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NNWSI WASTE PACKAGE PERFORMANCE ASSESSMENT

LAWRENCE LIVERMORE NATIONAL LABORATORY

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10/14/86

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1.0 Purpose and Objective of Studies

The purpose and objectives of performance assessment are to conduct integrated assessments of waste package designs in order to qualify those designs with respect to the containment and release requirements of 10 CFR 60. In addition, a source term of releases from the waste package as a function of time must be provided to total repository performance assessment for calculation of releases to the accessible environment. Therefore, performance assessment directly addresses the following information needs (taken from 8/7/86 version of NNWSI information needs):

Issue 1.4: "Will the waste package meet the performance objective for containment as required by 10 CFR 60.113?"

1.4.3 Scenarios and models needed to predict the time to loss of containment and the ensuing degradation of the containment barrier.

1.4.4 Estimates of the rates and mechanisms of containment barrier degradation in the repository environment for anticipated and unanticipated processes and events.

1.4.5 Determination of the time to loss of substantially complete containment of the waste packages for anticipated processes and events.

Issue 1.5: "Will the waste package and repository engineered barriers meet the performance objective for radionuclide release rates as required by 10 CFR 60.113?"

1.5.3 Scenarios and models needed to predict the rate of radionuclide release from the waste package and engineered barrier system.

1.5.4 Determination of the release rates of radionuclides from the engineered barrier system for anticipated and unanticipated processes and events.

1.5.5 Determination of the amount of the radionuclides leaving the near-field environment of the waste package.

Processes that affect release and containment failure do not occur independently but in an interrelated manner. Therefore, performance assessment calculations require that the effects of these interacting degradation and release mechanisms on waste package performance in an unsaturated tuff environment be calculated in an integrated manner. It is also recognized that waste package performance may not be calculated independently of the surrounding hydrologic environment. Further, differences in scale of interest may require an interfacing calculation between the engineered barrier system (EBS) boundary and the total system performance calculations. Since representation of the waste package environment is a necessary component of performance assessment calculations, it should be noted that changes in EBS definition will not affect the waste package performance assessment codes nor the strategies needed to produce those codes.

Performance assessment will integrate the processes affecting waste package life and releases into computational models. To address the reasonable assurance standard to be applied by NRC, these models will incorporate a methodology to provide for probabilistic analysis of waste package reliability. Subprocess models will be obtained from investigations performed by the other subtasks of the waste package task. The basic data needs of performance assessment are served by those investigations. Therefore, the activities of performance assessment are those necessary to integrate and process information from the other subtasks with computational models. As will be explained below, quality assurance levels are assigned to be consistent with waste package design phases. Data and submodels supplied by activities outside of performance assessment will be required to have quality assurance levels consistent with the levels assigned the performance assessment activity using the data or models.

Waste package performance assessment contains three broad categories of activities. These activities are as follows:

1. Development of a hydrothermal flow and transport model to test concepts to be used in establishing boundary conditions for performance calculations, and to interface EBS release calculations with total system performance calculations.

2. Development of a waste package systems model to provide integrated deterministic assessments of performance and analyses of waste package designs.

3. Development of an uncertainty methodology for combination with the system model to perform probabilistic reliability and performance analysis waste package designs.

The first category contains activities that aid in determining the scope of a separate, simplified set of hydrologic calculations needed to characterize the waste package environment for performance assessment calculations. These detailed hydrothermal calculations are included in the waste package performance assessment subtask as a matter of project history at LLNL, but do not represent direct performance assessment calculations. The last two activity categories are directly concerned with waste package performance calculations.

Work on performance assessment activities to date has concentrated on evaluation of codes for application to hydrothermal problems and waste package system simulation. In addition, planning of interfaces with other waste package subtasks and interaction with other interested NNWSI Project parties has been underway.

2.0 Rationale for Selected Studies

The following subsection will discuss the technical rationale for the performance assessment activities. Quality assurance assignment sheets for these activities are attached in the appendix of this document. The Quality Assurance element that applies to all performance assessment activities is Procedure 19.0; Software Quality Assurance. A detailed Software Quality Assurance Plan is currently being developed for Waste Package Performance Assessment. The rationale for level assignments requires some explanation.

Detailed hydrothermal flow and transport calculations will be necessary to determine the scope of hydrologic phenomena affecting waste package performance. Concepts developed during these modeling activities will be used to form a basis for constructing the waste package environment subroutines of the performance assessment system model. This activity will provide conceptual input to more simplified system model development but will not supply code used in performance calculations; therefore, it is assigned QA Level III throughout the Project.

Two groups of waste package performance assessment activities, development and application of the waste package system model (Activities I-20-5 through I-20-13) and development and application of uncertainty methodologies (Activities I-20-14 through I-20-19), show an evolution of quality assurance level beginning at Level III and ending at Level I. Using the development and application of the system model as an example should clarify this process. The rationale for this approach follows the evolution of the waste package designs. The first version of the system model is used to evaluate methods of analysis for use in a system model. Using the flow chart supplied with each level assignment, it can be seen that activities using this version of the systems model (Activities I-20-5 to I-20-7) are assigned a QA Level III. Similarly, uncertainty analysis activities I-20-14 and I-20-15 are QA Level III activities.

The next phase is the development and application of a system model for analysis of the advanced conceptual design (Activities I-20-8, -9, and -10). These activities will be based on an entirely new computer program using concepts learned in the earlier phase. New information and submodels from the other waste package subtasks will be incorporated into this program. The program will be used to analyze the advanced conceptual design. In this case, design alternatives will be evaluated. Therefore, these activities are assigned QA Level II. Similarly, uncertainty analysis activities (I-20-16 and I-20-17) based on this performance assessment system model will have QA Level II.

The final phase is the development and application of a system model to the license application design (Activities I-20-11, -12, and -13). Again, these will be based on new code, incorporating aspects of the earlier codes and final information and data from the other subtasks. This program will be used to provide estimates of waste package design performance for direct use in the license application. In addition, the code will also supply a source term for use in total system performance assessment. Therefore, these activities are assigned QA Level I. The uncertainty analysis activities using the final version of the system model will be used to produce the distributions needed to provide reasonable assurance for source term calculations and, therefore, also have QA Level I.

The rationale for the studies will be grouped by type, i.e., hydrothermal flow and transport, system model development and application, and uncertainty analysis. A rationale for each activity under these groups is presented. All of the activities of performance assessment are either code development or analyses of waste package problems. Therefore, the rationale for each activity basically answers the question of why a particular approach was selected.

2.2 Hydrothermal flow and transport

The durations of the hydrothermal flow and transport activities are as follows:

Activity No.	Activity	Duration (months)	Quality Level
I-20-1	Development of detailed near-field flow and transport model	25	III
I-20-2	Verification and validation of detailed flow and transport model	33	III
I-20-3	Sensitivity analysis of near-field flow and transport model	14	III
I-20-4	Analysis of source term attenuation in near-field host rock	22	III

These activities are not strictly in sequence, but overlap to some extent. For example, the development of the near-field model will be more or less continuous over the period discussed in Section 5. It will overlap with part of the verification and validation period, and the sensitivity analysis is likely to indicate areas that may require more work. The analysis of the source term will overlap to a small degree with the end of the sensitivity analysis section; however, this activity will basically require that the other activities are complete. Documentation of the detailed hydrothermal activities will be in the form of user manuals and application reports published as UCRL technical reports.

2.2.1 Development of near-field flow and transport model (I-20-1)

A near-field flow and transport model is necessary to understand boundary conditions of the waste package performance assessment model that are imposed by the immediate waste package environment. The development of this model may take place by modification of existing or development of new numerical simulations for flow and transport in the fractured host rock surrounding the waste package. The detailed simulation will be used in the development of a simplified flow and transport submodel for direct use in the performance assessment system model.

Numerical simulation of flow and transport in host rock is the only method sufficiently flexible to allow analysis of this aspect of the waste package environment. Other methods such as analytical solutions or even physical analogues are too restrictive to be representative.

Code development will consist of one continuous activity that must precede analyses using the code. As new information is obtained through either laboratory or exploratory shaft waste package environment tests, this information will be incorporated into the model. Therefore, this effort will heavily concentrate initially on development to produce a working code and developmental efforts will continue throughout the Project. Past work has concentrated on evaluating the applicability of available hydrothermal flow and transport codes. Codes considered included WAFE, TOUGH, and PETROS. All of these codes will require considerable modification to be applicable to the near-field environment.

As part of the code development process, a conservative method for analysis of flow and transport within the waste package will be selected. This method will be combined with the near-field host rock model to provide a more realistic source term for detailed transport calculations.

2.2.2 Model verification and validation (I-20-2)

Two basic methods will be used to verify the hydrothermal code. The first method is to verify the code by comparing analytical solutions with related problems. This method provides the best verification of a numerical code; however, it is limited by the existence of analytical solutions only for restrictive boundary conditions, geometries, etc. Therefore, in addition to comparison with analytical solutions, the code will be compared via benchmarking activities with other independently developed numerical codes such as TOUGH or WAFE using benchmarking activities. The verification activity will occur after the development of the first version of the hydrothermal code and after each major revision of the code.

Validation of the detailed model will be accomplished using data from exploratory shaft and laboratory waste package environment tests. These activities will test the code using physical approximations of the actual waste package environment. However, the experiments planned with the exploratory shaft and waste package environment activities will exercise the major components of this model. Model validation will be performed after the code verification is complete and after experimental results are available.

2.2.3 Sensitivity analysis of near-field flow and transport model (I-20-3)

Performance assessment calculations will require simplification of all process models included in the code. Without this simplification, a model that integrates the processes affecting waste package degradation could not be used to conduct the probabilistic reliability analysis required by NRC. To simplify a detailed calculational model, one must identify the most significant parameters affecting performance. The process of identifying these parameters is known as sensitivity analysis. After the model is verified and validated, sensitivity analysis will be performed to define the scope of phenomena needed to develop the simplified model for performance assessment.

2.2.4 Analysis of source term attenuation in near-field host rock (I-20-4)

Initially, release calculations made by the performance assessment models will provide release from the engineered barrier system, now considered to be the edge of the emplacement borehole. There are some indications that the first meter of tuff could provide significant sorption of many radionuclide species released from the waste package. The level of resolution required for analysis of the effect of the host rock immediately surrounding the waste package may require higher resolution than that practical for total system performance assessment.

These transport calculations are based on releases predicted by waste package performance assessment calculations. Therefore, the transport calculations are necessarily dependent on EBS release calculations. They will involve analysis of retardation in the first few meters of host rock, and high resolution analysis of extreme event scenarios. Uncertainties regarding the number of analyses required are difficult to discuss since they will depend on the outcome of the modeling activity. Again, these concepts will aid in determining the scope required of the system model waste package environment routine. These modeling and analyses activities will provide input to activities to analyze waste package EBS performance performed by SNL under WBS 1.2.1.4. Documentation will include UCRL reports, user manuals, and Milestone P204 (See Section 5.5).

2.3 Development of the systems model and analyses of waste package designs

The durations of the system model development and analysis activities are as follows:

Activity No.	Activity	Duration (months)	QA Level
I-20-5	Development of version I of system model	6	III
I-20-6	Verification and validation of system model version I	6	III
I-20-7	Testing of system model using waste package design concepts	46	III

Activity No.	Activity	Duration (months)	QA Level
I-20-8	Development of system model version II for analysis of anticipated and unanticipated events	4	II
I-20-9	Verification and validation of system model II	4	II
I-20-10	Analysis of advanced conceptual design with system model version II	7	II
I-20-11	Development of version III of system model for analysis of anticipated and unanticipated events	5	I
I-20-12	Verification and validation of system model version III	6	I
I-20-13	Analysis of license application design with system model version III	11	I

2.3.1 Development of version I (I-20-5)

The system model of the waste package is an essential step towards obtaining a license for the NNWSI repository design. To obtain a license, it will be necessary to provide evidence that the waste package design is capable of performing its function for the required time durations. Clearly, this is not possible through experimentation because it would take hundreds of years to physically test the waste package design. Consequently, the performance of the waste package design must be addressed theoretically, using the best data and predictive models to estimate the actual physical processes that will occur following closure of the repository.

This task involves the theoretical specification as well as the computer implementation of a waste package system model. The system model will deterministically calculate the performance parameters of interest given the specific design characteristics of the waste package. It will couple the various physical and chemical process models derived from the results of the other, more empirical, waste package task study efforts.

A computer implemented, theoretical system model to predict the performance of the waste package was used for many reasons. First, there are a number of synergistic physical and chemical processes, e.g., irradiative damage and heating, thermal expansion and stress, mechanical loading, corrosion, etc., which can lead to premature failure of the waste package. Since these processes are coupled, affecting one another's importance and rate of occurrence, it is not possible to assemble independent assessments of the likely history of particular waste package components or processes into a credible prediction of the total waste package performance. It is essential that a time-dependent, complete, and coupled system model of the waste package be used to coherently assess the behavior of the waste package in the repository environment.

Previous work on this activity has centered on evaluation of the waste package performance assessment code WAPPA for application to the NNWSI waste package. The formulation of this code appears inadequate for this purpose; and therefore, a new formulation is required.

The system model will be developed in parallel with the various physical and chemical process models. This is possible because, to a large degree, the process models within the system model will act more or less as black boxes, accepting certain physical parameters (e.g., time, temperature, water chemistry) as input, and returning one or more physical parameters (e.g., corrosion rate, thermal expansion, water chemistry) as output. The system model will couple these physical process models and determine their time-dependent behavior. Documentation of the development of this model will include UCRL reports, user manuals, and Milestone M276 (see Section 5.5).

2.3.2 Verification and validation of system model version I (I-20-6)

This effort involves the testing of the various physical and chemical process models (submodels) for use in the systems model. The submodels will be the result of extensive interaction with other, experimentally based, investigative efforts. As the submodels for a particular process (e.g., irradiative heating, waste material dissolution, mechanical loading) are developed, verification that the computer implementation of the submodels is in agreement with the theoretical model will be required. The theoretical submodels will be tested by comparison with analytical solutions and laboratory measurements to ensure that they do correctly represent their respective physical processes and that these processes are the correct ones for use in the system model.

This effort will be conducted in parallel with the system model development for reasons explained in Section 2.3.1. Documentation of this activity will be in the form of UCRL reports.

2.3.3 Testing of system model using waste package design concepts (I-20-7)

Once the system model and accompanying submodels have been independently developed, verified, and validated, it will become necessary to test the integrated model. This effort will involve running the system model with configurations formed of waste package design concepts. The results of this test will show logical or conceptual errors in the computer or theoretical model.

Another important aspect of testing the system model will be in the form of the sensitivity analysis. Sensitivity analysis will involve measuring the degree of sensitivity of the waste package performance measures calculated by the system model to the various waste package design input parameters, as well as the various internal data and process submodels of the system model. The results of this analysis will assist in improvement of the system model in succeeding versions, and also will provide useful information to the uncertainty analysis (see Section 2.4); therefore, it will provide conceptual input to activities I-20-8 to I-20-19. Although this activity begins with testing the first version of the system model, it will continue in order to provide a method for testing system model analysis methods throughout the duration of the project. Documentation of this activity will be in the form of UCRL reports.

2.3.4 Development of system model version II for analysis of anticipated and unanticipated events (I-20-8)

This effort is similar in nature to that described in Section 2.3.1. Some exceptions are that this version of the system model will be based upon the advanced conceptual design of the waste package, will be used to evaluate waste package designs, and will also address unanticipated events. Results of this study will be used in Activity I-20-9.

2.3.5 *Verification and validation* of system model version II (I-20-9)

This subtask is similar to that described in Section 2.3.2. Results of this study will be used in activity I-20-10. Documentation of this activity will appear as UCRL reports.

2.3.6 Analysis of advanced conceptual design with system model version II (I-20-10)

This subtask is similar to that *described* in Section 2.3.3. At this point the system model will be baselined and documentation will include user manuals developed as UCRL reports and Milestones M260 and M263 (see Section 5.5). This model will serve as a kernel for uncertainty methodology development activities to be used to analyze advanced waste package design performance (Activity I-20-16 and I-20-17). Also output of this activity will be used directly to evaluate waste package design alternatives (Activity I-20-11).

2.3.7 Development of version III of system model for analysis of anticipated and unanticipated events (I-20-11)

This effort is similar to that in Section 2.3.1 with the exception that this model will focus on the license application design of the waste package. The model developed under this activity will be used in Activities I-20-12 and I-20-13.

2.3.8 Verification and validation of system model version III (I-20-12)

This subtask is similar in content to Section 2.3.2. Results of this activity will be used in I-20-13. Documentation of this activity will appear as UCRL reports.

2.3.9 Analysis of license application design with system model version III (I-20-13)

This subtask is similar in nature to that described in Section 2.3.3. This model version will be baselined and applied to the license application waste package design. Results will form a portion of the EBS release and containment performance input to radionuclide source term construction performed under WBS 1.2 1.4 by SNL. Documentation will include UCRL reports and milestones M268 (see Section 5.5).

2.4 Uncertainty analysis

Uncertainty analysis activities are as follows:

Activity No.	Activity	Duration (month)	QA Level
I-20-14	Development of uncertainty analysis methodologies for testing with the system model	48	III
I-20-15	Verification of suitability of uncertainty methods using system model version I	7	III
I-20-16	Development of uncertainty methodology incorporating version II of the system model	20	II
I-20-17	Verification of uncertainty methodology and application to analysis of advanced conceptual design	6	II
I-20-18	Refinement of uncertainty methodology and incorporate final version of system model	7	I
I-20-19	Uncertainty analysis of license application design and derivation of source term for total system performance	15	I

There are two types of work in these activities--developing methodologies and applying the methodologies to waste package designs. There are three stages that correspond to the three design stages of conceptual design, advanced conceptual design, and license application design and to the three stages of system performance model development.

Uncertainty analysis is needed to address such questions as:

- With what reliability will the waste package meet its long-term performance goals?

- What will be the range and distribution of the waste package's perf‹rmance measures, which are in units of the performance goals?

- What are the values and the intrinsic variability of the source term of radionuclide releases over time from the waste package to the total repository system?

An analysis is needed and an experimental approach alone is unfeasible because:

- The purpose is to look for what is by design a rare event, the failure of the waste package to fulfill its performance goals.

- Many joint occurrences of events and coupled evolution of processes in the characterization of the range of likely or possible outcomes must be considered.

2.4.1 Development of uncertainty analysis methodologies for testing with the system model (I-20-14)

Development of an uncertainty analysis methodology involves examining existing methodologies, selecting or modifying some of them, and developing a computer code and a procedure for using the computer code. Development rather than off-the-shelf use of an existing methodology is necessary because of the unique set of conditions. The reliability and performance variability questions involve rare outcomes, long-term outcomes, continuous outcomes (release rates over time), and coupled processes and events.

Uncertainty analysis of conceptual designs of the waste package is performed to:

1. Test and guide improvement in the methodology.

2. Illustrate the format for describing the variability in the time history of the waste package source term.

3. Determine which factors among design, analysis, and data most limit the confidence in the predictions.

Uncertainty analysis on the license application design of the waste package is performed for the following reasons:

1. Reliability on meeting performance goals is information required by NRC regulations.

2. The cumulative probability distribution on cumulative release of radionuclides to 10,000 years is information required by NRC regulations.

3. The cumulative probability distribution on other performance measures will increase the confidence in the reliability results.

4. A description of the variability in the waste package source term time history will be provided as an input to total repository system reliability analysis.

This activity begins with examination of methodologies for possible use in the first uncertainty model, but it will continue in a similar function throughout the project. This activity will provide results about analysis feasibility and thus will provide a guide to subsequent development activities. This activity will require outside inputs at certain phases. These inputs consist of waste package design and the conceptual model development in the corresponding system performance model to start the uncertainty method development. Further, a waste package analysis and sensitivity analysis using the system performance model is required before putting the finishing touches on the uncertainty method development and computer code implementation. Results of this activity will be documented in UCRL reports. The results of this activity will be used in Activities I-20-15 to I-20-19.

2.4.2 Verification of suitability of uncertainty methods using system model version I (I-20-15)

There are uncertainties in which methodologies for uncertainty analysis will be selected and used. Provision is made in this activity for evaluating and selecting methodologies. Initial selection will depend on selection criteria such as feasibility and usefulness as a learning tool. An issue that is particularly important is which among models, data, and design features will most limit the accuracy and applicability of the first analysis cycles. Results of this activity will be in the format of UCRL reports and concepts learned in this activity will guide work in Activity I-20-16.

2.4.3 Development of uncertainty methodology incorporating version II of the system model (I-20-16)

This development will be based upon the concepts learned in Activities I-20-14 and I-20-15. It will incorporate the version of the system model to be used to assess performance of the advanced conceptual design. Results will be in the form of UCRL reports and will be used in Activity I-20-17.

2.4.4 Verification of uncertainty methodology and application to analysis of advanced conceptual design (I-20-17)

This activity will verify the methodology developed in Activity I-20-16. Application of the methodology to advanced conceptual design will be reported as a UCRL report. Concepts learned in this activity will guide work in Activity I-20-18.

2.4.5 Refinement of uncertainty methodology and incorporate final version of system model (I-20-18)

This activity will use the results of Activity I-20-17 to refine the uncertainty methodology for application to the license application design. The results of this development will be documented in a UCRL report and as part of milestone M273 (see Section 5.5).

2.4.6 Uncertainty analysis of license application design and derivation of source term for total system performance (I-20-19)

The activity will use the refinements of the uncertainty methodology made in Activity 1-20-18 to analyze the license application design. This activity will provide the loss of containment and EBS source term distributions to the total system performance calculations to be performed under WBS 1.2.1.4. The results will be documented in a UCRL report and, along with results of Activity I-20-18, will appear in milestone M273.

3.0 Description of Tests and Analyses

3.1 Introduction

The entire waste package performance assessment subtask consists of program development and analyses. As described in Section 2.0 of this plan, the activities of the subtask are divided into three groups: (1) hydrothermal flow and transport; (2) development and application of system model; and (3) development and application of uncertainty methodology. The plans for these activities will be discussed in detail in the following subsections of Section 3.0.

3.2 Hydrothermal flow and transport

3.2.1 Development of detailed near-field flow and transport model (I-20-1)

Numerical modeling of the coupled multiphase heat, fluid flow, and contaminant transport is necessary to predict the waste package environment and to provide a realistic source term to total system performance assessment. This detailed analysis will not be directly used in performance assessment calculations but will serve as a guide for a simplified model, which will be part of the performance assessment system model. The numerical simulations focus on understanding the fundamental mechanisms governing heat and fluid flow in partially saturated fractured rock. Understanding the roles that fractures and adjoining matrix blocks play as conduits to liquid and vapor phase transport is of particular interest. This interaction will influence the extent of dry out in the surrounding host rock and the rate at which rewetting can occur as the thermal output of the waste decreases. These processes impact assessment of waste package corrosion mechanisms and rates and will influence transport rates near the waste package after containment failure.

The approach to be used will be to construct a three-dimensional fully implicit, finite difference solution to the partial differential equations governing multiphase fluid flow in partially saturated fractured rock. Included in this formulation are equations for the transport of heat, and the phase changes required to simulate steam-water-air systems. The solution of the transport equation for contaminants will not initially be fully coupled with the flow model but will be partially driven by velocities calculated by the flow model.

Particular attention will be given to the role of fractures in characterizing the flow and transport problem. Fracture characterization will be attempted in two ways to obtain the most accurate model for the zone nearest the emplacement borehole. Synthetic characteristic curves that integrate the properties of matrix and fractures into single curves will be tested to examine the applicability of a single porosity model. Some simulations of discrete fracture response will be performed to determine how the response of a discretely modeled fractured media differs from the continuum approach. If significant, those effects will be built into the simulation.

Radionuclide transport modeling will be studied to address two basic questions. First, the effect of the thermal pulse on the concentration of ions adversely affecting performance of the waste package will be examined. Second, the attenuation of radionuclide transport due to retardation in the first few meters of host rock will be studied to understand how the near-field host rock may modify the source term resulting from release.

These issues will be resolved by hydrothermal modeling. The basic approach for model development will be to survey the existing literature and work already in progress on the NNWSI Project to identify applicable work. Based upon that work, a new model will be formulated, either as a new simulation or as a modification of an existing code, that will address the problems discussed above. This development effort will pause for verification and validation as appropriate data becomes available. Development will resume in order to modify the code as new data from site investigations or from retardation studies is obtained. Development will continue until verification and validation exercises indicate that an accurate, representative model has been obtained.

3.2.2 Verification and validation of detailed flow and transport model (I-20-2)

Verification exercises will determine the accuracy with which the numerical simulation solves the partial differential equations of flow and transport for a given geometry and set of boundary conditions. This task will be accomplished in two ways. First, since comparisons of the numerical solution with analytical solutions are only available for certain geometries and boundary conditions, it may be possible to use this method only for isothermal single-phase unsaturated flow or for steady-state solutions of more complex systems.

A second method of verification is to compare results with other independently developed, numerical hydrothermal simulations to test the model on more complex problems. This method will allow solutions to problems containing geometries and boundary conditions that are much nearer to actual waste package environment conditions to be verified. Comparison with other numerical simulations in many cases provides the only means to examine the accuracy of predicted results.

Validation exercises require comparison of results of simulations of field or laboratory experiments with the measurements taken during those experiments. Again two types of studies are planned. First, laboratory experiments will be conducted under controlled and often restrictive conditions that will exercise many of the features of the hydrothermal model. An example is a heat pipe experiment in partially saturated rock. In this case, partial validation is possible since the laboratory experiment is intended to track matrix saturation changes as a function of time and space, and the experiment will be conducted at temperatures that will cause a phase change.

More comprehensive validation experiments are planned for the exploratory shaft tests. In the waste package environment tests, a heater will be placed in host rock, and the changes in the saturation field in a fractured rock mass will be examined. Contaminant transport calculations will require validation using data to be obtained from tracer and sorbing species tests to be conducted as part of the exploratory shaft tracer tests.

3.2.3 Sensitivity analysis of near-field flow and transport model (I-20-3)

To derive simplified waste package environment models for performance assessment calculations, the most sensitive parameters of the hydrothermal flow and transport model must be identified. There are basically two methods under consideration for approaching this problem. The first is to vary individual parameters systematically, holding all others constant, and to record the changes observed in model results. This method is simple, and although not considered rigorous, it often provides the most practical approach. The most rigorous approach would be to develop an adjoint solution for the hydrothermal code. Both methods are currently under consideration. A decision on which method will be used will await the results of early model development. The results of this activity will provide the basis for the system model hydrothermal environment submodel.

3.2.4 Analysis of source term attenuation in near-field host rock (I-20-4)

After all other activities of hydrothermal modeling are completed, the detailed model will be used to analyze the transport of radionuclides in the first few meters of host rock. The selection of radionuclides will depend on the EBS source term calculations with the performance assessment code.

Basically, the study will consist of introducing partition coefficients that allow representation of the retardation mechanisms expected in the waste package environment. The solubilities of radionuclides in the groundwater will be used to limit the concentrations that can be predicted in the liquid phase transport.

3.3 Development of the system model and analysis of waste package designs

3.3.1 Development of version I of system model (I-20-5)

The first version of the system model, which has now been largely specified, is being reviewed. This model includes data flow descriptions that will provide the basis for development of the first version of the deterministic system model, named PANDORA-1 .

PANDORA-1 will consist of a main routine which presently drives seven physical and chemical process models:

1. radiation
2. thermal
3. mechanical
4. waste package environment
5. corrosion
6. waste form alteration
7. waste transport (within the waste package)

Each of the process models will, in turn, consist of subprocess models which interact among themselves and with subprocess models from other physical processes.

As stated, PANDORA will be a deterministic model; it will use point estimates of input quantities to arrive at point estimates of the performance indicators (i.e., time-to-loss-of-containment and rate of release). It is intended that PANDORA act as the core of another program that will perform the uncertainty analysis. This development will be partially reported in Milestone M276 (see Section 5.5) reported in final form in UCRL reports.

3.3.2 Verification and validation of system model version I (I-20-6)

PANDORA will consist of a driver routine that utilizes seven process models (submodels) to calculate the performance characteristics of the waste package. These submodels will effectively act as black boxes; input parameters, which may be the output parameters of other process models, will be fed into a submodel, and the submodel will return a set of parameters (e.g., radial temperature profile, gamma dose at a location, corrosion rate) related to that particular physical process. The physical process models will be stepped through time, and performance characteristics will be calculated at various time steps. In this way, the time-dependent behavior of the waste package and its radionuclide contents will be calculated deterministically.

PANDORA-1 will involve the use of some submodels that are quite sophisticated, while others may be rather simplistic. It is expected that subsequent versions of PANDORA, which will be developed as the waste package design evolves, will involve increasingly sophisticated physical process models. This evolution will depend heavily on the work of the other waste package subtasks. As each subtask completes experimental phases, thereby obtaining new empirical data and/or developing better formulations to represent the physical processes, the new data or formulations will be assimilated by the system modeling effort.

As each submodel is developed, there will be a verification and validation phase for that submodel. This testing stage will examine only the independent submodels, possibly examining limited aspects of submodel interactions. Results of this activity will appear in UCRL reports and will be used in Activity I-20-7.

3.3.3 Testing of system model using waste package design concepts (I-20-7)

Once the driver routine for PANDORA and the independent physical process models have been written, verified, and validated, the verification and validation of the performance of the entire system model will be started. This final step in the development of PANDORA will involve testing of the system model using the configuration of the waste package conceptual design.

The initial testing process will involve tests of the performance characteristics of the waste package using the nominal values specified in the conceptual design. However, sensitivity analysis will be used to further indicate the behavior characteristics of PANDORA. The sensitivity analysis program, PROMET, will be developed near the end of the PANDORA development process. PROMET will be a program that is designed to perform sensitivity analysis for PANDORA. It is essentially a shell that exercises PANDORA as a subroutine. The different approaches to performing the sensitivity analysis will be investigated while PANDORA is being developed. The choice of sensitivity analysis methodology will, to some degree, be dependent on the final design and operating characteristics of PANDORA.

The sensitivity analysis will also serve another purpose in the performance assessment subtask. Uncertainty analysis, which will provide the probabilistic calculation of the waste package performance characteristics, will utilize the results from PROMET to determine which input parameters, submodels, subprocess models, etc. have the greatest influence over the performance characteristics. In this way, the uncertainty analysts will be able to prioritize their examination of the effect of specifying distributions, rather than point estimates, for various inputs and parameters of PANDORA. Results of this study will be reported in UCRL reports and will be used in Activities I-20-8 to I-20-19. Milestone M260 (see Section 5.5) will be among the early reports from this activity.

3.3.4 Development of system model version II for analysis of anticipated and unanticipated events (I-20-8)

This effort will be similar to that of Activity I-20-5 with a few significant changes. First, this version of the system model, PANDORA-2, will be based upon the advanced conceptual design for the NNWSI waste package. Second, unlike PANDORA-1, this version of the system model will be designed to accommodate analyses of unanticipated events as well as anticipated events. Third, in designing this version of PANDORA, the results of the sensitivity analysis of PANDORA-1 will be used as a significant additional set of data to guide the development effort. Last, preliminary results of the uncertainty analysis of PANDORA-1 should be available before the design and development of

PANDORA-2 is complete. The information from the uncertainty analysis could prove to be quite useful in making design modifications to the deterministic model.

Each successive version of the system model, and therefore, PANDORA-2, will be treated as the development of an entirely new model. Each physical process model and subprocess model, as well as all auxiliary routines, will be thoroughly examined for appropriateness in each version. Also, decisions will be made regarding the most appropriate computer system environment, computer language, etc. to be used for each new version of PANDORA.

3.3.5 Verification and validation of system model version II (I-20-9)

This effort should be essentially of the same nature as Activity I-20-6. Results will be documented in UCRL reports and will be used in Activity I-20-10.

3.3.6 Analysis of advanced conceptual design with system model version II (I-20-10)

After the driver and physical process models for PANDORA-2 have been completed, and verification and validation of the integrated system model is complete, analysis using the parameters from the advanced conceptual design (ACD) will be performed. It is expected that the results of the performance assessment of the ACD will be fed back into the design process for the license application version of the NNWSI waste package.

During the analysis of the ACD with PANDORA-2, development and utilization of the second version of the sensitivity analysis program, PROMEI-2 will be planned. The results from this sensitivity analysis of version II of the system model will be utilized in Activity I-20-11 and reported in UCRL reports and Milestone M263 (see Section 5.5).

3.3.7 Development of system model version III for analysis of anticipated and unanticipated events (I-20-11)

The effort will be similar to Activities I-20-5 and I-20-8, with the exception that the development process will be based on the license application design of the NNWSI waste package. Results will be reported in UCRL reports and will be used in Activities I-20-12, I-20-13, I-20-18, and I-20-19.

3.3.8 Verification and validation of system model version III (I-20-12)

This effort will be similar to Activities I-20-6 and I-20-9. Results will be reported in UCRL reports and will be used in Activity I-20-13.

3.3.9 Analysis of license application design with system model version III (I-20-13)

This effort will be the final deterministic simulation of the license application design. Source terms and times to containment failure will be calculated in Activity I-20-19 using the results of this activity. Milestone M268 (see Section 5.5) will document this model.

3.4 Uncertainty analysis

There is some inherent variation in fabrication and environmental parameters and, hence, in the performance values of waste packages, even with uniform design and well-controlled fabrication and emplacement conditions. Uncertainty analysis addresses this problem by analyzing the reliability of the waste packages and be developing an explicit description of the inherent variation in waste package performance.

The plan for uncertainty analysis was developed based on the purposes of the analysis and the nature of the subject matter. The purposes of the uncertainty analysis are:

1. Analyze the reliability of the waste package performance with respect to its performance criteria:

   a. Time of essentially complete containment;

   b. Release rates for individual radionuclides for a period of 10,000 years;

   c. Total release as of 10,000 years.

2. Provide a cumulative probability distribution function (CDF) on the total release as of 10,000 years.

3. Provide a source term, including description of variability, to the total repository system performance assessment and reliability assessment.

Possible additional uses of uncertainty analysis are:

4. Provide CDFs of other performance measures.

5. Determine the data elements or modeling areas contributing most to the uncertainty (i.e., assess sensitivity of uncertainty) as a guide to additional tests or model refinement to reduce the uncertainty.

Assessment of reliability with respect to performance criteria means assessing the probability that the performance value is on the acceptable side (high for time of containment, low for releases and release rates) of the performance criteria. This assessment is one point on the CDF. A low probability that the waste package would not meet its performance criteria and a high confidence in this low probability are desirable.

When the assessment of the CDF to performance values is extended well beyond the performance criteria and correspondingly to higher probabilities of occurrence, it must be recognized that confidence in the CDF values becomes progressively less. Paradoxically, the better the waste package design and performance become, the less accurately its actual performance value can be predicted, even though a high confidence on lower bounds of performance may be realized. An example of an assessed CDF and a format for depicting confidence interval on the assessed CDF is shown in Figure 1. There are two types of uncertainty in waste package performance shown separately in Figure 1: the best estimate CDF represents the uncertainty due to inherent variability; and the higher and lower CDFs represent the confidence in the best estimate CDF due to a finite state of knowledge. Although separate, if desired, the CDFs can be merged using the calculational tools of probability theory to get one overall uncertainty.

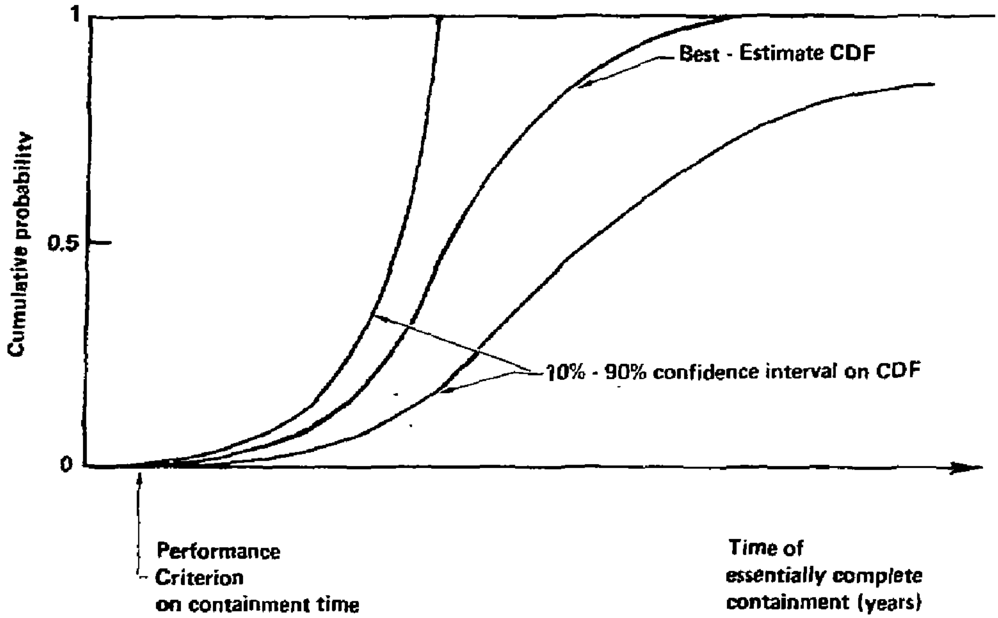

Fig. 1. Example of an assessed CDF depicting confidence intervals on the distribution.

The strategy for uncertainty analysis is to perform the analysis incrementally in three cycles because of the stages of information becoming available from other subtask tests and the stages in waste package design, i.e., conceptual design, advanced conceptual design, and licensing design. There will also be stages in the experience with the applicability of uncertainty analysis methodologies and in sensitivity-of-uncertainty results. This experience will guide further cycles in the methodology development process.

The stages and the step-by-step plan for carrying out the uncertainty analysis are as follows.

3.4.1 Development of uncertainty analysis methodologies for testing with the

system model (I-20-14)

3.4.1.1 Examine methodologies

First, various existing methods of reliability analysis will be examined for applicability and feasibility. Methods to improve on computational efficiency or accuracy will be explored or created.

Features of the waste package performance process that must and will be addressed in the selection of a suitable uncertainty analysis method include:

1. The identification and description of failure modes.

2. The continuous and multidimensional range of input parameters affecting package performance.

3. The coupling of parameters in processes.

4. The interactions of processes and the gradually changing conditions of the waste package.

Numerous methodologies exist to date. They will be reviewed and evaluated in order to choose the most promising ones. All of the methodologies require information on the distributions of values of the input parameters. These will be treated as probability distributions of random variables. Not all of the input parameters need to be treated as random variables. The parameters needing such treatment can be determined from results of the sensitivity analysis of the deterministic system model coupled with preliminary estimates of the amount of variability in the parameters.

Several methods are available to evaluate the CDF of a performance measure (such as total EBS release). One group of methods involves sampling from the probability distribution of the input variables and doing repeated deterministic calculations of the performance using these samples of inputs. In this way, a sample of output performance values is accumulated, which approximates the CDF of the output. The input sampling may be by purely random sampling, by stratified sampling such as Latin Hypercube sampling, or by stratified selection.

Other methods of evaluating the CDF include analytic methods of propagating moments of the input probability distributions to moments of the output probability distributions. In addition, some methods involve combined techniques of response surface analysis to get a simplified model of the deterministic process and then sampling inputs and using the simplified model.

To evaluate the reliability of the waste package in meeting its performance criteria, several methods are available. Sampling as in evaluating the CDF is possible but may be inefficient if the unreliability to be determined is very low. Biased sampling may be of some help in this case. Another approach determines the first few central moments of the output distribution from the sample used in evaluating the CDF and then extrapolated this distribution to high or low probabilities using the moments. This approach is easy but has a relatively large uncertainty due to the extrapolation.

Another group of methods for evaluating the reliability involves finding the dividing surface in the multidimensional input space between the "success" space (i.e., those combinations of inputs which give a successful performance outcome) and the "failure" space. One then integrates the joint probability measure of the input variables over the failure space to determine the probability of failure. Usually it is too tedious an exercise to determine the exact dividing surface between success and failure spaces, so one falls back on a simpler dividing surface between a "safe" space and an "unsafe" space. The unsafe space contains some undetermined part of the success space and all of the failure space. The idea is to find some simple method to qualify and delineate a safe space, even at the expense of conceding some possible success regions to the opposite space.

3.4.1.2 Select methodologies

Selection criteria, which may include combinations of feasibility, defensibility, manageable input data needs, usefulness in the analysis, accuracy, and usefulness, will be determined as a learning tool in the phased development process. One or several methodologies from those evaluated in Section 3.4.1.1 will be selected to answer the questions posed for the first version of the system model and the conceptual design.

3.4.1.3 Develop computer program

A computer program to implement the selected uncertainty analysis methodologies will be developed. This is expected to be a substantial project. It will be done in a methodical and documented manner of computer program development.

3.4.2 Verification of suitability of uncertainty methods using system model version I (I-20-15)

3.4.2.1 Develop input data on parameter probability distributions

Data describing the probability distributions of those parameters of the deterministic model that must be treated as random variables will be developed. Parameters that need such treatment can be determined from results of the sensitivity analysis of the deterministic system model coupled with preliminary estimates of the amount of variability in the parameters. The format of the data will depend on the uncertainty methodologies selected, and may include type of distribution, moments, and upper and lower limits on values.

The data on probability distributions will need to be provided by other subtasks in the Waste Package Task, which contain the data, experimental programs, and expertise on the individual processes and their parameters.

3.4.2.2 Estimate secondary uncertainties and gaps in the data in Section 3.4.2.1

Asking for a probability distribution is asking for more information than is contained in just a best-estimate value or a mean value. The basic measurements and analyses on measurements to support distribution information may be available only to a limited extent, thus leaving some uncertainty in the distribution information. This is known as secondary uncertainty to distinguish it from the uncertainty in the value actually obtained when sampling from the distribution.

3.4.2.3 Perform trial computer runs using hypothetical data to demonstrate functioning of program and to identify some major features of program performance, such as effects of probability distribution input values and of submodel performance

This step is exploratory, but important. Often in a large complex system of software or hardware, the implications of the whole are not obvious from knowledge of the parts or of the specification. Effects of the whole model on submodel performance, of submodel interactions, and of input data combinations should be explored. Some trial runs can be guided by knowledge of the internal structure of the model. These runs allow examination of expected major influences on the output from certain submodels or certain input uncertainty values. Other trial runs should be "black-box" input-output studies. Any unanticipated major influences on output should be studied until they can be understood.

3.4.2.4 Perform uncertainty analysis of conceptual design

This step will take the input data applicable to the conceptual design determined in Section 3.4.2.1 and do an uncertainty analysis of that design. The uncertainty analysis will include reliability analysis of the waste package meeting its performance criteria, CDFs of performance values, and source term over time with some description of its uncertainty.

3.4.2.5 Estimate the secondary uncertainty in the results in Section 3.4.2.4

This step will estimate the uncertainty in the probability distribution values and characterizations done in Section 3.4.2.4. The sources of this uncertainty include uncertainty in inputs, models, and limitations in sample size and algorithm accuracy due to time tradeoffs.

3.4.2.6 Estimate the major sources of this secondary uncertainty in the results in Section 3.4.2.4.

This estimation will provide some guidance to the next cycle of development. The estimation at this stage may be done by a combination of qualitative and subjective judgments and a limited amount of sensitivity-of-uncertainty computerized analysis.

The major purpose of the analyses in Sections 3.4.2.4 and 3.4.2.5 is to check the feasibility of the approach, that is, whether enough data is available to support it, how much manpower and computer time it takes, how large the uncertainties in the results are, and whether the uncertainties in the results can be meaningfully described.

3.4.2.7 Perform uncertainty analysis or sensitivity-of-uncertainty analysis for alternate design features as needed

This step can check out the implications on reliability arising from alternate design features or from design parameters that could be changed. At this cycle in the methodology development, any results and recommendations will need to be checked on a case-by-case basis to make sure they are significant and not the result of oversimplification of the model or input data. Results of this activity will be reported in UCRL reports, and concepts will be incorporated into Activity I-20-16.

3.4.3 Development of uncertainty methodology incorporating version II of the system model (I-20-16)

These activities will parallel those presented in Section 3.4.1 except that it will be necessary to address new questions that will arise with the analysis of the advanced conceptual design. Expected new questions concern the analysis of scenarios based on unanticipated events and combination of the results of analyses of anticipated and unanticipated events into a net reliability and a net COF for performance values. The source term will remain uncombined; separate source term descriptions conditional on the specified unanticipated events will be developed. Any new features due to the new advanced conceptual design must also be treated in the analysis. The degree of accuracy and/or the degree of defensibility required of the analyses will be increased at this cycle, consistent with the quality assurance level required for analysis of alternative designs.

Based on requirements and on methodology selection criteria, refinements or additions to the first cycle methodology may be added. If found desirable, an essentially different methodology may be selected. A new computer program for uncertainty analysis will then be developed. This development will be treated as a new computer program even if major parts of methods developed in Section 3.4.1 are adopted for reuse. The program will be developed following a methodical standard procedure of scoping, specification, design, and cooling. Results of this activity will be reported in UCRL reports and will be used in Activity I-20-17.

3.4.4 Verification of uncertainty methodology and application to analysis of advanced conceptual design (I-20-17)

This activity will parallel that described in Section 3.4.2; however, analyses will be made of the advanced conceptual design. Therefore, it will be necessary to develop input data on parameter probability distributions and on scenario probabilities. Secondary uncertainties will then be estimated, and gaps in the input data identified. Trial computer runs will then be performed using hypothetical data to demonstrate the functioning of the program and to identify some major features of program performance, such as effects of input uncertainties and submodel performance.

An uncertainty analysis of advanced conceptual design will follow trial runs. This will include estimation of the secondary uncertainty in the analysis results and the major sources of this secondary uncertainty. After identifying some techniques or representative problems for use in verification of uncertainty methodology, a limited verification of the uncertainty methodology will be conducted. Results of this activity will be reported in UCRL reports, and concepts will guide the work in Activity I-20-18.

3.4.5 Refinement of uncertainty methodology and incorporate final version of system model (I-20-18)

After analysis of the advanced conceptual design, it will be necessary to examine new questions as well as the nature and accuracy required of analyses. This activity will be guided by results of previous cycles of waste package analysis. At this time, it may be necessary to add methodologies or select alternate methodologies. After these questions are addressed, a new computer program for uncertainty analysis will be developed. Results of this activity will be used in Activity I-20-19 and will be documented in UCRL reports.

3.4.6 Uncertainty analysis of license application design and derivation of source term for total system performance (I-20-19)

As before, input data on parameter probability distributions and on scenario probabilities will be developed. Again, this will include estimating remaining secondary uncertainties in the input data. Trial computer runs will be made using hypothetical data to demonstrate the functioning of the program and to identify some major features of program performance, such as effects of input uncertainties and submodel performance. Some techniques or representative problems for use in verification and validation of uncertainty methodology will be identified, and a verification and validation of the uncertainty methodology will be performed.

Reliability analysis of license application design will then proceed, leading to the required complimentary cumulative distribution functions for performance measures. Further, an analysis will be conducted to derive the source term for total system performance, including description of the variability in the source term. Finally, estimates and descriptions of the secondary uncertainty in these results will be made. This analysis will then serve as input to total system performance assessment performed under WBS 1.2.1.4. Activity results will be reported in Milestone M273 (see Section 5.5).

3.5 Equipment

Performance assessment consists of computational activities; therefore, the equipment used in these activities are computer systems. Presently, performance assessment plans to use two computer systems. The system to be used for program development and testing is a network of Sun workstations and Ridge computers that are located in the Earth Sciences Department at Lawrence Livermore National Laboratory. These systems are UNIX-based computers linked by an Ethernet network. The UNIX operating system provides utilities to facilitate operating system software configuration management as required by software quality assurance requirements.

Application of the hydrothermal system model and uncertainty codes will be utilized in Magnetic Fusion Energy Computing Center (MFECC) computers at Lawrence Livermore National Laboratory. This center currently consists of two CRAY I computers, a CRAY X-MP computer, and a CRAY-2 supercomputer. These computers are being linked to a laboratory-wide Ethernet network which will communicate with the Sun workstation network via a UNIX shell at MFECC. This system will provide for the large number of system model executions (foreseen to be) required for uncertainty analysis. The Ethernet network will also allow the control of applications, as required by quality assurance procedures.

4.0 Application of Results

4.1 Detailed hydrothermal flow and transport

These calculations are necessary to provide an understanding of the hydrologic environment of the waste package. The results will be used as a basis for formulation of the waste package environment submodel of the performance assessment code. Cases simulated by this model will be used to verify that submodel. Further, sensitivity analysis of this model will help to determine the significant variables to be included in performance assessment calculations. The model will also be useful in the design of experiments fo the exploratory shaft waste package environment tests.

The releases calculated from the Engineered Barrier System may not be the most appropriate source term for total system performance assessment calculations. Therefore, this model will allow examination of radionuclide transport in the immediate vicinity of emplacement. Through these calculations, the environment submodel of the waste package performance assessment code can be modified to include the effects of retardation near the package if desired.

4.2 System model development and application

At present, three versions of the system model are planned. The first version is an initial test bed for deterministic waste package performance assessment modeling concepts. The second version will be used to analyze advanced conceptual design alteratives. The final version of the system model will deterministically calculate waste package performance. It will be used to analyze the license application design directly to develop bounding values of performance. In addition, it will be incorporated into the uncertainty methodology to provide a means for determining the complimentary cumulative distribution functions for time to waste package failure and for radionuclide release rates. The system models developed prior to the final version will provide a basis for testing analytical techniques and will be used to screen waste package designs.

4.3 Uncertainty analysis methodologies

The uncertainty methodology will be used to provide the direct input to the total system performance assessment in the form of a probabilistic source term. Further, it will be used to evaluate the reliability of the waste package with respect to the containment and release requirements of 10 CFR 60. This methodology will incorporate the successive versions of the system model to construct the required complimentary cumulative distribution function.

5.0 Schedule and Milestones

5.1 Discussion and assumptions

The subsections that follow present schedules for waste package performance assessment activities. These activities are grouped into three basic efforts: (1) hydrothermal modeling of near field flow and transport; (2) development of the waste package systems model; and (3) uncertainty analysis. The schedules presented are based on assumptions described and on a continued level of effort consistent with the 1988 WPAS submission.

Since performance assessment collects information to perform the required calculations, the schedule for activities presented is based on inputs from other waste package subtasks that are expected on a continuous basis. However, because the performance assessment system modeling effort will produce a series of three codes, deadlines exist for final input of information into the system code. Assumptions are also made regarding the time at which the advanced conceptual and license application waste package designs will be available. Data for validation and refinement of the waste package environment are expected from the exploratory shaft experiments. Finally, input from the total system performance assessment effort is expected to provide scenarios to be included in the waste package performance assessment. Variations in the delivery of these inputs will cause significant variations in the schedules presented for activities and milestones.

The following schedule presents dates by which input from activities other than performance assessment are needed to meet the milestone dates for performance assessment.

1. Waste package subtask inputs

a.	submodels for analysis of conceptual designs	11/86
b.	submodels for analysis of advanced conceptual designs	8/87
c.	submodels for analysis of license application design	6/88

2. Waste package designs

a.	conceptual design	currently available
b.	advanced conceptual design, preliminary input	11/87
c.	advanced conceptual design, final input	4/88
d.	license application design	6/89

3. Exploratory shaft (ES) data

a.	preliminary ES input	9/88
b.	final ES input	7/89

4. Scenarios for anticipated and unanticipated events

a.	preliminary input	11/87
b.	final input	7/89

5.2 Hydrothermal flow and transport modeling

The purpose of the near-field flow and transport modeling is to provide boundary conditions for performance assessment, a component of the waste package environment submodel, an interface between the waste package environment submodel, and a theoretical interface between the waste package and total system performance assessments. Therefore, the schedule above conforms to the requirements of the performance assessment calculations. The development of the flow and transport submodel is included as part of system model development activities. Activities I-20-1 and I-20-2, rovide the necessary theoretical basis for the submodel to be included in the system model. Activity I-20-3 occurs concurrently with the system and with uncertainty analysis of the license application design and helps to provide source terms to the total system performance assessment when the waste package performance assessment calculations are complete.

The following table presents the hydrothermal flow and transport activities and their durations:

	Analyses	Duration
I-20-1	Development of detailed near-field flow and transport model	7/86-8/88
I-20-2	Verification and validation of detailed flow and transport model	2/87-11/89
I-20-3	Sensitivity analysis of near-field flow and transport model	7/87-9/88
I-20-4	Analysis of source term attenuation in near-field host rock	1/89-11/90

5.3 Development of the systems model and analyses of waste package designs

The development of the system model parallels the schedule for development of waste package designs. The first version of the system model will utilize waste package design concepts that first appeared in the Site Characterization Plan. The second version will contain revisions reflecting new data from the investigation subtasks (e.g., metal barriers, waste form degradation, waste package environment, etc.) and will be used to analyze the advanced conceptual design. The final version will be used to analyze the license application design. This version will incorporate the conclusions of the investigation subtasks. Though all versions will undergo verification and validation, the final version will require the most effort in this area since it will be the most complex and will be used to produce input to total system performance assessment.

The schedule for system model activities is as follows:

	Analyses	Duration
I-20-5	Development of version I of system model	7/86-1/87
I-20-6	Verification and validation of system model version I	7/86-1/87
I-20-7	Testing of system model using waste package design concepts	1/87-11/90

I-20-8	Development of system model version II for analysis of anticipated and unanticipated events	6/87-10/87
I-20-9	Verification and validation of system model II	10/87-2/88
I-20-10	Analysis of advanced conceptual design with system model version II	2/88-9/88
I-20-11	Development of version III of system model for analysis of anticipated and unanticipated events	9/88-2/89
I-20-12	Verification and validation of system model version III	2/89-8/89
I-20-13	Analysis of license application design with system model III	8/89-7/90

5.4 *Uncertainty analysis*

The uncertainty methodology will incorporate model system versions. Therefore, reliability analysis of the waste package designs must be scheduled to allow for system model development. The final reliability analysis must await completion of all work that might impact system model process submodels.

The schedule for uncertainty analysis activities is as follows:

I-20-14	Development of uncertainty analysis methodologies for testing with the system model	11/86-11/90
I-20-15	Verification of suitability of uncertainty methods using system model version I	6/87-1/88
I-20-16	Development of uncertainty methodology incorporating the version II of the system model	1/86-9/88
I-20-17	Verification uncertainty methodology and application to analysis of advanced conceptual design	9/88-3/89
I-20-18	Refinement of uncertainly methodology and incorporation of final version of system model	3/89-10/89
I-20-19	Uncertainty analysis of license application design and derivation of source term for total system performance	10/89-1/91

5.5 Milestones

The only milestone for near-field flow and transport is presently as follows:

Title	Milestone	Date
Detailed flow and transport model documentation	P204	4/90

The level 1 and level 2 milestones for system model development are as follows:

1.	Design specification report on first version of system model	M276	8/86
2.	Report on system model I analysis of waste package conceptual designs	M260	4/87
3.	Report on system model II analysis of advanced conceptual designs	M263	12/88
4.	Final documentation of system model III and analysis of license application design	M268	2/91

Presently, there is only one level 1 milestone for uncertainty analysis:

Final report on waste package performance assessment and reliability analysis of license application design	M273	6/91

6.0 List of Activity Plans to Support this Study Plan

Waste package performance assessment activities will be grouped for production. As before, the groups will be: (1) development of the near-field hydrothermal flow and transport model; (2) development and application of the system model; and (3) development and application of the uncertainty analysis methodology. Production of these activity plans is prioritized with respect to their overall importance to waste package performance assessment. The following schedule presents production dates for activity plans.

6.1 Hydrothermal flow and transport model

Production Date for Activity Plans: 6/87

Activities Included in Plan:

Number	Title
I-20-1	Development of detailed near-field flow and transport model
I-20-2	Verification and validation of detailed flow and transport model
I-20-3	Sensitivity analysis of near-field flow and transport model
I-20-4	Analysis of source term attenuation in near-field host rock

6.2 Development and application of system model

Production Date for Activity Plans: 12/86

Activities Included in Plan:

Number	Title
I-20-5	Development of version I of system model
I-20-6	Verification and validation of system model version I

Number	Title
I-20-7	Testing of system model using waste package design concepts
I-20-8	Development of system model version II for analysis of anticipated and unanticipated events
I-20-9	Verification and validation of system model version II
I-20-10	Analysis of advanced conceptual design with system model version II
I-20-11	Development of version III of system model for analysis of anticipated and unanticipated events
I-20-12	Verification and validation of system model version III
I-20-13	Analysis of license application design with system model version III

6.3 Development and application of uncertainty methodology

Production Date for Activity Plans: 3/87

Activities Included in Plan:

Number	Title
I-20-14	Development of uncertainty analysis methodologies for testing with the system model
I-20-15	Verification of suitability of uncertainty methods using system model version I
I-20-16	Development of uncertainty methodology incorporating version II of the system model
I-20-17	Verification of uncertainty methodology and application to analysis of advanced conceptual design
I-20-18	Refinement of uncertainty methodology and incorporate final version of system model

Number	Title
I-20-19	Uncertainty analysis of license application design and derivation of source term for total system performance