The unleached phase equation may be solved internally, or data may be taken from another code, such as ORIGEN2. The dissolved-phase equation ignores dispersive transport.

Major limitations in the model are: (1) the code accommodates only a single liquid phase; fully saturated porous media are assumed; Darcy's-law kinetic energy is ignored in the energy balance; fluid viscosity is assumed to be a function of temperature or, alternatively, of concentration; salt dissolution is dealt with as a first-order reaction; adsorption is treated as a linear equilibrium process; dispersion is assumed to be a linear function of velocity; and dispersion and molecular diffusion are considered to be additive.

The partial differential equations are solved by dividing space into a three-dimensional grid and developing finite-difference approximations of the equations for that grid. The method is semi-implicit in that the dependent variables (pressure, temperature, and concentration) appearing in the space derivatives are expressed at the new time level. Because the equations are nonlinear (fluid properties depend on the dependent variables), the difference approximation is not totally stable. Hence, an iterative procedure is used to solve the equations, and convergence criteria are applied to changes in fluid density between iterations. Two methods are available for solution --ADGAUSS, a reduced-band-width direct-solution method, and L2SOR, a two-line successive overrelaxation method.

A.15.2 Development Stage

The code was developed recently and is fully operational on a CDC CYBER 76 machine. It has been used by INTERA and others for various applications, and has undergone limited verification and validation.

A.15.3 Documentation

SWENT has been fully documented in ONWI-457 (INTERA, 1983) in accordance with NUREG-0856.

A.15.4 Performance Specification Review

The findings of INTERA's review are contained in their documentation of SWENT in ONWI-457.

A.15.5 Code Design Review

A review of the code design was conducted by INTERA as part of their documentation of SWENT. The following remarks are based on information found in ONWI-457. "The use of second-order correct finite-difference approxima tions introduces block-size and time-step restrictions. These restrictions, though considerably less stringent than those of explicit methods, depend upon the magnitude of the dispersivity." "The comprehensive nature of the code may require more computer time and storage requirements relative to a code written specifically for simple problems." The code provides options for finite-difference approximations, either backward or central differences, both in space and time. The code was not designed for "double" or "dual" porosity systems. However, the code can be adapted to such simulations in one or two dimensions. Restart capabilities are provided along with two-dimensional contour mapping.

A.15.6 Verification

According to ONWI-457, there are no published analytical solutions for the complete coupled processes addressed by the code. However, 11 simple, idealized problems were available against which to check portions of the code in an uncoupled fashion. Consequently, fluid flow, heat flow, chemically inert component transport, and radionuclide transport coding were checked separately. These 11 cases are described in detail in Ward et al., 1981 and Intercomp, 1976, with the results summarized in INTERA, 1983.

Of the 11 cases studied, none involved three-dimensional solutions. Three separate cases addressed one-dimensional convection-dispersive transport with constant velocity of an inert component, heat, and a three-membered radioactivity chain, respectively. There were five separate two-dimensional tests. Of these, two involved well-injection problems (constant pressure or constant rate); one addressed inert-component transport; one addressed radionuclide transport along a single fracture, with molecular diffusion into the rock matrix; and one addressed fluid flow and heat convection in a confined, circular aquifer, with heat loss to the overburden and a uniform vertical temperature profile in the aquifer. All of the reported results of the SWENT calculations appeared to agree reasonably well with the analytical results. The effects of choosing coordinate geometries and boundary conditions were quite small for these cases.

A.15.7 Validation

The following three validation studies cited in INTERA, 1983 are briefly summarized in a single table in that document.

1. Leachate migration from landfill (Sykes et al., 1981), which "validated" fluid flow and trace component transport.
2. Injection, storage, and recovery of heat from a confined aquifer (Sykes et al., 1982), which "validated" coupled fluid and heat flow.
3. Uranium-front movement in the aquifer (Muller et al., 1981), which "validated" fluid flow and trace component transport.

In the above cases, comparisons between calculated results and field observations were reported to have "validated" certain processes modeled by SWENT. The term "validated" in this instance means good agreement under these particular conditions. Such "validaton" does not imply the general validity of those portions of the SWENT model in terms of performance assessment for nuclear waste storage purposes.

A.15.8 Proposed SRP Application

SWENT may be used in the following general problem areas:

1. Waste package thermal boundary analyses.

2. Temperature analyses within waste package components.
3. Repository subsystem thermal environment assessment.
4. Fluid conditions in repository regime.
5. Groundwater flow and hydrologic budget.
6. Radionuclide transport from repository boundary to biosphere.
7. Evaluation of potential human interference.

With the exception of the second item, these possible applications all derive from SWENT's capability to simulate coupled fluid, heat, solute, and radionuclide transport in a general aquifer system. It is not clear from the documentation whether SWENT could be used for analysis of transport processes occurring within the waste package, other than as an aid in establishing the boundary conditions as in the first application. Virtually all of these applications require the design of failure scenarios and the coordinated use of codes to provide source terms, geochemical effects, and the effects of flow through fractured media.

A.15.9 Relationship of Model to Other Codes

SWENT is a general-purpose, stand-alone code. For transport of radio nuclides, an internal leach submodel can be used to generate a source term or, alternatively, source terms can be obtained from an external code like WAPPA and entered as input. To the extent that solubility of radionuclides is a function of solution speciation, geochemical codes like EQ3/EQ6 will be required to determine initial solution properties and phase distributions, and to update them as solution and medium properties change and as the temperature and pressure change. Furthermore, SWENT's simulation capabilities will need to be augmented by codes more specifically designed for flow in unsaturated media (TRIPM) and fractured media (FTRANS). For some purposes, it may be possible to replace SWENT with simpler codes, such as LAYFLO and FE3DGW or TRIPM, which handles flow in both saturated and unsaturated porous media. Finally, to determine the radiological exposure to man, the output of SWENT can be used for dose-to-man codes like PABLM.

A.15.10 Application of Code to Other Problems

SWENT has been applied to a number of problems, including the following, by INTERA and other organizations (INTERA, 1983).

1. Nuclear waste isolation assessments in various geologic formations, including basalt deposits, salt domes, and bedded salt formations.
2. Heat storage aquifers.
3. Injection of industrial wastes into saline aquifers.
4. In situ solution mining.
5. Migration of contaminants for landfills.
6. Disposal of municipal waste.
7. Salt-water intrusion in coastal regions.
8. Brine disposal in underground aquifers.
9. Determination of aquifer transport parameters from well-test data.

A.15.11 Suitability of Model for SRP Applications

ONWI-457 lists some previous applications of SWENT to problems involving brine solutions and salt repositories. These applications should be reviewed for further information on their suitability to the SRP. Because SWENT does have the explicit capability to handle salt dissolution, at least in first-order reactions, it may be suitable for addressing questions related to dissolution of a salt repository host material embedded in a multilayered aquifer system. However, the limitations on brine concentration are not readily apparent in the code documentation. Furthermore, on page 57, ONWI-457 states without further elaboration that SWENT cannot be used in the waste package.

A.15.12 Peer Review

No documented peer review was found.

A.15.13 References

INTERA Environmental Consultants, Inc., A Three-Dimensional Finite-Difference Code for the Simulation of Fluid, Energy, and Solute

Radionuclide Transport, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-457 (April 1983).

Ward, D.S., R.B. Lantz, and S.B. Pahwa, Geosphere Model Validation, Vol. I: Verification of the Simulator for Waste, Energy, and Nuclide Transport, prepared for Sandia National Laboratories (1981).

Intercomp Resource Development and Engineering, Inc., A Model for Calculating Effect of Liquid Waste Disposal in Deep Saline Aquifers, Part I: Development, and Part II: Documentation, NTIS Pub. No. 26903, Washington, D.C. (1976).

Sykes, J.F., et al., Numerical Simulation of Flow and Contaminant Migration at CFB Borden Landfill, Vol. II: Geosphere Transport Model Validation, prepared by INTERA Environmental Consultants, Inc., Houston, Texas, for Sandia National Laboratories, 771-00G-04 (1981).

Sykes, J.F., et al., Numerical Simulation of Thermal Energy Storage Experiment Conducted by Auburn University, Vol. III: Geosphere Transport Model Validation, prepared by INTERA Environmental Consultants, Inc., Houston, Texas, for Sandia National Laboratories, 771-00G-05 (1981). Also published in Groundwater, 20(5):569-576 (1982).

Muller, A.B., N.C. Finley, and F.J. Pearson, Jr., Geochemical Parameters Used in the Bedded Salt Reference Repository Risk Assessment Methodology, Sandia National Laboratories Report SAND81-0557 and U.S. Nuclear Regulatory Comm. Report NUREG/CR-1997 (1981).

A.16 TEMP: MODIFIED STANFORD FINITE-LENGTH LINE-SOURCE CODE

A.16.1 Code Description

TEMP is a three-dimensional code that calculates temperatures generated by finite-length line sources of heat embedded in a geologic medium. The original TEMP code described in ONWI-94 (Kaiser, 1980) found a numerical solution to the heat flow equation. The code was then modified to include an analytic solution as an option. This modification is described by Wurm et al (1981). Their report describes only the modification and not the original TEMP code. The TEMP code (in both the modified and original forms) assumes isotropic thermal conductivity and constant thermal conductivity, rock density, and heat capacity throughout an infinite volume.

In the modified TEMP code, the numerical solution procedure must be used to find the temperature contributions from finite line sources within a certain cutoff distance from the observation point. (This distance was 150 feet in a typical case.) Then, either the numerical or analytic solution procedure can be used for distances greater than the cutoff distance. Wurm et al (1981) present the analytic solution, while the numerical solution is described in ONWI-94.

The cutoff distance is that distance beyond which the finite line source (representing a waste package) looks to a temperature sensor like a point source. The analytic solution procedure in TEMP consists of obtaining an analytic solution to the heat flow equation for a point heat source, with the source a function of time, and summing up the temperature contributions from all the sources beyond the cutoff distance. This analytic solution procedure was incorporated into TEMP to reduce computing time without sacrificing accuracy.

The numerical solution procedure in TEMP consists of: (1) obtaining the analytic solution (consisting of an integral over time) to the heat flow equation for a line source of finite length, with the source a function of time, (2) dividing the interval of integration into four subintervals, (3) applying the numerical technique of Romberg integration to each of the four subintervals, (4) summing up the integrations over the four subintervals to obtain the temperature increment at an observation point from a single finite-length line source, and (5) summing up the increments from all the appropriate line sources in the array.

Input consists of system geometry; thermal conductivity, heat capacity, and density of the geologic medium; time dependence of the heat sources; times at which the heat sources are emplaced; and initial temperature. Output consists of temperature as a function of three spatial dimensions and time.

Limitations of the modified TEMP code include: (1) it assumes constant thermal conductivity and thermal diffusivity throughout an infinite homo geneous medium, thus ignoring the significant inhomogeneity introduced by the repository chambers; (2) thermal conductivity is taken to be independent of temperature; and (3) radiative and convective heat transfer are taken to be negligible. The modified TEMP is written in FORTRAN and can be run on either a CDC or a VAX computer.

A.16.2 Development Stage

The modified TEMP code is operational on CDC and VAX computers.

A.16.3 Documentation

The documentation provided by Wurm et al (1981) is very incomplete and is not in the NUREG-0856 format. Specifically: (1) there is no standard software summary; (2) the problem being solved is not well described; (3) the numerical procedure is not at all described; (4) there is no discussion of assumptions and limitations; (5) variables are defined, but their dimensions are not presented; (6) the analytic solution is not derived; (7) there is no user's manual; (8) there is no discussion of verification and validation; (9) there is no chronology of code versions, and (10) there is no description of a code maintenance and quality assurance program. Because Wurm et al (1981) was apparently never intended to be a complete document in the NUREG-0856 format, its incompleteness and departure from that format cannot, in all fairness, be criticized.

ONWI-94 (Kaiser, 1980) is well written and relatively complete, but it is not fully in the NUREG-0856 format in that: (1) it has no standard software summary, (2) there is no discussion of assumptions and limitations, (3) validation is not discussed, (4) there is no chronology of code versions, and (5) there is no description of a maintenance and quality assurance program.

A.16.4 Performance Specification Review

No external performance specification review has been documented.

A.16.5 Code Design Review

No external code design review has been documented.

A.16.6 Verification

Verification studies were not reported in Wurm et al.[2] One bench marking test is reported in ONWI-94[1] -- a comparison of salt temperatures calculated by TEMP and by HEATING5. Agreement was within ~10%. Other comparisons, not reviewed by Argonne, appear in Refs. 4 and 5.

A.16.7 Validation

Validation studies were not reported by Wurm et al. or in ONWI-94.

A.16.8 Proposed SRP Application

The modified TEMP code is intended for repository assessment. It can be used to predict temperatures in different geologic media and to investigate alternative storage geometries (vertical or horizontal canister emplacement and spacing) to find an optimal configuration of waste packages.

A.16.9 Relationship of Modified TEMP to Other Codes

The modified TEMP code is basically a stand-alone code. However, its output temperatures, appropriately adapted, should be usable as input to temperature-effects codes like SPECTROM-58, SALT4, or VISCOT.

A.16.10 Application of Modified TEMP to Other Problems

No other applications are known.

A.16.11 Suitability of Modified TEMP for Salt Repository Application

The possibility of radiative heat transfer in salt (since salt is transparent in the infrared), the possible temperature dependence of thermal conductivity, and the nonhomogeneity of thermal properties in the vicinity of the repository are all potential problems in applying TEMP to salt repository assessment.

A.16.12 Peer Review

No peer review has taken place.

A.16.13 References

Kaiser Engineers, Inc., Finite-Length Line Source Superposition Model (FLLSSM), prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-94 (March 1980).

Wurm, K.J., S.G. Bloom, and R. Freeman-Kelly, Modification of the TEMP Computer Code - FY 81, Battelle Memorial Institute, Columbus, Ohio, SPAC-25 (Sept. 30, 1981).

McNulty, E.G., Comparison of TEMPV4 Results with Those Published in Westinghouse AESD-TM3-3131, Office of Nuclear Waste Isolation Memorandum, Battelle Memorial Institute, Columbus, Ohio (1983).

McSweeney, T.I., Comparison of TEMPV3 with Infinite Line Source Analytical Solution, Office of Nuclear Waste Isolation Memorandum, Battelle Memorial Institute, Columbus, Ohio (1983).

A.17 VISCOT: A TWO-DIMENSIONAL AND AXISYMMETRIC NONLINEAR TRANSIENT THERMO-VISCOELASTIC AND THERMOVISCOPLASTIC FINITE-ELEMENT CODE FOR MODELING TIME-DEPENDENT VISCOUS MECHANICAL BEHAVIOR OF A ROCK MASS (ONWI-437)

A.17.1 Code Description

VISCOT is a two-dimensional (plane or axisymmetric) finite-element code for calculating time-dependent, nonlinear deformations of a rock mass in response to geostatic and thermal stresses (INTERA, 1983). The rock mass is modeled as viscoelastic or viscoplastic. Input consists of a description of the geometry of the physical system being modeled, initial and boundary conditions, material properties (Young's modulus, Poisson's ratio, coefficient of thermal expansion, mass density, and other parameters used in modeling the rock mass), and temperatures at the nodes. In the transient case, the nodal temperatures are specified at successive times. Output consists of the predicted displace ments, stresses, and strains, plus a summary of the input data.

VISCOT obtains the output from the input by using a Bubnov-Galerkin finite-element technique with an explicit Euler time-stepping scheme to solve a system of equations consisting of the force equilibrium equation, the stress-strain relation, and the equations that describe the viscoelastic or viscoplastic deformation. VISCOT is restricted to simulating systems that are either two-dimensional planar or axially symmetric. Additional limitations are: (1) mechanical and thermal properties must be isotropic, (2) the rock mass is treated as a continuum (i.e., VISCOT is inapplicable when there is significant fracturing), and (3) large deformations cannot be accurately simulated. VISCOT is written in Fortran IV for use on a CDC CYBER 176 computer.

A.17.2 Development Stage

VISCOT is ready for use.

A.17.3 Documentation

The code documentation in ONWI-437 (INTERA, 1983) is in the NUREG-0856 format and is generally quite good. However, it has one major inadequacy plus a number of minor deficiencies. The major inadequacy is that ONWI-437 does very little to help the code user develop an intuitive physical understanding about the kinds of processes the model is supposed to simulate. Yet the user needs to have such an understanding to provide appropriate input to and to understand the output from VISCOT. The existing documentation needs to be supplemented to more clearly display the logic employed by the code and to enhance understanding of possible applications.

A.17.4 Performance Specification Review

An internal review of the first draft of ONWI-437 has been completed by INTERA and ONWI. No other external review is documented.

A.17.5 Code Design Review

INTERA and ONWI have performed an internal review of ONWI-437. No other code design review is documented.

A.17.6 Verification

ONWI-437 describes five VISCOT verification tests -- four involving comparisons with analytic solutions and one with the results of an alternative computational procedure. VISCOT performed well in the comparison with the results of the alternative procedure and in three of the four comparisons with analytic solutions. However, in the fourth such comparison -- that for the case of a rectangular plate subject to a parabolic temperature distribution (p. 49) -- VISCOT did not do well. Specifically, Table 4-3 (p. 52) shows that:

1. One VISCOT output value for the stress component σ_{xx} was +6.8311, while the corresponding analytic value was -6.7537. This may be a typographical error.
2. A second VISCOT-produced value for σ_{xx} is 2.4450, while the corresponding analytic value is -6.7551. This represents a greater than 100% difference.
3. The last two σ_{xx} VISCOT values in the table (-0.3221 and -0.3791) differ from the corresponding analytic values (0.7862 and 0.7862) by more than 100%. Nonetheless, the text describes the VISCOT and analytic values as being "in good agreement" (p. 49). While this is true for most of the corresponding values listed in Table 4-3, it is clearly not the case for all.

The three discrepancies noted above need to be explained.

A.17.7 Validation

The VISCOT code has not been validated.

A.17.8 Proposed SRP Application

VISCOT will be used for repository assessment. It can do room-scale calculations to generate input for the prediction of room-closure rates, stability, and floor heave in rock masses such as granite, basalt, tuff, or salt. VISCOT can also calculate the stress within the backfill material within a salt repository and can be used for studies of the volume adjacent to the waste package.

A.17.9 Relationship of Model to Other Codes

To accomplish a complete thermomechanical analysis, a SCEPTER thermal analysis code must be used to provide input temperatures to VISCOT.

A.17.10 Application of the Code to Other Problems

None are documented.

A.17.11 Suitability of Model for Salt Repository Application

In applying the VISCOT model (i.e., the mathematical model on which the code is based) to a salt repository, there may be problems in that (1) the model cannot treat three-dimensional deformation, (2) it cannot simulate an anisotropic or fractured material, (3) small deformations are assumed by the model, and (4) the assumptions listed on page 19 may not all be satisfied for salt.

A.17.12 Peer Review

No formal peer review of VISCOT has been carried out.

A.17.13 References

INTERA Environmental Consultants, Inc., VISCOT: A Two-Dimensional and Axisymmetric Nonlinear Transient Thermoviscoelastic and Thermoviscoplastic Finite-Element Code for Modeling Time-Dependent Viscous Mechanical Behavior of a Rock Mass, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-437 (1983).

A.18 WAPPA: A WASTE PACKAGE PERFORMANCE ASSESSMENT CODE (ONWI-452)

A.18.1 Code Description

WAPPA is designed for evaluating waste-package design performance in a repository in a geologic medium (INTERA, 1983). The code determines the integrity of the barriers designed to isolate the wasteform from the repository as a function of time. It computes the heat and radionuclide fluxes at the waste-package/repository interface as a function of time. The code can handle solid wasteforms surrounded by up to 17 barriers, including a backfill layer. The wasteforms must be homogeneous, brittle, and uniformly leachable. Spent-fuel-clad assemblies and "cermet" wasteforms (INTERA, 1983) are not accurately treated because of their structural inhomogeneities and deviations from the required cylindrical symmetry.

From a systems point of view, WAPPA transforms output data from codes that provide information on the nuclide inventory and the heat generation rate within a particular wasteform as a function of time and from codes that provide information on temperature, mechanical stress, and fluid-flux boundary conditions as a function of time at the waste-package/repository interface into heat and nuclide fluxes at that interface for use by other codes that treat transport in the near field. Although all of the codes involved in this sequence of processing input and output information are operated independently of each other, the waste-package/repository system is naturally coupled, and the boundary conditions at the waste-package/repository interface cannot be determined in a self-consistent manner without proper treatment of the coupling.

WAPPA assumes cylindrical symmetry, which seems satisfactory for a single, isolated waste package, but ignores the possibility that the distribution of waste packages within the repository may significantly alter that symmetry. The consequences of this limitation have not been addressed.

The code consists of five process models that treat five processes: radiation, thermal, mechanical, corrosion, and leaching. The radiation and thermal process models are driven internally from the nuclide inventory and heat generated within the wasteform. The corrosion and leaching process models are driven externally by external mechanical stresses and fluid fluxes. Corrosion is treated only from the outside inward, that is, no internally originating corrosion is considered. Corrosion rates can be enhanced by radiation, but possible degradation of the mechanical properties of the barrier materials by radiation damage is not treated. The corrosion model begins operation when the user-input data indicates that the backfill has been wetted. In other words, the user must provide a time when the repository becomes saturated. The leach model begins operation when all of the barriers have been breached and fluid from the repository contacts the wasteform, which itself is continuously subject to radiation and mechanical damage.

The code operates over a sequence of up to 30 time steps covering a geologic period of about one million years. During each time step, the five process models operate independently of each other and degrade the barriers. At the end of each time step, the effects of all processes on the barriers are integrated, and the status of all barriers is updated. During the next time step, the process models operate on the updated barriers. In this way the operation of the process codes is coupled together. A restart option allows the user to add or insert additional time steps to obtain better time-resolution if desired.

The radiation process model requires a user-specified data set containing nuclide inventory and heat generation data as a function of time for the specific wasteform of interest. These data must be obtained from a detailed code like ORIGEN2 (Croff, 1980) that treats the characteristics of a wasteform after irradiation of the waste products. The radiation process model takes data directly from a look-up table if the time steps are properly chosen (20 for ORIGEN2) or interpolates for other times. Gamma ray attenuation by the package components, radiation damage to the wasteform, corrosion and leach enhancement related to radiolysis processes all require empirical input data.

The thermal process model treats heat flow across concentric annuli based on power input from the ORIGEN2 code or its alternatives. The three basic forms of heat transfer are considered.

The mechanical process model calculates radial and axial stresses, and canister and wasteform fracturing. Required inputs include state of stress at the waste-package/repository interface and thermal input from the thermal process model. Only tensile-stress fracturing of the wasteform is treated.

The corrosion process model is composed of five corrosion submodels: general corrosion, localized pitting and crevice corrosion, stress corrosion, galvanic corrosion, and dry oxidation. Of these, pitting and crevice corro sion, and stress corrosion are assumed to be catastrophic. That is, if they are operative for a particular barrier within a given time step, that barrier is assumed to be breached or completely destroyed during that time step. Three important limitations to the corrosion process model are:

1. Internal corrosion is ignored, which may be a nonconservative assumption.
2. Only galvanic corrosion between pairs of metal barriers is considered. Single-barrier galvanic corrosion is ignored, which may be nonconservative assumption.
3. Effects of corrosion films are ignored, which is presum ably a conservative assumption.

The leach process model calculates the mass transport of nuclides across the waste-package/repository interface as a result of both diffusive and advective transport. The backfill is treated by this model as a "mixing cell." In other words, the backfill is assumed to be instantaneously and uniformly wetted by new fluid entering from the repository or contaminated fluid entering from the interior waste package. The boundary condition at the interface is assumed to be of the "swept-away" type; that is, any nuclides crossing the interface are immediately swept away so that no accumulation occurs. This means the effluent from one waste package can never influence an adjacent waste package in a repository. The consequences of ignoring possible cumulative effects (nonzero nuclide concentrations in the near field) have not been addressed.

Sophisticated numerical methods are not used by any of the process models. Most are closed-form analytical expressions requiring empirical input data. The leach model solves four simple simultaneous equations using the

Gauss-elimination technique. Further, the model assumes swept-away boundary conditions, so that the concentration of nuclides in the repository at the interface with the waste package is always assumed to be zero.

The WAPPA code is written in ANSI-77 FORTRAN. It has been installed on a CDC 7600 machine and consists of approximately 12,000 lines of code. It runs very fast, requiring only a few seconds of central processing unit (CPU) time for a fully dimensioned problem. The code output includes both summary and detailed outputs. The latter includes status of barriers as a function of time and nuclide concentrations as a function of radius. Tabulations of heat and nuclide fluxes at the waste-package/repository interface are also given.

A.18.2 Development Stage

WAPPA is a newly developed but fully operational and documented code.

A.18.3 Documentation

The code has been documented by INTERA in ONWI-452 (INTERA, 1983) in accordance with NUREG-0856.3 The theory of each of the five process models contained within the WAPPA model is explained in detail, as is the verification procedure. A detailed user's manual is provided, along with a code listing on microfiche. The documentation is quite complete, although not without problems. First, although the overall structure of the code is clear enough, the interactions between the five independent process models are difficult to unravel. The information is all there, but it tends to be buried in the description of the individual process models. One is not always sure which interactions are included and how they are implemented.

The mechanical model, for example, assumes that when the backfill stress limit is exceeded, the backfill "fails" and is treated as an incompressible fluid. It does not say what happens, if anything, to all of the other properties of the backfill in this "failed" state. Also in the mechanical model, the influence of stress on the solubility of the wasteform is not mentioned. As another example, emphasis is placed on the need to have more flexibility in the choice of corrosion film growth models. Yet, nowhere is there any discussion of how the growth of films influenced the outcome of any calculations. In fact, it appeared that such films were calculated but that their effects were subsequently ignored. Although most of the physical processes treated by the five process models are described in ONWI-452, the physical process descriptions are not adequate in many cases to give a clear picture of what is going on. For example, the backfill barrier is described in terms of a "mixed-cell model" in which "new" and "old" fluids are instantaneously mixed. Presumably what is meant is that the resistance to flow in the backfill media is much lower than that in the remainder of the waste package so that any deviation from cylindrical symmetry is removed. Still, one is left wondering whether only radial flows are considered or whether more complex flows in the repository are envisioned, with the backfill region intended to serve as a transition from the more complex flow pattern to one of radial flow only within the interior waste package.

A.18.4 Performance Specification Review

ONWI-452 lists the performance specifications for WAPPA, but no external review has been documented. The documentation in ONWI-452 lists the assumptions and limitations of each of the process models as well as of the code verification tests. However, the justification for why certain processes are treated while others are ignored is often missing.

A.18.5 Code Design Review

ONWI-452 lists code inputs, outputs, and methods of solution for each of the process model codes. The input data consist of waste-package design data, empirical data for various process rates, radio nuclide inventory and heat generation rate data, and boundary condition data for the waste-package/repository interface. The availability of the empirical rate data for the various corrosion processes seems uncertain, both because of the extent of the data required and because of the uncertainty of applicability of what are often short-term data to long-term processes. As noted in the code documentation,1 short-term data may indicate that certain package materials are not subject to pitting or crevice corrosion. Yet, in the long term, such processes may arise and could lead to catastrophic failure of the barrier. Radionuclide and heat input data are relatively readily available from runs of ORIGEN2 or similar codes.

Specification of the time-dependent boundary conditions is probably the input requirement posing the greatest difficulty. This information will probably only be available through the operation of near-field repository heat transfer, fluid transport, and mechanical stress codes, whose input requirements will be difficult to satisfy. In view of the intrinsically coupled nature of the waste-package/repository system, it remains to be clearly defined how the boundary conditions at the interface will be handled.

A.18.6 Verification

Two types of verification were performed for each of the five process models included in the WAPPA code. First, the results of hand calculations performed for simple problems were compared with the results of executing each of the process models and their submodels in a stand-alone fashion. All results agreed to within the accuracy of the hand calculations. Second, using a complex 17-barrier waste-package test problem, the entire integrated WAPPA code was executed and the results compared with the results obtained by manually feeding the input data obtained from the integrated WAPPA package code into the process models executed in the stand-alone mode. Comparisons again were very good, indicating that the integrated WAPPA code properly transmitted data to and from each process model during each time step. Three or four separate time steps were generally used for this comparison.

For example, the radiation process model is composed of four linked submodels, namely, the source, attenuation, damage, and radiolysis submodels. According to ONWI-452, computations performed by each of these submodels were checked with hand calculations. But, only the results of the numerical integration performed by the attenuation submodel were reported. These results compared very well with the results of the hand calculations.

The integrated WAPPA code was then executed for the complex 17-barrier test problem mentioned above and the results compared at three different time steps with the radiation process model code operated in a stand-alone fashion by simulating input data from the integrated WAPPA code at the three time steps. The results verified that the radiation process model code was properly integrated into the entire WAPPA code.

The thermal process model contains temperature and heat flow algo rithms, which were verified by comparing hand calculation results with those from code runs in the stand-alone mode. The 17-barrier waste package test problem was used for this purpose. Predicted temperatures and heat flows from the stand-alone code and from the hand calculations were in good agreement for the one simulation time used (t = 0). Predicted temperatures and heat flows from the stand-alone code and from the integrated WAPPA code were in good agreement for the four simulation times used (t = 0, 1, 100, 1000 years). Correct solutions for conductive and radiative heat transport across individual annuli over a range of material properties were verified. Logic options for various types of heat flow through the various barrier materials were also checked. Only temperature-independent properties for conductive and radiative heat transport were checked. Temperature-dependent convective heat transport was also checked.

The mechanical process model code was verified through a series of stand-alone and integrated system tests. Ten test cases compared hand calculations with stand-alone code executions. For example, waste-package-element stress fields were verified for radial and axial pressure loadings, thermal gradients, and residual stresses caused by initial displacement. The code correctly treats a fractured portion as an incompressible fluid. The system-integrated test demonstrated that (1) material properties are degraded based on radiation damage information from the radiation process model, (2) temperature gradients leading to thermal stresses are properly transferred from the thermal process model, and (3) the corrosion process model properly passes updated barrier thicknesses. Other details regarding integrated system performance were also verified.

The corrosion process model code contains many logic options and tracking/flagging variables. These options and variables as well as the results of calculations using the simple algebraic expressions in the code were verified by hand calculations. System integration testing indicated that the interfacing of data between this process code and the entire WAPPA code is correct.

The leach model tests verified the coding of the leaching, diffusion, and backfill equations and solution methods by comparison with hand calculations. Integrated system tests verified the interface between the WAPPA system and the leach process model code.

There remains one point of uncertainty in the code verification procedure; namely, how do we convince ourselves that the integrated system code has been fully verified? That is, under the concerted action of all of the processes, are the various barriers breached when they are supposed to be, and is the effect of each breach properly handled in subsequent time steps by all of the process models? The answer to this question may already be contained in ONWI-452, but it is not easy to extract from the documented verification tests of each of the WAPPA process model codes. A clearer demonstration that the integrated system has been verified is needed.

A.18.7 Validation

No Validation exercises have been documented.

A.18.8 Proposed SRP Application

Two applications of WAPPA are planned: (1) corrosion analyses of metallic barriers surrounding the wasteform and (2) assessment of leach rates. WAPPA is designed specifically for these proposed applications. The corrosion process model embedded in WAPPA actually consists of several submodels of individual corrosion processes. WAPPA also contains a leach process model for estimating the flux of nuclides at the waste-package/repository interface. The effects of radiation and thermal output from the wasteform on the corrosion and leaching processes are included in the WAPPA codes. However, certain processes that may be important are not considered.

A.18.9 Relationship of Model to Other Codes

Although WAPPA is a stand-alone code, it does require input data on nuclide inventories and heat generation rates for specific wasteforms (and their constituent irradiation histories) from a source code like ORIGEN2. WAPPA contains a leach model that can provide leachate fluxes at the waste-package/repository interface. These data can be used directly by geochemical and radionuclide transport codes like PHREEQE, EQ3/EQ6, and SWENT. SWENT, however, contains its own leachate model, which can be used in place of the WAPPA leachate model output. WAPPA also provides information on heat flow through the waste package that can be used to drive thermal/mechanical codes and fluid/energy transport codes. It should be borne in mind that WAPPA assumes cylindrical symmetry of both input and output data, and uses a swept-away boundary condition at the waste-package/repository interface.

Both fluid and heat flux boundary conditions must be specified at the waste-package/repository interface. This requirement will necessitate the iterative operation of WAPPA and appropriate transport codes. Simple transport codes like STAFLO and DOT can be used for this purpose. For more complex simulations involving coupled processes (flow in fractured and/or deformed porous media; coupled fluid, energy, and radionuclide transport; solute transport and adsorption) codes like STAFAN, CFEST, SWENT, TRIPM, and FTRANS may be required.

Finally, the waste-package-barrier corrosion processes that are assumed in WAPPA to operate from the outside inward begin only after the surface of the outer barrier has been wetted. Hence, the user must predict the time at which such wetting occurs.

A.18.10 Application of Code to Other Problems

No applications of WAPPA to other problems have been documented.

A.18.11 Suitability of Model for Salt Repository Application

Most of the barrier destruction processes accounted for in WAPPA are expressed in terms of empirical constants. Of special concern in a salt repository are the various barrier corrosion process rates and radionuclide leach rates that would govern the life of the waste package during an invasion of concentrated brine solutions at various temperatures. To the extent that such empirical data exist, WAPPA is applicable to salt repositories. The code documentation does not address the issue of the availability of specific salt repository data.

A.18.12 Peer Review

No peer review has been documented.

A.18.13 References

Croff, A.G., ORIGEN2 -- A Revised and Updated Version of the Oak Ridge Isotope Generation and Depletion Code, Oak Ridge National Laboratory Report ORNL-4628 (July 1980).

INTERA Environmental Consultants, Inc., WAPPA: A Waste Package Performance Assessment Code, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-452 (April 1983).

A.19 SCOPE: SIMPLIFIED CODES FOR PERFORMANCE EVALUATION OF RADIONUCLIDE TRANSPORT

A.19.1 Code Description

The computer programs that make up the SCOPE system can be separated into three groups. The first group, the LADDY systems, comprises four programs that simulate ground-water transport of the radionuclides from radioactive material in a ground-water system from the repository to the biosphere. Program EXPOSE represents the second group; it uses the results of LADDY to calculate the integrated exposure to radionuclides in accordance with regulations set up by the U.S. Environmental Protection Agency (EPA) in 40 CFR Part 191 (currently in draft form). The third group consists of the dose codes PABLM and ALLDOS. These dose codes use the results generated by LADDY to provide a detailed estimation of the potential radiation doses to people. LADDY replaces its predecessor BAIRN in the document PNL-4737.

A.19.2 Development Stage

SCOPE is a recent development from PNL. LADDY (or BAIRN) follows the calculation structure developed in the code GETOUT (ONWI-433) with new radionuclide transport equations provided by the University of California, Berkeley (see code UCB-NE-10.2 - ONWI-359). EXPOSE simply integrates the output profiles from LADDY for each nuclide over a specified time period. PABLM and ALLDOS were developed earlier and are provided within SCOPE to provide the ability to calculate individual and population doses from releases of radionuclides from the repository.

SCOPE is fully operational on the VAX 11/780 computer, and LADDY can be down-loaded to a DEC PC350.

A.19.3 Documentation

Documentation of SCOPE is provided in PNL-4737. PABLM and ALLDOS, which were earlier developments, are documented in PNL-3209 and PNL-3524, respectively.

A.19.4 Performance Specification Review

Internal peer review associated with clearance of the PNL report was conducted. SCOPE is a system code made up of three codes (UCB-NE-10.2, PABLM and ALLDOS), which have been peer reviewed and documented.

A.19.5 Code Design Review

Internal peer review associated with clearance of the PNL report was conducted. SCOPE is a system code made up of three codes (UCB-NE-10.2, PABLM and ALLDOS), which have been peer reviewed and documented.

A.19.6 Verification

The code uses LADDY the UCB-NE-10.2 formulation of the transport equations. The UCB-NE-10.2 codew was one of the codes used in the INTRACOIN study. This code was found to provide excellent agreement with the results from a variety of other codes using differing solution techniques. Informal comparisons of the SCOPE results with INTRACOIN and the results presented in the NAS-Waste Isolation System Panel Report have been made. The comparison is excellent. These comparisons will be documented in future updates of the code.

Documents verifying ALLDOS and PABLM are limited. Appendix C of the NAS-WISP Report provides the only documented comparison of several dose codes--PABLM is one of the codes used.

A.19.7 Validation

No validation of SCOPE has yet been reported.

A.19.8 Proposed ONWI Application

SCOPE is available to model radionuclide transport in a porous, sorbing medium. The LADDY portion of SCOPE in effect replaces the code GETOUT.

The SCOPE system provides a good survey type code for an initial performance evaluation of different post-closure scenarios. The inputs required for such simulations are radionuclide inventory, ground-water flow characteristics, medium retardation factors, and nuclide leaching rates.

A.19.9 Relationship of Model to Other Codes

SCOPE links radionuclide transport, radiation dose and exposure calculations in a single package.

A.19.10 Suitability of Model for Salt Repository Applications

As with most radionuclide transport codes, a flowing groundwater condition is assumed. Normally in a salt repository, the flow rates are extremely slow (possibly zero). SCOPE will be used for worst case analysis of the salt repository.

A.19.11 Peer Review

External peer review of SCOPE is planned to be conducted in FY 84-85 along with other performance assessment codes.

A.19.12 References

Napier, B. A., et al., PABLM-A Computer Program to Calculate Accumulated Radiation Doses from Radionuclides in the Environment, Pacific Northwest Laboratory, Richland, Washington, PNL-3209 (March, 1980).

Petrie, G. M., et al., Simplified Codes for Performance Evaluation (SCOPE) of Radionuclide Transport, Pacific Northwest Laboratory, Richland, Washington, PNL-4737 (September, 1983).

Strenge, D. L., et al., ALLDOS--A Computer Program for Calculation of Radiation Doses from Airborne and Waterborne Releases, Pacific Northwest Laboratory, PNL-3524 (October, 1980).