January 31, 1989

PROGRAM PLAN FOR
MODELING AND VALIDATION EXERCISES
UNDER THE
NMSS/RES MEMORANDUM OF UNDERSTANDING (MOU)

NRC PROJECT TEAM
INTRAVAL RPOJECT

PROGRAM PLAN FOR MODELING AND VALIDATION EXERCISES UNDER THE NMSS/RES MEMORANDUM OF UNDERSTANDING (MOU)

INTRODUCTION

The NRC accepted an invitation from the INTRAVAL Project Secretariat to participate in INTRAVAL (Letter from E. Beckjord, RES to K. Andersson, SKI dated Sept. 9, 1987). INTRAVAL is an international endeavor focusing on validation issues associated with simulating hydrologic flow and radionuclide transport for radioactive waste reporting sites. This ongoing effort is being incorporated as Task 1 of the NMSS/RES Memorandum of Understanding (MOU). Under the MOU, NMSS and RES staff will be developing an in-house flow and transport modeling expertise for performance assessment modeling. This expertise will come from evaluating and modeling observed processes at experimental field sites and in controlled laboratory experiments. The NRC staff will improve its understanding of the controlling phenomena for flow and transport in the geosphere. NRC staff participation in INTRAVAL will benefit the MOU by; 1) comparison and development of validation criteria for different conceptual models for flow and transport through the different participants analyses, 2) peer review of NRC analyses and modeling of flow and transport of radioactive waste, and 3) interaction with and ability to influence experimental programs in other countries.

NRC participation will focus on test cases which, at this time, are considered to be most relevant to NRC licensing needs. The test cases initially selected for analysis are:

1. Apache Leap unsaturated tuff experiments
   (University of Arizona - FIN D1662)

2. G-tunnel borehole experiment in unsaturated tuff
   (USGS - DOE Funding)

3. Synthetic migration experiment
   (Cooperative Effort Among NRC - PNL - NAGRA)

4. Alligator Rivers natural analog experiment
   (ANSTO International Cooperative Project)

5. Las Cruces unsaturated flow and transport experiment
   (New Mexico State University - FIN B8934)

NRC participation includes fourteen staff members (see Table 2) and a number of RES contractors (SNL/NRC, MIT, PNL, and UofA) at different levels of involvement. This program plan structures and defines the staff participation for the flow and transport modeling exercises and the NRC participation in INTRAVAL.

BACKGROUND

NRC will need to review and accept the validity of DOE's assumptions and simulations of ground-water flow and radionuclide transport at Yucca Mountain. The validity of ground-water flow and radionuclide transport models is still an issue that is being examined in all countries involved in nuclear waste disposal. A clear explanation of validation needs and goals was presented in the following excerpt from the INTRAVAL First Progress Report;

"Previous experiences from attempts to validate geosphere transport models have lead to an increased confidence in the models. They have, however, also lead to an awareness that model validation is a difficult issue, which cannot be resolved by simply comparing model results with experimental data. This procedure will most likely create alternative explanations of the experiments that cannot be unambigously confirmed or rejected because of insufficient information.

In order to increase the possibilities to be conclusive in validation, there is a need to utilise information from different types of experiments on different temporal and spatial scales. There is also a need to increase the interaction between modellers and experimentalists in order to gain reassurance that the experimental data are properly understood and that the experiences of modellers regarding the type of data needed from the experiments are accounted for.

One must recognise that validation of models is an integrated part of the scientific process with the necessary components:

- identification of outstanding issues requiring experimental/technical resolution,

- identification of experimental procedures to address these issues,

- peer evaluation and review.

These different aspects of the model validation process are well suited to be tackled in an international group. Confrontation of ideas, larger range of experimental data, as well as contacts between modellers and experimentalists from several countries should serve as a driving force for progress.

Considering the fact that nuclear waste disposal programmes in many countries now gradually leave a generic stage and enter a stage of application it is clear that the need for "validated" models will increase. The detailed validation strategies will vary between different countries and their programmes for nuclear waste disposal due to e.g. different time schedules as well as dissimilar performance measures and criteria for waste repositories. It is, however, foreseen that the INTRAVAL project will provide a framework for international co-operation which can meet important demands in the development of strategies for geosphere transport model validation."

OBJECTIVES

NMSS and RES (memorandum from R. Browning DHLW, NMSS to G. Arlotto, DE, RES dated May 13,1988) have committed staff involvement to INTRAVAL that will address; 1) improve understanding of the validity of models for flow and transport of radionuclides, 2) better understanding limitations of current experimental techniques used in site characterization and parameter estimation, 3) better defining experiments needed to distinquish between different conceptual models, 4) improving performance assessment capability within NMSS and RES, and 5) allowing for peer review of NRC staff analyses similar to the analyses that will be required during the DOE's liscence application.

PROGRAM DESCRIPTION

As described above, the INTRAVAL participation will focus on five test cases. While staff simulation efforts will concentrate on these test cases, it is anticipated that additional benefit will be derived from following the efforts of the other project teams involved in the other test cases (e.g., fracture flow and transport phenomena). This supplemental effort will consist primarily of attendance and participation at INTRAVAL Meetings. The MOU program work is limited to the situation exercises related to the five specific test cases described earlier.

Each validation/simulation exercise may involve different technical issues or phenomena, however, the steps taken to reach a conclusion will require the following three programmatic steps:

Step 1: Test Case Definition and Validation Strategy

The staff effort for each test case will begin with a review of the INTRAVAL test case definition. Based on this review, a strategy will be developed as a guide for the hypothesis testing and simulation effort to be performed in Step 2. The strategy will include; 1) clear description of phenomena to be analysed/validated, 2) initial identification of data needs and uncertainties, 3) identification of performance measures, 4) discussion of relevance to performance assessment, and 5) initial estimate of goodness-of-fit expected between experimental and simulation results (as quantitative as possible). The validation strategy will be documented and reviewed prior to proceeding to the next step of the test case exercise.

Step 2: Initial Simulations

Based on the validation strategy developed in Step 1, initial simulations will be performed. The goals of these simulations will be; 1) determine the adequacy of computer programs to simulate the test case, 2) determine the appropriateness of the performance measures, 3) better define uncertainties and data needs, and 4) define a rigorous validation test.

Step 3: Validation Simulation and Conclusions

Based on the previous results, a validation simulation will be designed, executed and analysed. The results of the simulation will also consider other INTRAVAL results to support or reject the validity of the model. Regardless of the the validation finding, the final analyses will involve; 1) technical rational for the finding, 2) discussion of the results of other conceptual models used by other INTRAVAL participants, 3) recommendations for future experiments, and 4) discussion of unresolved issues and possible resolution.

INITIAL TEST CASE EXERCISES

Specific exercises for the five test cases are expected to be:

Apache Leap -

Exercise 001; Fracture and matrix flow will be analysed using field experimental data. The initial approach will assume a porous media where fractures may be accounted for as high conductivity zones and/or a bi-modal characteristic curve. Computer programs such as TOUGH and SUTRA will be used. Staff equivalent porous media simulations will be compared with discrete fracture models of other INTRAVAL participants (University of Arizona).

Exercise 002; Two-phase flow and heat transport in a porous media will be examined using the core experiment data. The computer program TOUGH and a semi-analytic solution (to be developed in-house) will be used. Staff two-phase flow simulations will be compared with other two-phase flow models of other INTRAVAL participants (SNL/NRC and USGS).

Exercise 003; Fracture and matrix flow will be analysed with the laboratory block experiment data. The initial approach will assume a porous media where fractures may be accounted for as high conductivity zones and/or a bi-modal characteristic curve. Computer programs such as TOUGH and SUTRA will be used. Staff equivalent porous media simulations will be compared with discrete fracture models of other INTRAVAL participants (University of Arizona and SNL/NRC).

G-Tunnel -

Exercise 004; The G-tunnel experiment examines the effect of wet and dry drilling on heat and fluid flow in unsaturated tuff. Analyses will concentrate on fracture and matrix flow under slightly elevated temperatures. Two-phase flow will be analysed assuming porous media with fractures accounted for as a high conductivity zone and a bi-modal characteristic curve. The computer programs TOUGH and SUTRA will be used. Comparisons will be made with of a model which includes two phases (TOUGH) and a model which includes a single phase (SUTRA) for simulating unsaturated flow and heat transport.

Synthetic Migration Experiment -

Exercise 005; The synthetic migration experiment is designed to examine the uncertainties of performance predictions arising from incomplete knowledge of the hydrogeologic system. The limitations of current predictive simulation techniques are to be examined in this test case. Computer models such as SWIFT II, SUTRA and DPCT could all be used. Comparison of predictive modeling techniques of the NRC staff with other techniques used by other INTRAVAL participants.

Alligator Rivers Analog -

Exercise 006; The Alligator Rivers analog is focused on the long term (hundreds of thousands of years) and large scale (hundreds of meters) migration of radionuclides from an unranium ore body. Analyses will examine dispersive and retardation mechanisms. Computer programs such as SWIFT II, SUTRA, DPCT and EQ3/EQ6 will be used. (The significant time involved in detailed geochemical modeling (i.e., use of EQ3/EQ6) may require that NRC staff follow the work being done by other contributors to INTRAVAL such as Dimitri Sverjensky from Johns Hopkins University.) Comparison of various retardation mechanisms (e.g., retardation coefficient, Freundlich isotherm, detailed geochemistry) and examination of dispersion phenomena over long times will be made within the NRC staff effort and with other INTRAVAL participants.

Las Cruces Trench -

Exercise 007; The Las Cruces trench experiment was designed to examine the affect of spatial variability on the infiltration and subsequent moisture redistribution in a porous media. The analyses of this test case will examine how spatial variability in hydrologic properties affects horizontal and vertical flow and transport in heterogeneous unsaturated media. It is anticipated that deterministic models such as TOUGH and SUTRA will be used. (Time commitments of the NRC staff may dictate that participation be limited to following the stochastic and deterministic modeling being done by NRC contractors such SNL/NRC, PNL and MIT.) Comparison of stochastic and determinsitic models will be performed.

Test case exercise scheduling and staff commitments are presented in Tables 1-7. (Due to NRC participation in INTRAVAL prior to the MOU, progress on the Apache Leap test case has already been made and is reflected in the Tables.)

Documentation

It is anticipated that due to the complexity of both the validation issues and test cases, the staff effort will be an iterative process consisting of a number of simulation excercises which analyse a particular issue. At the conclusion of each exercise (Steps 1-3), a progress report will be written to document the results. A notebook for each test case exercise will be maintained for the duration of the project which will provide a record for the various simulation activities and the technical findings. The emphasis of the test case notebooks will be to maintain a clear ongoing technicl documentation of the work.

Additionally, an annual summary report will be prepared which documents the important findings from the INTRAVAL project. The objective of this documentation is to incorporate and document the collective INTRAVAL findings (i.e., obtained through attendance at meetings and review of INTRAVAL documentation) as they pertain to individual test cases and to the licensing of an HLW repository in the United States (i.e., scaling of hydrologic and transport properties for the INTRVAL cases should be directly applicable to scaling issues at Yucca Mountain).

Meetings

The INTRAVAL Project involves a variety of problems that examine a number of flow and transport validation issues under a variety of hydrogeologic conditions and at differing spatial and time scales. The NRC staff and their contractors do not have the resources to be involved in every test case and will only be able to try a limited number of modeling exercises for selected test case. However, through active participation at INTRAVAL Workshops, the NRC Staff will be able to maximize this effort by closely following the simulation analyses of all test cases via the cooperative nature of this international project.

An integral part for benefiting from the cooperative effort on INTRAVAL is the participation in workshops and associated field trips. The workshops are the primary way technical ideas are exchanged and peer review of staff analyses is accomplished. NRC staff and contractors attending the workshops and field trips will brief NRC staff and management on their technical findings.

Staff participation will primarily be coordinated through bi-weekly meetings to be held in OWFN. RES will be responsible for distributing an agenda the Friday prior to the meeting.

NRC PROGRAM MANAGER

The NRC program manager will coordinate staff simulation work and documentation on the modeling exercises and be responsible for communication with the NRC representative to the INTRAVAL Project Secretariat.

Contractor Participation

This program plan describes NRC staff participation, however, it is important to note that it is dependent on a significant contribution from NRC contractors. These contractors are responsible for developing an experimental data base at Apache Leap and Las Cruces Trench sites. RES is also currently providing partial funding to the multi-national cooperative agreement for the Alligator Rivers Analog Project. NRC contractors (i.e., MIT, PNL, SNL, and UofA) will also be using different models for simulating these test cases.

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Table 2 MOU staffing requirements (reported as staff weeks).

					RES											NMSS	NRC
TASK	TN	TM	GB	LK	TOTAL	RC	NE	WF	JB	JV	NC	DC	JH	KM	SC	TOTAL	TOTAL
INTRAVAL	4				4								1		2	3	7
Las Cruces	7	2	2	2	13		6	7	4			2		2		21	34
G-Tunnel	5	5			10		4	4	3					1		12	22
Apache Leap	10	10	4	5	29		6	16	5			3		2		32	61
Alligator R.		5	6	5	16				7		7			2		16	32
Synthetic Migration		4			4	14				3						17	21
Travel	4	4			8	2										2	10
Training	2	2			4											0	4
Totals	32	32	12	12	88	16	16	27	19	3	7	5	1	7	2	103	191

TN - Tom Nicholson

TM - Tim McCartin

GB - George Birchard

LK - Linda Kovach

RC - Richard Codell

NE - Norman Eisenberg

WF - Bill Ford

JB - John Bradbury

JV - John Buckley

NC - Neil Coleman

DC - Don Chery

JH - Joe Holonich

KM - Keith McConnell

SC - Seth Coplan

Table 3. Task plan and staff commitments (reported in weeks) for the Apache Leap Test Case.

FY 1989	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
EXERCISE 001 (Field Experiment)									
Step 1 (Strategy) Staff Effort - 0 weeks									
Step 2 (Simulation) Staff Effort - 0 weeks									
Step 3 (Validation) Staff Effort - 4 weeks		X	XXX						
Total Exercise Effort - 4 weeks TM(1), TN(1), WF(1), JB(.5), DC(.5)									
EXERCISE 002 (Core Experiment)									
Step 1 (Strategy) Staff Effort - 7 weeks		X	X	X					
Step 2 (Simulation) Staff Effort - 14 weeks		X	X	X	X				
Step 3 (Validation) Staff Effort - 5.5 weeks					X	X	X	XXX	
Total Exercise Effort - 26.5 weeks WF(6), TM(5), TN(4), NE(3), JB(2), GB(2), LK(2), DC(1.5), KM(1)									
EXERCISE 003 (Block Experiment)									
Step 1 (Strategy) Staff Effort - 7 weeks			X	X	X	X			
Step 2 (Simulation) Staff Effort - 18 weeks			X	X	X	X	X	X	
Step 3 (Validation) Staff Effort - 5 weeks							X	X	X
Total Exercise Effort - 30 weeks WF(9), TN(5), TM(4), LK(3), JB(3), NE(2.5), GB(2), DC(1.5), KM(1)									

XXX - Progress Report Due

Table 4. Exercise plan and staff commitments (reported in weeks) for the G-Tunnel Test Case.

	FY 1989								
	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
EXERCISE 004									
Step 1 (Strategy)		X	X	X	X				
Staff Effort - 11 weeks									
Step 2 (Simulations)				X	X	X	X	X	X
Staff Effort - 11 weeks									
Step 3 (Validation)									
Staff Effort - 0 weeks									

Total Exercise Effort - 22 weeks
TM(5), TN(5), WF(4), NE(4), JB(3), KM(1)

Table 5. Exercise plan and staff commitments (reported in weeks) for the Synthetic Migration Test Case.

	FY 1989								
	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
EXERCISE 005									
Step 1 (Strategy)	X	X	X	X	X	X			
Staff Effort - 7 weeks									
Step 2 (Simulations)				X	X	X	X	X	X
Staff Effort - 14 weeks									
Step 3 (Validation)									
Staff Effort - 0 weeks									

Total Exercise Effort - 21 weeks
RC(14), TM(4), JV(3)

Table 6. Exercise plan and staff commitments (reported in weeks) for the Alligator Rivers Analog Test Case.

	FY 1989								
	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
EXERCISE 006									
Step 1 (Strategy)			X	X	X	X	X	X	
Staff Effort - 15 weeks									
Step 2 (Simulations)				X	X	X	X	X	X
Staff Effort - 17 weeks									
Step 3 (Validation)									
Staff Effort - 0 weeks									

Total Exercise Effort - 32 weeks
JB(7), NC(7), GB(6), TM(5), LK(5),
KM(2)

Table 7. Exercise plan and staff commitments (reported in weeks) for the Las Cruces Trench Test Case.

	FY 1989								
	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
EXERCISE 007									
Step 1 (Strategy)			X	X	X	X	X	X	
Staff Effort - 14 weeks									
Step 2 (Simulations)				X	X	X	X	X	X
Staff Effort - 20 weeks									
Step 3 (Validation)									
Staff Effort - 0 weeks									

Total Exercise Effort - 34 weeks
TN(7), WF(7), NE(6), JB(4), TM(2),
LK(2), GB(2), DC(2), KM(2)

PROGRAM PLAN FOR TASKS 2 AND 3

OF THE MOU ON PERFORMANCE ASSESSMENT ACTIVITIES

SOURCE TERM AND TOTAL SYSTEM PERFORMANCE MODELING

DETAILED PROGRAM PLAN FOR PERFORMANCE ASSESSMENT ACTIVITIES
UNDER THE NMSS/RES MEMORANDUM OF UNDERSTANDING

JANUARY 31, 1989

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Appendices

Detailed Program Plan for Performance Assessment Activities Under the NMSS/RES Memorandum of Understanding

I. Introduction

This detailed program plan describes the first phase of Task 2 and Task 3 of the performance assessment (PA) activities to be carried out under the NMSS/RES Memorandum of Understanding (MOU) of September 1, 1988. This plan expands on the memorandum of December 9, 1988, which implements the MOU. This plan describes in greater detail the work to be performed under various subtasks, how the various subtasks relate to each other, the schedule for that work, and the individuals responsible for the work.

The purpose of Task 3 of the MOU activities is to perform a total system performance assessment for the proposed Yucca Mountain Repository, and by doing so, to extend the NRC capability to model repository performance pursuant to the regulatory review of the Yucca Mountain Project. Task 2, the source term modeling effort, is broken out as a separate activity, but is an essential part of the overall PA activities in Task 3; therefore, Tasks 2 and 3 will be treated together except for the purposes of making work breakdown schedules and personnel assignments.

The September 1, 1988 MOU describes the three Tasks comprising the MOU activities in broad outline. The December 9, 1988 implementing memorandum describes the various subtasks, persons assigned to various subtasks, and staff time commitments. This plan provides more detail about these matters and how the work is envisioned to proceed. An important aspect of the Task 2 and 3 MOU activities, delineated in the September 1, 1988 MOU, is that these Tasks are to proceed in two phases. Phase 1, to be completed in FY 89, is intended to be accomplished with a minimum of technical input and interaction with NRC contractors, except for work documented and products delivered (including computer codes) to the NRC. Phase 2, to be accomplished in FY 90 and beyond, is intended to incorporate significant products to be delivered by NRC contractors, most notably the Tuff Performance Assessment Methodology currently under development by Sandia National Laboratories under FIN-A1266. Phase 1 is intended to result in a framework for PA modeling, with the limited resource allocated to perform this activity, only a rudimentary demonstration of a PA modeling capability is anticipated. Phase 2 is intended to provide a more complete, accurate, sophisticated, and realistic PA modeling capability.

II. Goal and Scope of Tasks 2 and 3

The primary goal of Phase I of Task 2 is to provide a simplified radionuclide source term in the form of a table or a computer code, to the overall system performance activities in Phase I of Task 3. The goal of Phase I of Task 3 is to conduct a preliminary performance assessment of the high level waste repository at Yucca Mountain, Nevada. As explained in I above, only a rudimentary performance assessment is intended for Phase 1 of the MOU, because of limited resources and time and because input from NRC contractors, that could contribute greatly to the goals of the MOU, is not currently available.

The performance assessment is considered to be comprised of two parts: (1)quantitative estimation of total system performance through the use of predictive models and (2)documentation, including detailed subsidiary modelling where appropriate, to support the assumptions, data, and modelling approaches used to obtain quantitative estimates of performance. Tasks 2 and 3 of the MOU will include both of these activities.

The total system performance measure for a high level waste repository can be expressed by a complementary cumulative distribution function (CCDF) of radionuclide releases to the accessible environment, weighted by a factor approximately proportional to radiotoxicity, integrated over an appropriate period of time (10,000 years is the current regulatory requirement). This performance measure is estimated by following the steps outlined in the information flow diagram (Figure 1.). These steps are described briefly below for the Phase I effort:

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

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

3. Consequence Analysis - The consequence in terms of cumulative release of radionuclides to the accessible environment over a specified time period (usually 10,000 or more years) is calculated for each scenario and usually numerous realizations of possible parameter values. In addition to being incorporated by way of cumulative releases into the CCDF (step 4), certain types of consequences might also be considered separately to compare to standard for maximum doses to individuals and for maximum concentration in groundwater.

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

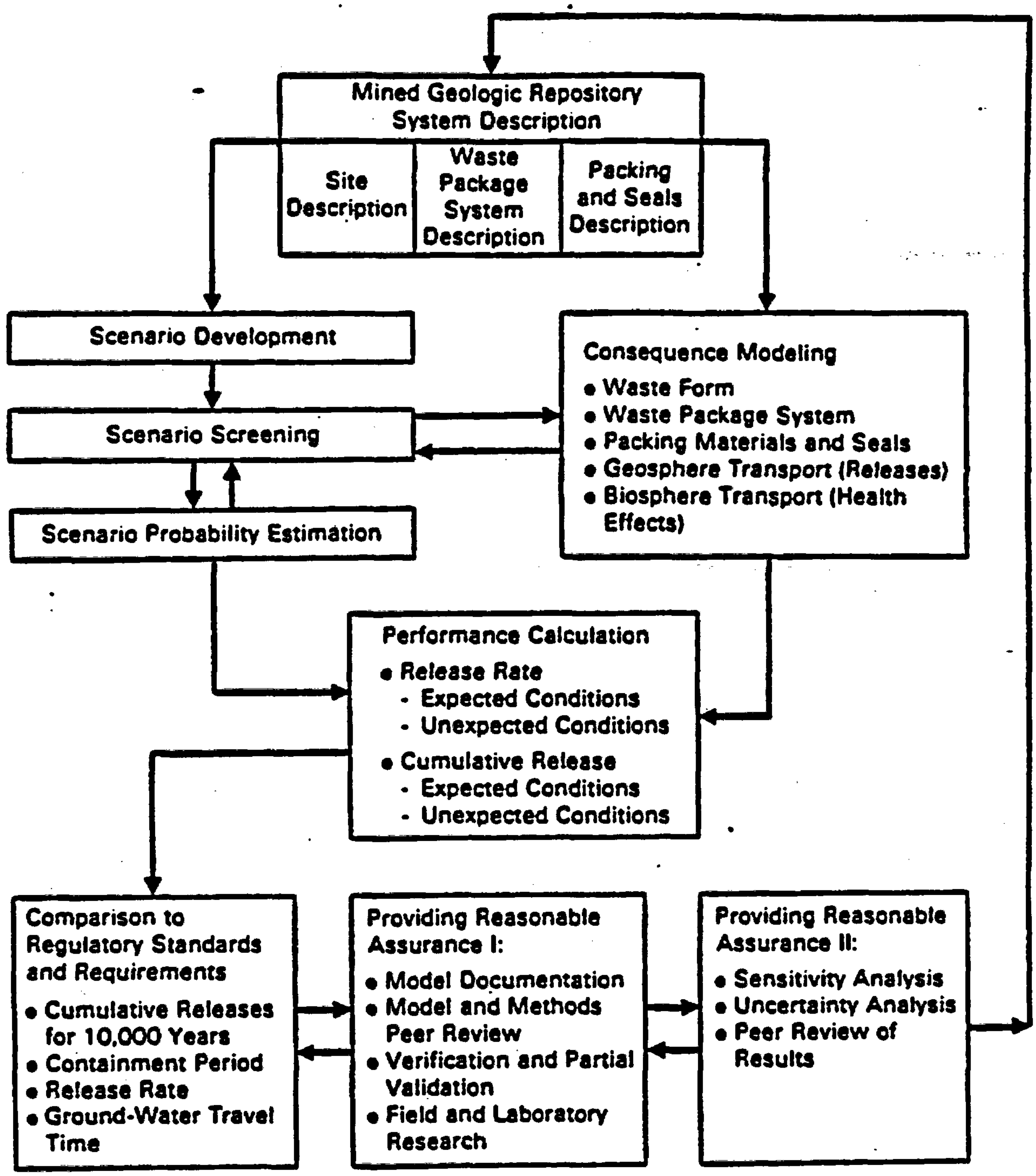


FIGURE 1. COMPONENTS OF THE STRATEGY FOR ASSESSING THE POSTCLOSURE PERFORMANCE OF THE GEOLOGIC REPOSITORY SYSTEM

5. Sensitivity and Uncertainty Analysis - Sensitivity analysis investigates the change in performance measures caused by incremental changes in the values of input parameters and data. Uncertainty analysis attempts to quantify the uncertainty in performance estimates in terms of the major sources of uncertainty, including uncertainty in input parameters, uncertainty in modeling (both the conceptual model of the geometry and characterization of the system and the process model of what physicochemical processes occur and how they are manifested), and uncertainty about future states-of-nature.

6. Documentation - This is largely self explanatory; however, the most effective documentation must make the assumptions used in the analysis, their basis, and the implications of their use explicit and clear.

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

Because of the complexity of the calculation of the CCDF it is likely, but not absolutely necessary that the generation of the CCDF be performed by a computer code. At a minimum such a code would need to: (1)sequence through all the scenarios to be considered, (2)choose the consequence models and parametric distributions corresponding to the scenario being analyzed, (3)sample the parameter space appropriate to the given scenario, (4)estimate consequences based on the models and parameter values for the scenario, (5)combine the parametric and scenario probabilities and the calculated consequences to generate a CCDF.

III. Planning Assumptions

The NRC staff will carry out Phase I. However, resources allocated by NRC management appear to be insufficient.

Other than existing reports and papers and computer code packages already delivered, there will be no contractor input available for Phase 1.

CNWRA involvement in Phase 1 will be primarily as an observer, but will become more active as the CNWRA PA capability expands.

All work will be conducted under the NQA-1 Category III. J. Holonich is responsible for managing QA for these activities.

IV. Technical Description of the Work

This section states our current view of the mechanisms that appear to control the performance of the Yucca Mountain repository. In many cases, the mechanisms are poorly understood, requiring further research and more sophistication than can reasonably be expected in the Phase I effort. The processes are nevertheless listed here with the understanding that they will be considered to the extent possible in the Phase I study. In some cases, we may simply choose to ignore a mechanism entirely, if such an assumption leads to a conservative estimate of performance. In many cases, we will rely only on reported ranges of parameters governing these phenomena rather than a truly independent estimate.

Task 2 - <u>Source Term Modeling</u>

The engineered barrier for inhibiting releases of radionuclides consists of multiple layers of protection. The release rate model will consider at least the following mechanisms:

1. Waste Package Lifetime - The estimate of the loss of waste package integrity will consider such factors as corrosion and mechanical damage; exactly what factors will be used in the computation of an estimate of performance is yet to be determined. Corrosion will be caused by contact of the canister with liquid water, either by immersion, dripping, or by direct contact with the rock. We will consider various mechanism that lead to the presence of liquid water and to increased concentrations of corrosive minerals in the water. We will investigate the likelihood of pitting and other types of corrosion as opposed to simple corrosion. While a very conservative

assumption would be that all waste packages fail instantaneously, such an assumption might lead to an unrealistically high importance given to highly radioactive, but relatively short-lived radionuclides, and would not further the understanding of performance assessment at the Yucca Mountain site. We might however consider the instantaneous loss of all waste package integrity as a highly unlikely, very severe scenario in the Phase I study.

2. Oxidation of UO_2 - We will investigate the conditions that might be present and which lead to the exposure of the uranium dioxide fuel to dry oxidizing conditions. Oxidation of fuel could be caused by exposure to atmospheric oxygen, to groundwater with high oxygen potential, and possibly from exposure to dissociated water vapor. Some of the fuel might have been converted to a higher valence state before being placed in the canisters. The oxidation state of the fuel is important, because the oxidized fuel is much more soluble than the unoxidized fuel, which could lead to increased release rates if and when the fuel is exposed to liquid water at a later time. For the Phase I study, we might consider as a bounding case that all fuel has been instantaneously converted to the most soluble state.

3. Dissolution of radionuclides - We will investigate how water comes in contact with the fuel following canister failure. Part of the problem will focus on mechanisms outside of the engineered barrier leading to large enough quantities of liquid water to allow direct contact between the waste package and the water (e.g., increased quantities of infiltration because of climate change, non-uniform percolation from the earth's surface to the repository level, perching of water along horizontal rock structure). Part of the analysis will focus on repository-related changes such as the evaporation of water by the heat generated within the waste, with subsequent condensation at some distance away and flow-back through fractures.

   Given that there will be a source of liquid water, we will explore ways that the water can get inside of the canisters and come in contact with the clad and exposed fuel. We will consider estimating, most likely with highly simplified models, the approximate time span during which heat generated by radioactive decay might keep any water infiltrating the canisters from remaining in liquid form.

   For those conditions for which liquid water does come in contact with the waste, it is important to consider the mechanisms of release of radionuclides from the intergranular boundaries and cladding gap, and the dissolution of the waste matrix. For the last mechanism, we will investigate the ramifications of the reprecipitation of radionuclides less soluble than the uranium oxide matrix. This consideration will take into account conceptual models for transport away from the fuel (e.g., canisters filled with water, water dripping onto the waste), the fraction of the fuel converted through oxidation to a more soluble state, and the accessibility of the fuel to the water through the failed or partially intact cladding. We will also consider the possibility that the oxidation state of the liquid water will be diminished because of sacrificial corrosion of the canister and associated metal structure. For Phase I we may choose to consider as a very conseravative case probably producing maximum releases of radionuclides, that liquid water comes directly in contact with the bare fuel almost instantaneously, and that the water is in its most corrosive, oxidizing state.

Task 3 - Overall System Performance Assessment

Phase I of Task 3 will consider only simplified models of transport of radionuclides from the engineered barrier to the accessible environment. The emphasis of this task will be on calculating the cumulative release of radionuclides at the accessible environment for a period of at least 10,000 years, in terms of their compliance with the regulatory standards of 40 CFR 191 as incorporated in 10CFR60.112. We may also consider the maximum exposures to individuals to determine compliance with the individual protection limits of these rules (although the standard for the time being has been remanded). We will pay no particular attention to the performance measures for radionuclide release rate at the engineered barrier, waste package lifetime, or groundwater travel time in the Phase I exercise.

The main modeling effort in Task 3 is centered on the flow and transport model. The model should consider the following phenomena to the degree that can be handled under the constraints of Phase I work:

1. Infiltration of precipitation at the land surface.
2. Flow through the unsaturated zone, both in the matrix and in fractures. The conceptual model should consider the possibility of perched water on interfaces.
3. Flow through the saturated zone. This model should consider both matrix diffusion and fracture flow.
4. Retardation mechanisms. This model should take into account the physical and chemical effects on the migration of dissolved substances in the rock; e.g., matrix diffusion, chemical sorption.
5. Decay of radionuclides, especially chains. This model should take into account different retardation factors for parent and daughter radionuclides in the same chain.

Other phenomena such as convection and vapor phase transport might be considered in more detail in the Phase II study.

Appendix D contains a summary of technical issues to be addressed during Phase I. Also included is a discussion of the various issues. These issues will be addressed primarily by considering the results of work done previously and reported in the open literature. In some cases particular issues may be addressed by incorporating particular phenomena, processes, or features in the models used to compute repository performance. In other cases we may, as time and resources permit, perform subsidiary calculations to treat particular issues, so that even though the issue is not treated explicitly in the calculation of performance, we will be able to evaluate the effect of such issues on our estimates of performance.

V. Work Breakdown Structure

Task 2 - Preliminary Source Term Modeling

Subtask 2.0 - Technical Management

1. Purpose and Scope
   The purpose of this subtask is to provide a means for first-line technical management of the source term activity.
2. Expected Products
   The products of this subtask will be interaction with line and project management, the MOU coordinators, and the technical staff working on tasks 2 and 3.
3. Relationship to other Subtasks
   This subtask provides leadership and coordination of all the other subtasks of Task 2 of the MOU.
4. Scheduling Considerations
   This subtask is active during the entire duration of Task 2, Phase 1.
5. Methods anticipated to perform work
   Meeting and consultation with affected persons.
6. Staff
   R. Codell

Subtask 2.1 - Problem Definition

1. Purpose and Scope
   The purpose of this subtask is to determine, by reaching a common understanding among the involved staff: (1)what the objectives of Task 2 are, (2)what the technical issues are, (3)what potential technical approaches might work, (4)who does what and when it is needed, (5)what products are required.
2. Expected Products
   The detailed program plan for the conduct of Task 2 is the primary product.
3. Relationship to other Subtasks
   This subtask sets the stage for accomplishing all the other subsequent work.
4. Scheduling Considerations
   The detailed program plan is required by the end of January 1989.
5. Methods anticipated to perform work
   The planning and documentation activities required to accomplish this subtask will be performed primarily by the Task Leader for Task 2. However, in order that the planning be effective, it is essential that all involved staff provide technical and planning input and provide comments on the detailed program plan.

6. Staff
   All

Subtask 2.2 - Background Literature Review

1. Purpose and Scope
   The purpose of the background literature review is: (1)to determine what facts are known and published that have a bearing on determining an approach to modeling the source term for a HLW repository at Yucca Mountain, (2)to determine what computational methods and tools are available for this purpose, (3)to determine what data on site parameters needed to model the source term are available, (4)to become familiar with the modeling approaches used by others for the same or similar problems. Information specific to Yucca Mountain is of the highest priority; as time permits, auxiliary information on modeling approaches, codes not specifically adaptable to Yucca Mountain, related parametric data, etc. should be evaluated.

2. Expected Products - See above

3. Relationship to other subtasks
   We expect that the models used in the Phase I study will come principly from the literature, especially previous performance assessments for Yucca Mountain and other High and Low-level repository studies.

4. Scheduling Considerations
   The background literature review will commence as early as possible. The limitations of staff resources and a short schedule for delivering a product dictate that we must rely heavily on previously published reports to extract useful models of processes important to the source term. While the literature review will continue throughout the Phase I effort, it will be important to glean useful models and parameter ranges by April to complete the Modeling Requirements subtask.

5. Methods anticipated to perform work
   No special guidance is necessary, except perhaps to point out that there are several indices of references relating to the Yucca Mountain site in general and performance assessment in particular.
6. Staff - ALL

Subtask 2.3 - Review/expand system definition and Scenario Analysis
Subtask 2.4 - Define Modeling Strategy
Subtask 2.5 - Code Selection and testing
(These tasks will be considered together in this program plan)

1. Purpose and Scope
   Based on the literature review, the assigned staff will develop a system definition of the Yucca Mountain repository source term, and the range of scenarios which will be applied to the performance analysis. The assigned staff will define the modeling which must be performed on the expanded system definition and range of scenarios which will lead to a reasonable source term to be used in the overall performance analysis. This modeling strategy will take into account the following:
   a. Phenomena important to modeling the source term and availability of models of the phenomena
   b. Probability that model can be tested in allowable time for inclusion into the total systems performance model.

Based on their conclusions, the staff will either use presently existing computer programs or write a new one for expressing the source term for the overall performance assessment model.

2. Expected Products - We expect to develop a computer program to be included in the overall system performance model, that implements a model of the source term.

3. Relationship to other Subtasks - The model will be coupled directly to the overall system performance model in Task 3.

4. Scheduling Considerations - The model must be completed before the total systems performance analysis can be completed.

5. Methods anticipated to perform work - We could develop empirical models based on reported behavior of canisters and fuel and analytical approximations to heat transfer in rock. The most sophisticated modeling is likely to be analyses with geochemical reaction path and speciation codes for examining chemical states of water in the very near field, including reactions inside the canisters with spent fuel. We may occasionally resort to using multiphase heat transfer codes such as TOUGH for near field environmental determinations.

6. Staff - R.Codell, J.Randall, K.Chang, J. Bradbury, T. Mo

Subtask 2.6 - Document Results
Staff - All

Task 3 - Preliminary total system performance assessment

Subtask 3.0 - Technical Management.

1. Purpose and Scope
   The purpose of this subtask is to provide a means for first-line technical management of the total system performance assessment activity
2. Expected Products
   The products of this subtask will be interaction with line and project management, the MOU Coordinators, and the technical staff working on Tasks 2 and 3.
3. Relationship to other Subtasks
   This subtask provides leadership and coordination of all the other subtasks of Task 3 of the MOU. This subtask is also intended to assure that the activities and products of Task 2 are thoroughly coordinated with those of Task 3.
4. Scheduling Considerations
   This subtask is active during the entire duration of Task 3, Phase 1.
5. Methods Anticipated to Perform Work.
   Meetings and consultation with affected persons. 6. Staff - N. Eisenberg, R. Codell, J. Randall.

Subtask 3.1 - Program definitions and program planning

1. Purpose and Scope
   The purpose of this subtask is to reach a common understanding among the involved staff as to: (1)what the objectives of Task 3 are, (2)what the technical issues are, (3)what potential technical approaches might work, (4)who does what and when it is needed, (5)what products are required.
2. Expected Products
   The detailed program plan for the conduct of Task 3 is the primary product.
3. Relationship to other Subtasks
   This subtask sets the stage for accomplishing all the other subsequent work.
4. Scheduling Considerations
   The detailed program plan is required by the end of January 1989.
5. Methods anticipated to perform work
   The planning and documentation activities required to accomplish this subtask will be performed primarily by the Task Leader for Task 3. However, in order that the planning be effective, it is essential that all involved staff provide technical and planning input and provide comments on the detailed program plan.
6. Staff - All

Subtask 3.2 - Background literature review

1. Purpose and Scope
   The purpose of the background literature review is: (1)to determine what facts are known and published that have a bearing on determining an approach to modeling repository performance at Yucca Mountain, (2)to determine what computational methods and tools are available for this purpose, (3)to determine what data on site parameters needed to model the performance assessment are available, (4)to become familiar with the modeling approaches used by others for the same or similar problems. Information specific to Yucca Mountain is of the highest priority; as time permits, auxiliary information on modeling approaches, models not specifically adaptable to Yucca Mountain, related parametric data, etc. should be evaluated.

2. Expected Products - see Purpose and Scope above

3. Relationship to other subtasks
   The background literature review forms the basis for the remaining work in Task 3. The system definition, scenario analysis, and determination of modeling approach all are based on information in the literature. The literature review will provide the basis for decisions about computations, as well as providing the basis for putting the modeling into technical and regulatory perspective. We expect that the models used in the Phase 1 study will come principally from the literature, especially previous performance assessments for Yucca Mountain and other High and Low-level repository studies.

4. Scheduling Considerations
   The background literature review will commence as early as possible. The limitations of staff resources and a short schedule for delivering a product dictate that we must rely heavily on previously published reports to extract useful models of processes important to the source term. While the literature review will continue throughout the Phase 1 effort, it will be important to glean useful models and parameter ranges by July to complete the Total System Modeling subtask.

5. Methods anticipated to perform work
   No special guidance is necessary, except perhaps to point out that there are many references relating to performance assessment in general and the performance assessment of Yucca Mountain in particular.

6. Staff - ALL

Subtask 3.3 - System Definition

1. Purpose and scope
   The purpose of the System Definition subtask is twofold: (1)to provide a description of the proposed repository at Yucca Mountain in

physicochemical terms sufficient to enable us to simulate its performance and (2)to provide a summary of the scientific information known about the behavior of the proposed Yucca Mountain repository to enable placing estimates of performance in technical and regulatory context. At a minimum the system description must consider the geologic, hydrologic, and geochemical processes and systems operating at Yucca Mountain so that transport of radionuclides through the geosphere can be estimated quantitatively. The natural systems must be described in sufficient detail so that the scenario analysis can be performed.

2. Expected Products

(1)an integrated, mechanistic description of the physicochemical systems at Yucca Mountain influencing waste isolation and, especially, transport of radionuclides through the geosphere; (2)parameter values and distributions of parameter values important for estimating radionuclide transport and other aspects of repository performance; (3)a summary of factors not included in the system description used to calculate performance and an estimate of the significance of such omissions on the estimates of performance.

3. Relationship to other subtasks

The subtask is based on subtask 3.2 Background Literature Review. It provides the basis for the analyses in subtasks 3.4, 3.5, and 3.6. 4. Scheduling considerations

This subtask should begin in January, based on the early part of the Literature Review, and should be complete by the end of February, so that the subsequent, dependent analyses can commence.

5. Methods anticipated to perform work

Analysis and synthesis of scientific information about Yucca Mountain and the proposed repository there. Abstraction of the essential elements to be included in the system description must be derived from careful evaluation of the information available.

6. Staff - All, but Codell.

Subtask 3.4 - Scenario Analysis

1. Purpose and scope

The purpose of this subtask is to provide information on potential scenarios at the Yucca Mountain repository to guide the modeling of total system performance and to provide the probabilities to be incorporated in the CCDF.

2. Expected Products

(1)A list of processes and events or a list of scenarios that should be considered in an analysis of performance, (2)a screening of these to determine the most important, (3)estimates of probability of occurrence. In addition the scenario analysts will confer with the system modeler, flow and transport modeler, and Task leader to determine which scenario classes to treat explicitly in the computational models and which to defer to Phase 2. Scenario analysts will also confer on what features, processes, and parameters should be incorporated in consequence models to effectively treat various scenario classes.

3. Relationship to other subtasks

This subtask derives from subtasks 3.2 and 3.3. It is a prerequisite to defining the modeling requirements (subtask 3.5). Synthesized data on scenario class probability will be used in the computations of total system performance (subtasks 3.7 and 3.8). Insights into the treatment of scenarios and scenarios omitted from the estimation of performance will be documented in subtask 3.9.

4. Scheduling considerations

This subtask must be largely complete by the end of March so that subtask 3.5 can commence.

5. Methods anticipated to perform work

(1)evaluation of "scenario literature" for the Yucca Mountain repository, (2)synthesis of a coherent set of scenarios or scenario classes, (3)estimation of probabilities of basic events and processes based on the geologic record or historical record (other methods as appropriate), (4)combinatorial analyses to estimate probabilities of scenarios used for the performance computation.

6. Staff - J. Trapp, D. Fehringer, other staff as needed.

Subtask 3.5 - Determination of Modeling Requirements

1. Purpose and scope

The purpose of this subtask is to synthesize the knowledge gained in subtasks 3.2, 3.3, and 3.4 to articulate the nature of the modeling to be conducted for the remainder of Task 3.

2. Expected Products

This subtask will produce a major product the "Modeling Requirements Document", which will articulate the type of modeling to be pursued for the remainder of Task 3 and, more important, the rationale for such an approach.

3. Relationship to other subtasks

This subtask depends on the information and analysis conducted in subtasks 3.2 - 3.4. The Modeling Requirements Document is a means to reach general agreement on the modeling approaches to be used in subtasks 3.6 - 3.8. It is anticipated that a substantial amount of the reasoning documented in the Modeling Requirements Document will be incorporated into the Final Report for Task 3, Phase 1.

4. Scheduling considerations

This subtask requires substantial completion of subtasks 3.2 - 3.4. It is scheduled to be completed in April 1989. Completion of this subtask is required before total system modeling and subsequent subtasks can begin in earnest (subtasks 3.6 - 3.8).

5. Methods anticipated to perform work

Key staff will evaluate what modeling approaches to adopt based on: (1)the importance of various processes, features, and scenarios as disclosed by the literature review; (2)the existence of available and adaptable quantitative methods; (3)the practical constraints of limited time and personnel, as well as the limitations of the available computer environments. A determination will also be made as to what type of computation will be included in the direct calculation of the performance measure(s), which modeling will be conducted as analyses supporting the calculation of the performance measures, and which modeling will be deferred to Phase 2.

6. Staff - N. Eisenberg, J. Randall, J. Pohle.

Subtask 3.6 - Total System Modeling

1. Purpose and scope

The purpose of subtask 3.6 is to assemble the computational tools to enable computation of the performance measure(s) for the repository at Yucca Mountain. Important components of this activity include: (1)computerization of parametric distribution and other data bases required to obtain performance estimates, including information related to scenarios; (2)testing and selection of codes to calculate consequences (e.g. codes calculating geosphere transport of radionuclides); (3)coding of an executive program to exercise the consequence models with the appropriate data bases or adoption/adaptation of an existing executive code for calculating CCDF's and other total system performance measures. In addition, testing and selection of codes and assembly of data bases required to perform analyses supporting the estimation of performance will be accomplished under this subtask.

2. Expected Products

An integrated methodology in the form of a computer code and the data bases required for it to operate. The integrated methodology would, at a minimum, calculate a CCDF for Yucca Mountain. This integrated methodology will be described in "Total System Performance Assessment Methodology Report," which is a major deliverable (it is anticipated that much of this documentation will be incorporated in the Final Report).

3. Relationship to other subtasks

This is the most important aspect of the MOU Tasks 2 & ; this central activity incorporates and focuses all previous work and is the basis for all subsequent work.

4. Scheduling considerations

This subtask can begin in March and must be completed in July.

5. Methods anticipated to perform work

Data bases will be encoded; formats will be selected to be compatible with a broad range of codes and uses. Consequence codes will be tested and compared to each other in terms of accuracy, ease of use, running time, and other relevant attributes. Total system performance assessment codes and approaches will be tested and evaluated. Choices on codes will be made based on testing results.

6. Staff - N. Eisenberg, J. Randall, R. Codell, J. Pohle, W. Ford, K. McConnell, J. Bradbury.

Subtask 3.7 Total System Code Test and Debug

1. Purpose and scope
   Test and debug the methodology assembled in subtask 3.6.

2. Expected Products
   A tested computer code to compute the CCDF and tested codes to perform supporting analyses, if any.

3. Relationship to other subtasks
   Must follow completion of subtask 3.6.

4. Scheduling considerations
   Start in May and finish in July.

5. Methods anticipated to perform work
   Run the computer code and evaluate results.

6. Staff
   N. Eisenberg, J. Randall, J. Pohle.

Subtask 3.8 - Final Run to generate Preliminary CCDF

1. Purpose and scope
   Generate performance estimates for Yucca Mountain repository.

2. Expected Products
   CCDF's, perhaps other performance measures.

3. Relationship to other subtasks
   Must follow subtask 3.7.

4. Scheduling considerations
   Start and finish in August.

5. Methods anticipated to perform work
   Run the code(s); assemble the results.

6. Staff - N. Eisenberg, J. Randall, R. Codell, J.Pohle

Subtask 3.9 - Document Results

1. Purpose and scope
   Self evident.

2. Expected Products
   The Final Report - the major deliverable for the Phase 1 activity.

3. Relationship to other subtasks
   Reports on all the others.

4. Scheduling considerations
   Begin in June and terminate in September.

5. Methods anticipated to perform work
   Analyze results of modeling and write up.

6. Staff - all.

Schedules and Resource Allocations

Appendix A. Major Milestones

Appendix B. Gantt Charts

Appendix C. Staff-Loading Charts

APPENDIX A

Major FY89 Milestones

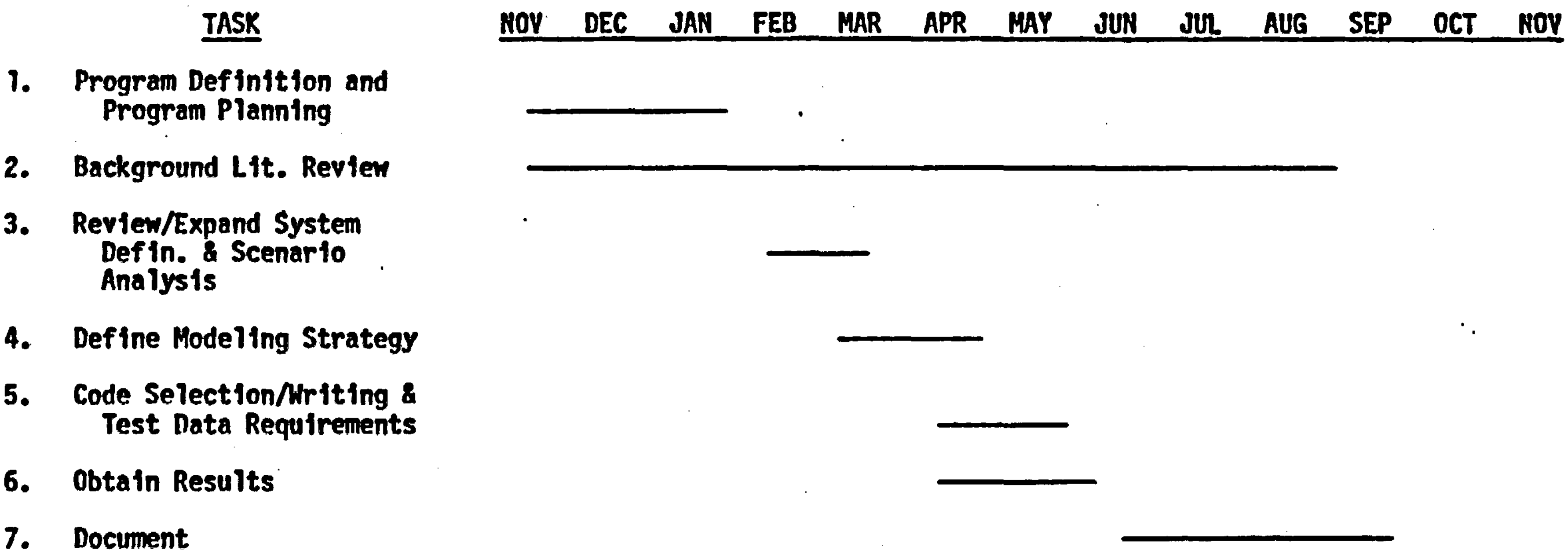
Task 2. Source Term

2.1 January 1989	Detailed Program Plan
2.2 April 1989	Modeling Requirements for Source Term
2.5 April 1989	Mid-Term Briefing for NRC Management
2.3 May 1989	Source Term Subroutine Delivery to Task 3
2.4 September 1989	First Annual Source Term Report
2.6 September 1989	End-of-Year Briefing for NRC Management

Task 3. Preliminary Total System Performance Assessment

3.1 January 1989	Detailed Program Plan
3.2 April 1989	Modeling Requirements Document
3.5 April 1989	Mid-Term Briefing for NRC Management
3.3 July 1989	Total Systems Performance Assessment Methodology Report
3.4 September 1989	First Annual Report for Performance Assessment Modeling
3.6 September 1989	End-of-Year Briefing for NRC Management

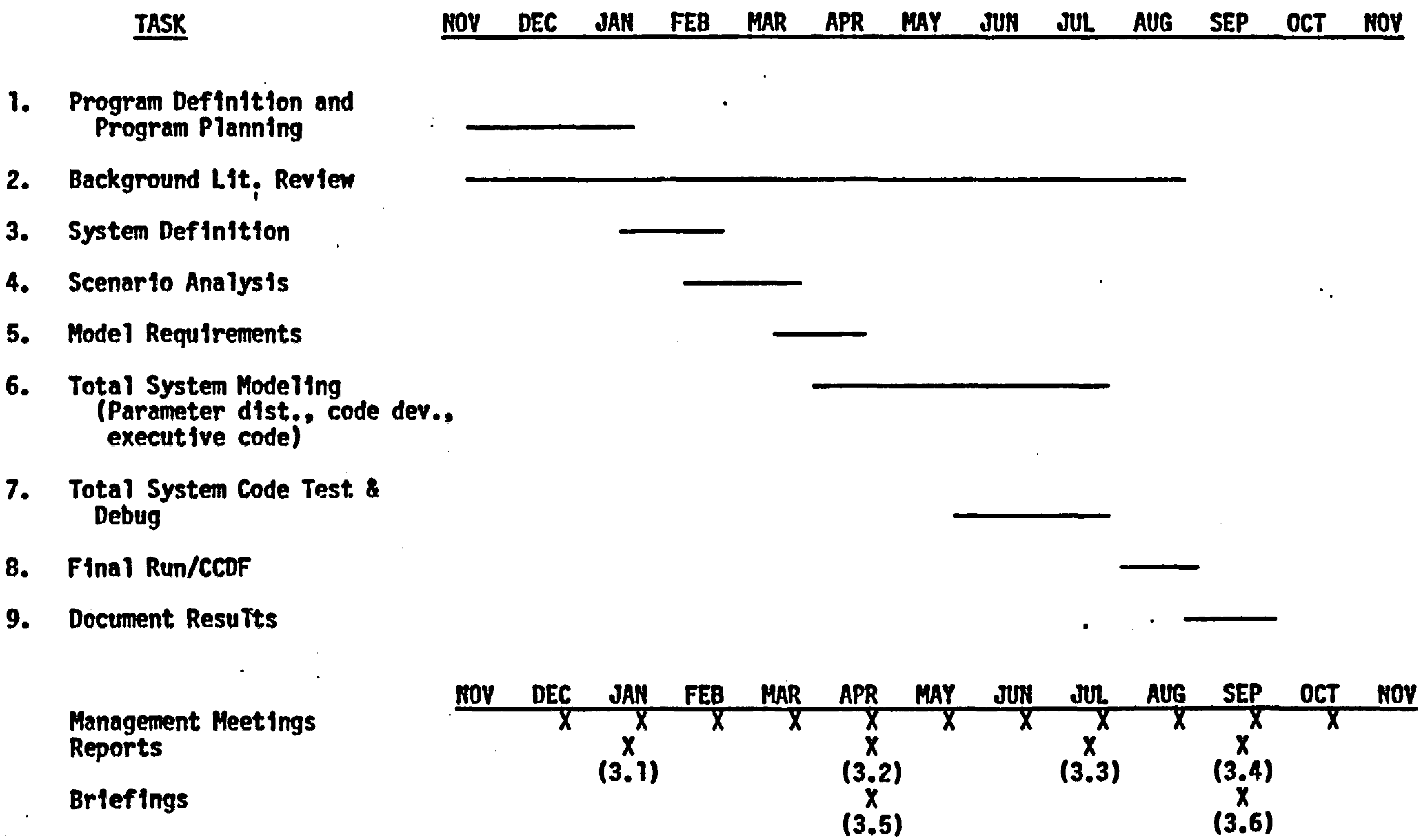
TASK 2 - SOURCE TERM



	NOV	DEC	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV
Management Meetings	X	X	X	X	X	X	X	X	X	X	X		
Reports			X (2.1)			X (2.2)					X (2.4)		
Subroutine							X (2.3)						
Briefings						X (2.5)					X (2.6)		

Note: Numbered milestones are keyed to listing on Enclosure A.

TASK 3 - PRELIMINARY TOTAL SYSTEM PERFORMANCE ASSESSMENT



Note: Numbered milestones are keyed to listing on Enclosure A.

TASK 2 - SOURCE TERM	TL	ANAL	GE	HY	RM	CE	WPA	TOTAL
0 TECHNICAL MANAGEMENT	2.4							2.4
1. PROBLEM DEFIN/PROGRAM MANAGING	0.8	1.0	0.4	0.4	0.4	0.4	0.4	3.8
2. BACKGROUND LIT. REV.	1.2	3.0	0.8	0.8	0.4	0.4	0.4	7.0
3. REVIEW/EXPAND SYSTEM DEF.	0.4	1.0	0.0	0.0	0.0	0.0	0.4	1.8
4. DEFINE MODELING STRATEGY	0.8	2.0	0.4	0.4	0.4	0.4	0.8	5.2
5. CODE SELECTION/WRITING &	0.8	4.0	0.0	0.0	0.0	0.0	0.4	5.2
TOTAL SYSTEM MODELING	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6. OBTAIN RESULTS	4.0	4.0	0.4	0.4	0.4	0.4	0.4	10.0
7. DOCUMENT	1.2	2.0	0.0	0.0	0.0	0.0	0.4	3.6
TOTAL	11.6	17.0	2.0	2.0	1.6	1.6	3.2	39.0

TASK 2 KEY
TL - TASK LEADER. R. CODELL
ANAL - SYSTEM ANALYST. J. RANDALL
GE - GEOCHEMISTRY. T.Mo
HY - HYDROLOGY. W. FORD
RM - ROCK MECHANICS, J. BUCKLEY
WPA - WASTE PACKAGE ANALYST. K. CHANG

TASK 3 - TOTAL SYSTEM PA	TL	SM	ST	FT	SC	HY	GE	GC	TOTAL
0 TECHNICAL MANAGEMENT	4.0	0.0	2.4	0.0	0.0	0.0	0.0	0.0	6.4
1. PROBLEM DEFINITION/PROGRAM PLANNI	0.8	2.0	0.0	0.4	0.4	0.4	0.4	0.4	4.8
2. BACKGROUND LIT. REV.	0.8	4.0	0.0	0.8	0.8	0.8	0.8	0.8	8.8
3. SYSTEM DEFINITION	0.8	4.0	0.0	0.8	0.8	0.8	0.8	0.8	8.8
4. SCENARIO ANALYSIS	0.4	3.0	0.0	0.8	1.2	0.4	0.4	0.4	6.6
5. MODEL REQUIRE. TOTAL SYSTEMS MODE	0.4	3.0	0.0	0.8	0.0	0.0	0.0	0.0	4.2
6. REQUIREMENTS FROM:	0.8	8.0	1.6	2.4	0.0	1.2	0.4	0.4	14.8
A. PARAMETER DISTRIBUTIONS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
B. CODE SELECTION/TESTING	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C. EXECUTIVE STRUCTURE CODING	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7. TOTAL SYSTEM CODE TEST & DEBUG	0.8	3.0	0.0	0.8	0.0	0.0	0.0	0.0	4.6
8. FINAL RUN/CCDF	0.4	2.0	0.8	0.4	0.0	0.0	0.0	0.0	3.6
9. DOCUMENT RESULTS	1.2	4.0	1.2	1.2	1.2	0.4	0.4	0.4	10.0
TOTAL	10.4	33.0	6.0	8.4	4.4	4.0	3.2	3.2	72.6

TASK 3 KEY
TL - TASK LEADER. N. EISENBERG
SM - TOTAL SYSTEM INTEGRATION AND MODELING. J. RANDALL
ST - SOURCE TERM INTEGRATION. R. CODELL
FT - FLOW & TRANSPORT MODELING. J.Pohle/W.Ford
SC - SCENARIO ANALYSIS. J. TRAPP, D. FEHRINGER
HY - HYDROLOGY. W. FORD
GE - GEOLOGY. K. McCONNELL
GC - GEOCHEMISTRY, J.Bradbury

Appendix D. Summary of Technical Issues to be considered in Phase I

The following is a summary of technical issues and some discussion of them where appropriate. These are listed because the literature reviews, modeling activities, and analyses conducted by the staff for Phase I should attempt to resolve these issues by providing a concrete, rational basis for decisions. In Phase I of this effort, it may be appropriate to simply ignore an issure for the sake of expediency or conservatism. In most cases, we pose the question of whether we can neglect the mechanism a priori, or if it is necessary to connence the work taking it into account, at least initially.

1. Should we consider that the waste package protects the nuclear waste, or for Phase 1 should we simply ignore this protection and presume that the fuel is unprotected and directly exposed to adverse forces in the repository?

   Discussion
   The waste packages should remain intact for many years. Neglecting this protection places a heavy emphasis on highly radioactive and dangerous, but short-lived nuclides such as Cs-134, Cs-137, Sr-89, Sr-90 and H-3, which probably would not be of much concern if a realistic treatment of the waste package were used. We therefore could inappropriately divert attention from the more serious problem of treating long-lived radionuclides such as transuranics and actinides.

2. Should we explicitly model the releases of gaseous radionuclides to the atmosphere in calculating repository performance for Phase I?

   Discussion
   Radionuclides such as I-129 and C-14 may be released in gaseous form, and would be present in the in the air-filled pores and fractures of unsaturated rock. This raises two issues regarding transport of these radionuclides. First, the gaseous releases would partially equilibrate with the water phase in the unsaturated zone, and probably end up partially as water-borne contaminants. Second, it isn't clear that the regulatory agencies will actually end up including any atmospherically released radionuclides in the cumulative release totals or, if included, how. DOE is petitioning EPA for such an exemption, and to reinstate a separate table for atmospheric pathways, which would allow much greater releases than allowed for the water pathway. Given this regulatory uncertainty, should we include gaseous releases in models used to generate the CCDF for Phase I? The release of these radionuclides is not expected to produce significant health effects; this is a further reason for delaying calculation of such releases to a later Phase.

3. Should we assume that the repository is saturated, or at least that water comes in contact with the waste package immediately?

Discussion
In many respects, this would be a worst-case assumption, and probably should be considered as an extreme case for Phase I. Yucca Mountain was chosen partially on the basis that it is a relatively dry site, and is likely to remain that way for a very long time. We could consider the site unsaturated, but examine conditions which lead to saturation under low probability conditions. Even under unsaturated conditions, there may be ways that water could come into contact with the waste package, either by contact with water in the rock pores or fractures. We could consider the extent to which the waste packages would be subjected to this water, and what mechanisms either increase or diminish this contact.

4. Should we consider that the uranium in the spent fuel is in its most soluble state?

Discussion
The oxidation state of the uranium largely determines its solubility. Under reducing conditions, solubility is likely to be low. When oxidized, the solubility could be much greater. Ground water at YMP is oxidizing, but there are several factors protecting the uranium from oxidation:

- The fuel is stored in a canister, probably filled with an inert gas.
- The fuel is clad in highly corrosion-resistant zircaloy or stainless steel.
- The oxygen in the water, even if it were to come in contact with the canister, might be consumed by corrosion of the metal in the waste package, cladding and auxiliary structure (e.g., tubes and racks).

The fuel could be oxidized under dry, hot conditions if canister integrity is lost. In fact, the oxidation of the fuel through small cladding imperfections is likely to cause total failure of the cladding because the uranium dioxide swells. If the fuel then is saturated with water at a later time, it might already be in a very soluble state. Which of these possible concepts should be implemented in the calculation of performance in the Phase I study?

5. How should we consider unsaturated conditions for flow and transport in the calculation of performance?

Discussion
We must consider unsaturated flow, but it may not be necessary to incorporate very complicated models into our performance assessment. For example, we may want to explore with a complicated model the phenomena leading to saturated flow along discontinuities in the rock in order to place boundaries on the length and flowrate through fast pathways to the accessible environment. Once we have chosen the pathway, however, we could use a simple one dimensional model with constant flux and no other hydraulics.

6. What kinds of models should we use for retardation along the geological pathways and what is an acceptable treatment of the chemical behavior of radionuclides in the geosphere?

   Discussion
   The use of retardation coefficients in calculating radionuclide migration has frequently been criticized. As a practical matter what alternatives are available for calculating transport? Can the error in estimates of radionuclide releases to the accessible environment be quantified? To what degree? Can subsidiary geochemical calculations be useful in quantifying the uncertainties in using simplified chemical models? How important is the fact that the medium is unsaturated and how does the degree of saturation affect conclusions about the appropriateness of a given chemical modeling approach? Should the model of the saturated zone include matrix diffusion? Could retardation be completely neglected in Phase I?

7. Over what length of time should we calculate the performance of the repository?

   Discussion
   For a "realistic" treatment of the repository performance, the cumulative radionuclide releases may be zero or insignificant during the regulatory period of 10,000 years. Should we extend the period of consideration to determine how the repository might realistically release radionuclides to the environment? If so, how long should we extend the period of consideration?

8. The remanded EPA standard requires calculation of three performance measures: (1)CCDF of cumulative radionuclide releases to the accessible environment over 10,000 years; (2)concentration of radionuclides in certain groundwater at 1000 years; (3)dose to maximally exposed individuals at 1000 years. Which of these performance measures should we aim toward calculating in Phase 1?

   Discussion
   If doses are calculated, what models of usage should we have concerning the doses to people living close to the repository and consuming food and water impacted by radioactive releases from it?

9. For what set of scenarios should we calculate performance in Phase 1?

   Discussion
   Should we calculate performance for only the "base case" scenario or should we include disruptive scenarios? If so, which disruptive scenarios? Do consequence models exist to treat important classes of disruptive scenarios?

10. What form of sensitivity and uncertainty analysis, if any, should be performed in Phase 1?

Discussion
Sensitivity and uncertainty analyses can be very resource intensive tasks. However, these are very important parts of the performance assessment. For the Phase 1 activities what approach to these analyses is appropriate? Can we conceptualize some scaled-down version that would be doable and meaningful with the scarce resources allowed?

11. What form of waste should be assumed for the Phase 1 analysis?

Discussion
Spent reactor fuel, and to a smaller extent, vitrified high-level radioactive waste, will be stored in the repository. Since nearly all of the waste will be in the form of spent fuel, should only this waste form be considered in Phase 1 of this study?

12. What design for the engineered barrier system should be assumed for the Phase 1 analysis and, in particular, what type of canister material should be assumed?

Discussion
The spent fuel waste form will consist mainly of zirconium alloy or stainless-steel clad UO_2, some of which will be stored in racks, and put into metal canisters. The canisters will probably be constructed of stainless steel, although other alloys are also being considered. For the present study, should we consider only stainless steel canisters? Should we assume for Phase I that there are neither canisters nor cladding present (see issue 1)? The canisters will be stored in the repository rock either horizontally or vertically, probably in lined holes with an air gap between the canister wall and the rock. Should only the vertical orientation with the air gap present be studied in the present work?

13. How should the modeling of the repository treat the spatial distribution of waste packages and the likely temporal (and therefore spatial) distribution of waste package failure?

Discussion
Although it is attractive in many situations to consider point sources as the origin of groundwater pollution, some essential behavior of the repository may be lost by making such an assumption. Further, it may be difficult to argue that conservative estimates of performance are obtained for all performance measures. Some models (e.g. the AREST code) have considered the temporal distribution of waste package failure and found that it has a pronounced effect on performance. What is the appropriate level of detail for the treatment of these facets of the model of repository performance for Phase 1.

14. Should doses to individuals and populations be calculated as a consequence in Phase I or should this complication and refinement of the consequence modeling be deferred to later?

Discussion

Although several standard codes are available to calculate doses and the resulting health effects, such modeling does complicate the treatment of consequences and adds to the already large burden of work to be done. In addition, considerable contention might develop around the assumptions used regarding future population densities, land use, and ecology at the site

15. What is the appropriate degree of sensitivity and uncertainty analysis for this effort? How should these analyses differ between Phase I and Phase II? What methods should be used to perform these analyses?

Several methods are available for performing sensitivity and uncertainty analysis, including Monte Carlo methods, stratified sampling methods (e.g. Latin Hypercube), and the adjoint method to investigate sensitivity to parameters determining performance. Methods for uncertainty analysis are less well developed, especially for quantification of conceptual model uncertainty. Given the limited resources available for the Phase I effort it is unlikely that a substantial amount of quantitative sensitivity and uncertainty analysis is possible; however qualitativie analyses should be undertaken to the extent feasible. Also it may be possible to perform semiquantitative analyses by using extreme values of parameters to remove the effects of certain processes from equations used to predict performance (e.g. velocity equal to zero to remove the effect of advection on radionuclide migration).

ENCLOSURE B

The following is a compilation of statements prepared by the staff members participating in Phase 1 of the MOU Task 2 and 3 modeling activities. The requested information was:

> "Prepare a short paragraph (3-5 sentences) summarizing the work you intend to perform as part of the MOU acitivities. This should state (succintly) the purpose, scope, content, planned approach, and key products and/or milestones for the work."

MOU Phase 1 Task Description for
Richard Codell

R. Codell is the Task Leader for Task 3, Source Term Modeling, of the MOU activities. Responsibilities include first line technical management of the work, coordination of the various technical activities, communication with NRC management, participation in the drafting of deliverable documents as one of the principal authors, and technical analysis as appropriate and required. The Task Leader will participate in decisions regarding modeling approaches to be used to calculate the source term, subsidiary analyses to support modeling approaches, analysis of data for input to the models, descriptions of the modeling results and their implications. Key technical issues in which the Task Leader is expected to be involved include:

- Evaluation of the literature dealing with performance of the whole and the component parts of the engineered barrier.

- Selection of the model for barriers to release of radionuclides from the waste to the edge of the engineered barrier.

- Adapting currently existing computer programs of source term models or alternatively creating ad hoc computer programs for the present task

- Selection of scenarios that affect the release of radionuclides at the edge of the engineered barrier.

- Integration of the source term model with the total system performance model to assure it is compatible, philosophically and computationally with Task 3.

- Limited technical management of the overall system performance model effort

- Limited computer programming of the overall system performance model computer program.

- One of the principal authors of the Detailed Program Plan and Modeling Requirements Document.

- Responsible for interim and end-of-year briefings of NRC management on progress of Task 2 and 3 studies.

- A principal author of the "Total System Performance Assessment Methodology Report"

- A principal author of the "First Annual Report for Performance Assessment Modeling"

MOU Phase 1 Task Description
for
Norman A. Eisenberg

N. A. Eisenberg is the Task Leader for Task 3, Total System Performance Assessment, of the MOU activities. Responsibilities include first-line technical management of the work, coordination of the various technical activities, communication with NRC management, participation in the drafting of deliverable documents (one of the principal authors), and technical analysis as appropriate and required. The Task Leader will participate in decisions regarding: modeling approaches to be used to calculate performance, subsidiary analyses to support modeling approaches, data sets to be employed, descriptions of the modeling results and their implications. Key technical issues in which the Task Leader is expected to be involved include: (1)selection of the model for geosphere transport of radionuclides (the heart of the consequence portion of the total system model); (2)selection of scenarios, estimation of their probabilities, and adaptation of consequence modeling to properly reflect the scenario; (3)interpretation of the CCDF and intermediate results; (4)integration of the source term work conducted under Task 2 to assure it is compatible, philosophically and computationally, with Task 3. In addition to being a principal author of this "Detailed Program Plan," the Task Leader will be a principal author of the "Modeling Requirements Document," which will provide the documentation and rationale for the modeling approach chosen, he will be a principal in the April "Briefing for NRC Management" and will coordinate the presentations of other participants, he will be a principal author of the "Total System Performance Assessment Methodology Report," which will describe the modeling approach executed for Phase 1, he will be a principal author of the "First Annual Report for Performance Assessment Modeling," which will contain an updated version of the information contained in the two previous written deliverables, and he will play the same role for the "End-of-Year Briefing for NRC Management" as for the mid-year briefing.

INDIVIDUAL PROGRAM PLAN FOR
CONTRIBUTIONS TO THE MODELING ACTIVITIES SUPPORTING
THE MEMORANDUM OF UNDERSTANDING ON
HLW PERFORMANCE ASSESSMENT ACTIVITIES BY THE NRC STAFF

John D. Randall, RES/DE/WMB

The performance of repositories of high-level radioactive waste (HLW) is influenced by many individual process and by interactions among those process. Under the subject MOU, the NRC staff will be developing capabilities for selecting and using models of those processes.

My duties in this effort involve the integration of individual process models (of waste package failure, radionuclide release from the waste package, transport of radionuclides through the geosphere to the accessible environment, and possibly biosphere transport of radionuclides to man and dose to man) to insure that the models are physically reasonable and that they are compatible, both physically and mathematically, with each other. In doing this work, I plan to prepare a software package that provides a means of data communication among selected computer programs that implement the individual process models, that provides a means of specifying data needed by the individual programs, and that processes data produced by the programs in such a way that the NRC staff can interpret the data easily.

One of the outputs of this integrating software package will be a cumulative complementary distribution function (CCDF) that will summarize comparisons of estimates of cumulative radionuclide releases from a repository of HLW to the accessible environment with limits on these releases set by 40 CFR 191, the overall HLW performance standard set by EPA. If time permits, the integrated software package also will be designed to present comparisons of predicted and EPA-specified doses to individuals.

In preparing the integrating software package, I first plan to examine existing software packages that have been developed for the same purpose. Examples of such packages are Sandia's code coupler (used under NRC's HLW research project, FIN A1266) SYVAC (from Canada), AREST and PANDORA (developed for DOE), CONVO (developed for EBS evaluations for NRC), LISA (developed by CEC), and CNWRA's fast probabilistic methodology (recently proposed to NRC). If none of these packages proves to be suitable for the purposes of the MOU, I will develop a new one.

As I carry out my duties of integrating HLW process models into a methodology that will be useful to the NRC staff in its performance assessment activities, I plan to work closely with other NRC staff involved with the MOU's Tasks 2 and 3. This interaction will provide me with the information that I will need to have in order to decide what needs to be done in order to prepare that integrates individual process models in such a way that the integrated results will provide meaningful estimates of repository performance.

MOU/KM

NOTE FOR: NORM EISENBERG

FROM: KEITH MCCONNELL

SUBJECT: WORK RELATED TO MOU

I visualize my role in work related to the MOU on performance assessment modeling to be basically a support role providing input into the various subtasks outlined in the program plan. Principally, I see my largest input coming in the System Definition subtask helping to provide basic information about structural features that may be significant factors in the modeling effort proposed. Specifically, I am currently doing a literature search on emplacement hole stability and fracture networks in association with fault zones. An additional area that I may be able to provide, through John Trapp, a limited amount of information is in the identification of important scenarios. In the total system modeling effort, my role, as I see it, is to attempt to interrelate three-dimensional geologic models used in repository definition and numerical models of total system performance.

cc: Phil Justus
John Trapp

MOU Phase 1 Task Description
For
William H. Ford

William Ford will provide ground water support to Tasks 2 and 3 of the MOU activities. Responsibilities will include the compilation of site ground water data, compilation of available computer codes, development of modeling approaches, and setting up and running models. William Ford will contribute to written reports as necessary.

NOTE TO: Norman Eisenberg

FROM: John Bradbury

SUBJECT: MY MOU ACTIVITIES

I am presently involved in getting Bill Murphy from the Center to hold a workshop on EQ3/6. It is intended that this workshop will be held at NRC headquarters and that it will involve only NRC staff interested in using the code. Present plans are for a half day presentation on the capabilities of the code, and input and output requirements. Following this presentation there will be a couple of days of hands on modeling directed/assisted by Bill. It appears that this workshop might be held in February.

After getting the instruction in the Use of EQ3/6, I plan to start applying it to the various subtasks planned. The version of EQ3/6 that Bill will supply us may not have all the capabilities that I might require in this effort. For example, I am interested in subroutine that handles stable isotope geochemistry. I may have to produce this subroutine myself or get it elsewhere.

We have in house computer programs (MINTEQ and HYDRAQL) which handle speciation and sorption. I plan to get familar with these codes and apply them to portions of the tasks.

NOTE TO: Norman Eisenberg
SPS,HLGP,HLWM

1-31-89

FROM: Tin Mo
HTS,HLGP,HLWM

SUBJECT: My MOU Activities

MAJOR ACTIVITIES:

I am the Project Manager for the Technical Assistance Contract (FIN A-1756), "Geochemical Sensitivity Analysis for Performance Assessment", with the Sandia National Laboratory (SNL). In this capacity, I am presently coordinating with David Brooks,(CNWRA Program Element Manager for the Geologic Setting), to hold a workshop on Geochemistry Sorption Sensitivity Analysis. The CNWRA staff will lead the workshop and the NRC and SNL staff will participate . As part of the workshop proceedings, the SNL staff will conduct technology transfer sessions for the tools and methodologies for geochemical sorption sensitivity analysis.

As part of the contract deliverables, I have received a geochemical computer code on speciation (HYDRAQL) along with other codes. I intend to get familiar with all these codes that are now available in-house with particular emphasis on HYDRAQL.

The metabolism and dosimetry, health effects and risks to the members of the general public due to the HLW radionuclides released to the accessible environment may vary widely depending upon the physicochemical forms of the bioavailable radionuclides released. I will coordinate and provide the critical linkage between the geochemical transport (release source terms) / speciation codes/models (e.g. HYDRAQL) via the radiation exposure pathways codes (e.g. PATH 1) and the dose and health effects codes such as BIOPATH, DOSHEM, PABLM or other national and international codes and models used in the HLW management communities of the world. I now have available in-house the PATH 1 and DOSHEM codes. I will evaluate the capabilities of these codes and if suitable apply them to portions of the MOU tasks 2 and 3. I may need to update the DOSHEM code so that the dose conversion factors, algorithms and subroutines used are consistent with the most recent recomendations of the International Commission on Radiological Protection (ICRP) Publications 26/30 concerning the Annual Limits of Intake (ALI's) for the HLW radionuclides and other guidance on radiation protection for radioactive waste disposal in the ICRP publication #46.

The EPA Biosphere model and the other models/codes currently used in assessing the risks from proposed HLW repositories and performance assessment do not properly account for the long term accumulation of radionuclides in different parts of the biosphere as these models and codes are designed originally to assess the environmental impacts of routine or accidental releases of radionuclides from nuclear power plants or fuel cycle facilities. These releases are typically of short duration (tens of years) compared to those of a much longer duration (tens of thousands of years) that can be expected from a geologic repository. I will

MOUANDBS

NOTE FOR: Norm

FROM: John T.

SUBJECT: MOU and other stuff

For Year 1.

- ° Review scenario reports--basic work already done.
- ° Provide list of conditions with stipulated probabilities for external processes and events as surrogate scenarios initiation processes and events.
- ° Suggest combinations for analysis.
- ° Review and comment on other stuff going on.

John

Suggest consideration of the following base cases. These would encompass a whole series of scenarios. At same time ignore gas and drilling.

1. "Expected" system conditions assuming
    a. .1 mm/year flux
    b. 1 mm year flux
    c. 10 mm year flux

2. Uniform change
    a. .1 to 1 mm/year over 10,000 years
    b. .1 to 10 mm/year over 10,000 years
    c. 1 to 10 mm/year over 10,000 years

3. Assumed waste package failure
    a. All at 1000 years
    b. All at 5000 years

4. Tectonic effects--total failure and crushing / smearing of 1% waste packages
    a. @ 100 years
    b. @ 1000 years
    c. @ 5000 years

5. Distributed flux
    a. 95% flux in 5% of area

6. Repository temperature
    a. See attached

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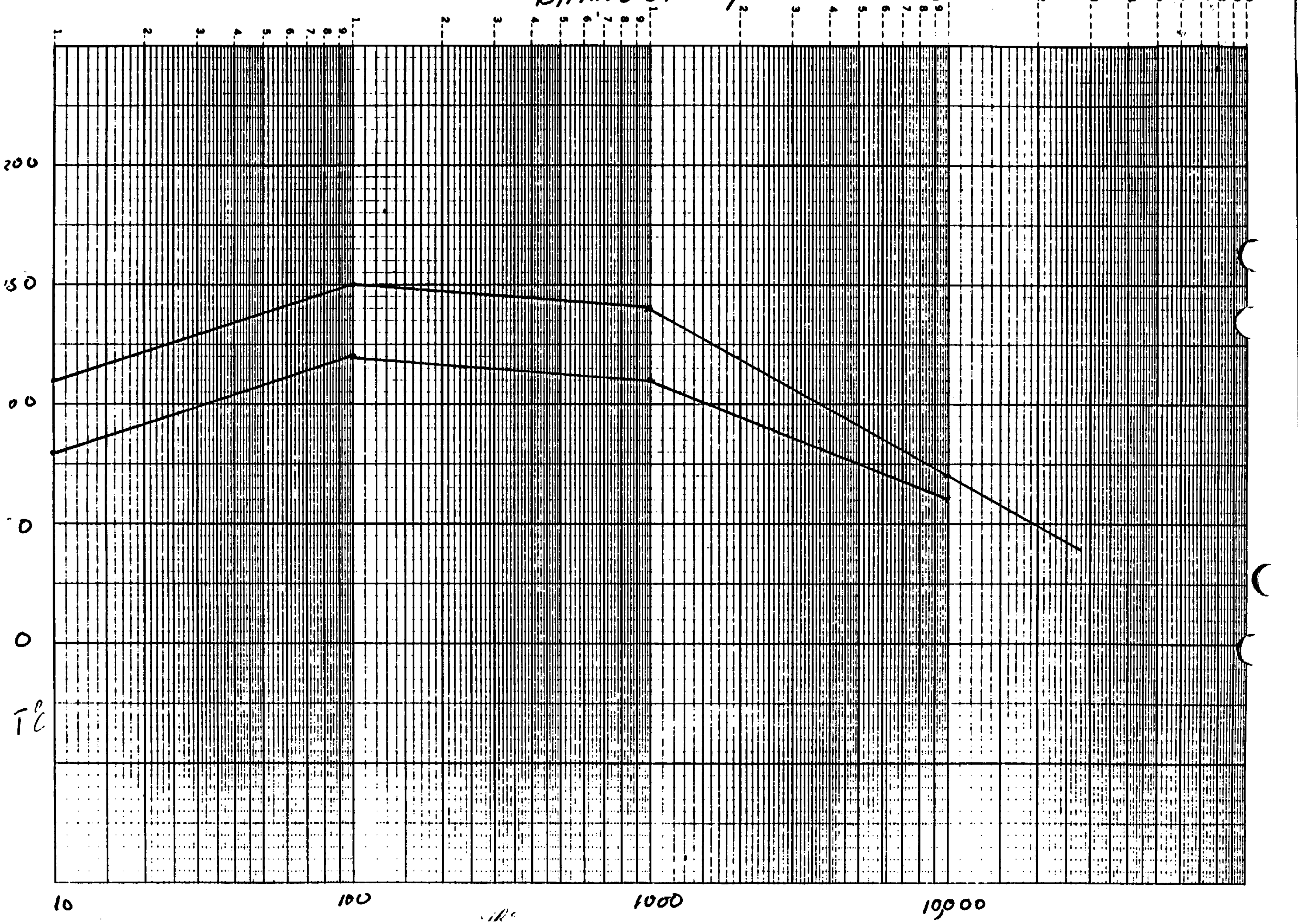

Work to be Performed Under Task 2 of the MOU by J. Buckley

The only area which requires rock mechanics/design input as presented in the MOU is Source Term Modeling (waste package lifetime). RM/D input may include:

1. Determine mechanical load on waste package.

MOU Phase I Task Description for K. Chang

Purpose: To provide a waste package performance assessment code capable of estimating a conservative bound on performance of DOE's waste package design.

Scope: The work scope will include a brief literature review of existing codes being used by DOE and others for waste package performance analyses and formulation of a simple code which may be used by NRC to check whether DOE's waste package design can satisfy NRC's regulatory requirements.

Content: The literature review will summarize the capabilities of the various codes being used by DOE and others and recommend if any of these codes may be used for NRC's purpose. The code to be used by NRC would probably be able to address only the most probable failure modes expected of the waste packages.

Planned Approach: The code to be developed likely be a simplified version of a more elaborate code in existence. Simplifications can be made by imposing additional assumptions on existing models/codes such that less calculation is required to arrive at more conservative approximated solutions.

Complex phenomena such as interaction between failed packages and failed packages and geochemistry will not be addressed.

Key Products:
1. Review report on existing codes
2. A PC code for source term