CONTRIBUTION TO THE PROGRAM PLAN FOR PHASE 3 ITERATIVE PERFORMANCE ASSESSMENT ACTIVITIES

CONDUCTED JOINTLY BY OFFICE OF NUCLEAR MATERIAL SAFETY AND SAFEGUARDS, OFFICE OF NUCLEAR REGULATORY RESEARCH, AND CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

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ABSTRACT

This contribution to the draft program plan primarily describes the involvement of the Center for Nuclear Waste Regulatory Analyses (CNWRA) in Phase 3 of the Iterative Performance Assessment (IPA). This contribution is based on guidance provided by staff members of the Nuclear Regulatory Commission (NRC), and frequently shows planned NRC staff participation in the proposed work. The IPA is a collaborative effort conducted jointly by NRC Office of Nuclear Material Safety and Safeguards (NMSS), the NRC Office of Nuclear Regulatory Research (RES), and the CNWRA. This report contains the following:

- An outline for seven proposed tasks within IPA Phase 3, including: (i) Task 1: System Code, (ii) Task 2: Scenario Analysis, (iii) Task 3: Flow and Transport, (iv) Task 4: Source Term, (v) Task 5: Disruptive Consequences, (vi) Task 6: Sensitivity and Uncertainty Analysis, and (vii) Task 7: Dose Assessment

- A listing of proposed subtasks (the Appendix) that summarize the potential participation of CNWRA technical staff members including: (i) Overall Task, name and number; (ii) Lead Person; (iii) Key Personnel; (iv) Justification for Work; (v) Description of Work; (vi) Anticipated Effort; and (vii) Anticipated Schedule

Further dialogue with the NRC will be required to complete definition of scope, establish an overall budget and schedule for the work, and designate lead persons for each of the seven tasks. Hence, this document contains only a draft of the CNWRA contribution to the overall plan for IPA Phase 3.

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ACKNOWLEDGMENTS

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1 INTRODUCTION

Iterative Performance Assessment (IPA) is considered to be a repetitive process of technical analyses to obtain quantitative estimates of repository performance based on data and models available at the time of assessment. Phase 3 is one such iteration and is a collaborative effort conducted by the Nuclear Regulatory Commission (NRC) Office of Nuclear Material Safety and Safeguards (NMSS), the NRC Office of Nuclear Regulatory Research (RES), and the Center for Nuclear Waste Regulatory Analyses (CNWRA). Because performance assessment (PA) is quantitative, IPA is based primarily on the use of predictive models in conjunction with computer codes. IPA has many facets, including the system descriptions and supporting databases, scenario analyses, consequence analyses, performance measure calculations, sensitivity and uncertainty analyses, and comparisons to the performance objectives of 10 CFR Part 60 (release and/or dose based objectives). These analyses are repeated as new data becomes available from site characterization.

The overall objective for the IPA activity is to develop, maintain, and enhance the NRC staff capability to effectively review the U.S. Department of Energy (DOE) high-level waste (HLW) PAs in its application for HLW disposal. In addition to the primary objective, there are other objectives of the IPA that include:

(i) Evaluating the DOE site characterization program, including field studies, laboratory studies, and analyses

(ii) Providing information for regulatory guidance and other regulatory products related to PA, especially the License Application Review Plan (LARP)

(iii) Providing information for the evaluation of the Federal regulations for a HLW repository, primarily 40 CFR Part 191 and 10 CFR Part 60

The IPA will achieve these objectives by illustrating how site characterization data and general information can be used to determine regulatory compliance. In the course of such exercises, the need for additional site characterization data and regulatory guidance will be revealed. Sensitivity and uncertainty analyses are key to identifying those data, assumptions, or regulatory interpretations with the greatest potential for introducing uncertainty into demonstrations of compliance. Similarly, auxiliary analyses provide information regarding sources of uncertainty in the models used in various stages of the IPA. In this document, the contribution of the CNWRA to the plan for IPA Phase 3 is outlined with the above objectives in mind.

2 BASIS FOR THIS CONTRIBUTION

The basis for this contribution stems primarily from three sources:

(i) The NRC Overall Review Strategy (ORS) for the anticipated License Application (LA) (Johnson, 1993), and the LARP (Nuclear Regulatory Commission, 1994a)

(ii) The NRC Performance Assessment Strategic Plan (PASP) (Nuclear Regulatory Commission, 1994b)

(iii) Recent NRC guidance for IPA Phase 3 by NRC NMSS staff members

In overview, the ORS is a broad document that highlights both pre-LA and LA reviews to be conducted within the mandate of the NRC. The PASP defines the goals, objectives, and activities of PA from the present to the time the DOE submits the LA. The recent NRC guidance is specific to near-term IPA activities, and the recently completed Phase 2 highlights the accomplishments of the IPA. Each of the four items is discussed in the following sections.

2.1 OVERALL REVIEW STRATEGY

The NRC ORS for the anticipated LA outlines the need to develop the capability of the NRC to conduct pre-LA and LA reviews. The IPA is a key component of the NRC review capability that will be used to perform effective reviews of the DOE PA activities. These PA activities are anticipated to be crucial components of the overall demonstration of compliance with the performance objectives of 10 CFR Part 60.

In the ORS, IPA activities are described in the context of the long-range LARP and PA Strategic Plan, as well as the periodic LARP and PA plans (Figure 2-1). All of the plans guide development of NRCs license application review capabilities during the pre-LA phase.

In the ORS, IPA is described as a "tool for technical integration, because it provides the structure for examining couplings between phenomena that might not be adequately evaluated, within the limits of a specific technical discipline." Hence, IPA is a multidisciplinary activity with data inputs, assumptions, and code development. By being multidisciplinary, IPA relies on the expertise of staff members throughout the NRC and CNWRA organizations. By combining the activities of a wide variety of staff members, IPA contributes to programmatic integration of NRC activities.

In the ORS, IPA is also described as providing a quantitative basis for identifying those areas that are most important to compliance. IPA is expected to play a role in revising Key Technical Uncertainties (KTUs) that have been developed in the LARP. The IPA is expected to feed the knowledge and insights of its integrated technical analyses periodic Total System Performance Assessments (TSPA) back into the NRC Systematic Regulatory Analysis (SRA) process. By doing so, the results from IPA can help the NRC revise its research user needs in a more systematic and comprehensive way that is more directly linked to the NRC pre-LA and LA review needs. Similarly, IPA activities are to be planned using the LARP to ensure that specific areas are investigated and considered in calculations of repository performance and determinations of compliance. The LARP is to be used to appropriately focus IPA activities to contribute in a logical fashion to the NRC pre-LA and LA reviews.

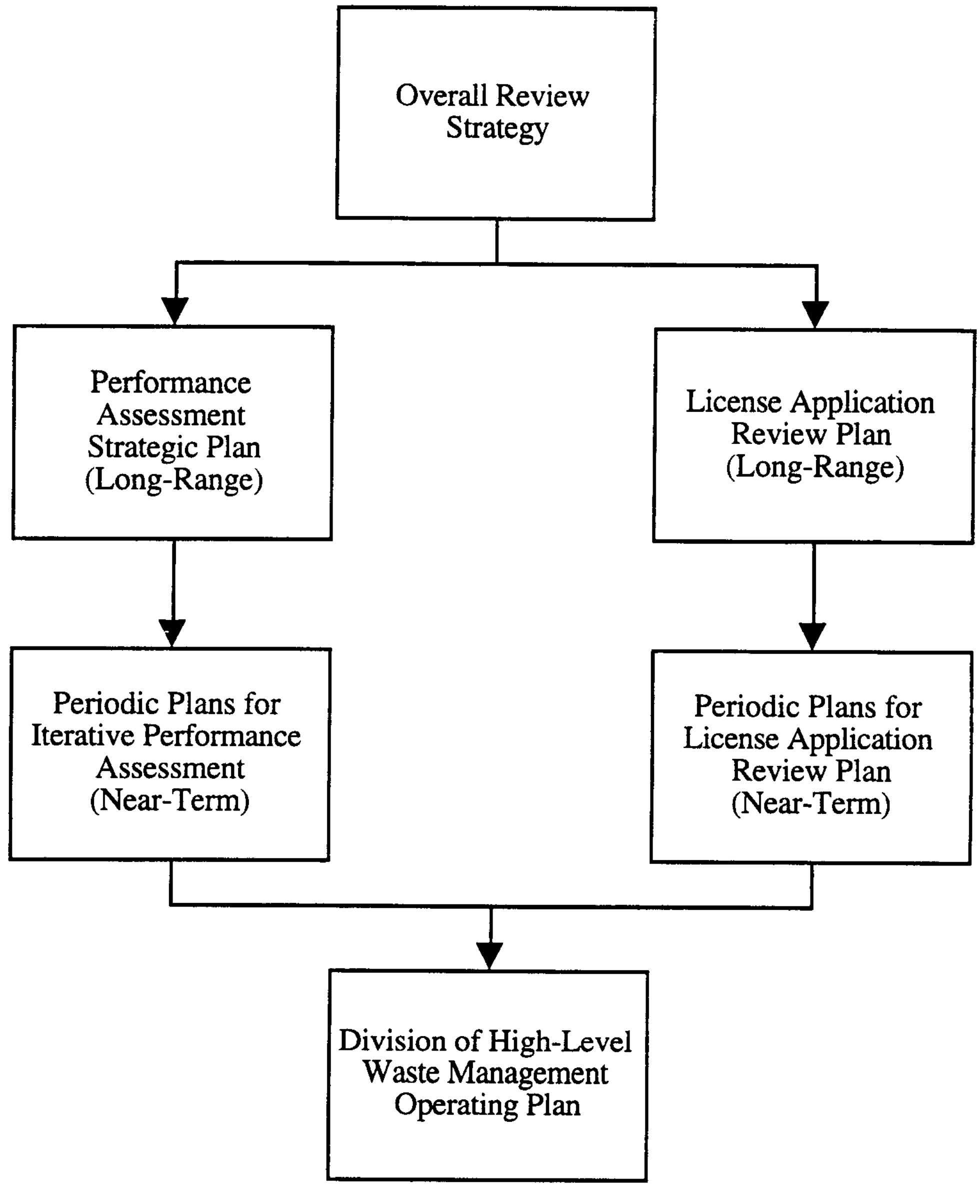

Figure 2-1. Plans which guide the development of NRC's license application review capabilities during the pre-license application phase (adapted from Johnson, 1993)

2.2 PERFORMANCE ASSESSMENT STRATEGIC PLAN

The NRC PASP defines the goals, objectives, and activities of PA from the present to the time the DOE submits the LA. The PASP describes the role of PA in achieving the basic goals of the NRC Division of High Level Waste Management (DHLWM) program. In particular, recent PA activities that demonstrate the benefits from the recently completed IPA Phase 2 exercise are highlighted. Based on the current state of PA and IPA, the PASP outlines a plan for future activities in five basic area:

(i) Legislative mandates

(ii) Interactions with the DOE

(iii) SRA and preparation of the LARP

(iv) Technical assessment capability

(v) Support to the HLW program

IPA is described to be one of four components of the PA technical assessment capability [item (iv) in the above list]. In addition to IPA, geological model and code development, geochemical model and code development, geotechnical model and code development, hydrological model and code development, and engineered barrier system (EBS) model and code development are included in the PASP technical assessment capability. As such, IPA is only one aspect of the NRC overall PASP.

Within the PASP, IPA is identified as being a key element in establishing the NRC capability to effectively conduct pre-LA and LA review. IPA is described as providing a basis for the development of an independent capability to perform a quantitative total system assessment of performance based on the performance objectives described in 10 CFR Part 60. IPA is further described as consisting of three components: (i) synthesis of data and information, (ii) modeling and computation to estimate performance of the repository and important subsystems, and (iii) auxiliary analyses that are often conducted on a finer level of detail and on narrower topics. The goals of IPA are to develop and maintain: (i) staff expertise, (ii) a suite of analysis tools, and (iii) support and management infrastructure required to conduct reviews of the DOE PAs. In addition, IPA provides the framework by which staff explore the impact of different phenomena and processes of the repository system, thereby gaining insights into performance issues. These insights can be used to critique and guide the DOE during pre-LA activities, guide the NRC pre-LA activities, and contribute to the NRC strategy for conducting the LA review.

The PASP also outlines the various component disciplines required in IPA, including geology, hydrology, geochemistry, climatology, waste package design, waste-form behavior, rock mechanics, thermohydraulics, and corrosion science. A TSPA requires the integration of these various disciplines in an organized manner. To date, PA methodologies have been formulated around the organization of scenarios, modeling methods, and sensitivity and uncertainty analyses. This framework is useful for integrating the multidisciplinary information into a unified PA.

In the PASP, it is noted that the focus of IPA Phases 1 and 2 have been on the production of TSPAs, which have been found to be resource intensive. For future work, IPA is expected to place greater emphasis on the development of appropriate assumptions and data sets, and on the utilization of existing computer codes being developed and/or enhanced in other NRC-funded activities. Examples of these codes include: (i) Engineered Barrier System Performance Assessment Codes (EBSPAC) being supported by the EBS model and code development activities, (ii) SEISM1 code being supported by the geological model and code development activities, (iii) UDEC/3DEC/ABAQUS codes being supported by the geotechnical model and code development activities, and (iv) PORFLOW code being supported by the hydrological model and code development activities. It is expected that IPA can incorporate the results of these efforts into a single assessment of repository system performance.

2.3 GUIDANCE FOR IPA PHASE 3

Recently, the NRC has provided informal guidance to the CNWRA for the preparation of this document. The guidance specifies four major objectives for IPA Phase 3:

(i) Improved analysis of site characteristics and engineered components

(ii) Improved system code methodology and implementation

(iii) Quantitative evaluation of the DOE TSPAs

(iv) Analysis of KTUs identified in the LARP

The first two objectives emphasize building and maintaining independent NRC PA capabilities, and the last two objectives emphasize the IPA contributions to the NRC overall pre-LA activities. Each of these major objectives is discussed further.

The first objective can be considered a continuation of auxiliary analyses such as those conducted in IPA Phase 2. The new emphasis is that the auxiliary analyses will increasingly investigate subsystem PA issues through more discipline-specific modeling. The added emphasis is consistent with the discussion in the PASP and is based on the notion that more detailed information will soon be expected from the DOE as the site characterization activities proceed. The increased level of detail will require more detailed analyses and lead to improved understandings of the phenomena and processes, and improved critique of the DOE site characterization activities. More advanced mechanistic models can be developed as improved data allow. These mechanistic models can then be used to develop abstracted results that can be incorporated into the total system code.

The emphasis on increased PA activities in the areas of site characterization and engineered components is consistent with trends in the DOE program in which effort is being devoted to the Multi-Purpose Canister (MPC), Exploratory Studies Facility (ESF), design of *in situ* heater tests, and analysis of the effects of thermal load on optimizing overall system performance. More detailed analyses are expected to provide a valuable contribution to the NRC evaluations and comments on the DOE Advanced Conceptual Design (ACD) of the Geologic Repository Operations Area (GROA) and Waste Package, engineering studies of surface and subsurface facilities, and design considerations for thermal loadings and emplacement modes.

In addition to DOE-sponsored activities, NRC-sponsored activities are expected to generate improved data, models, and computer codes. These improvements, likewise, are expected to be incorporated into PA. Specific examples include EBSPAC and a number of models that are being developed to predict waste package corrosion and release. The corrosion portion of EBSPAC includes models of localized corrosion, stress corrosion cracking, and mechanical failure. Within the EBS element activities, the Substantially Complete Containment Example (SCCEX) problem has been completed. It is the goal of IPA to utilize the pertinent portions of these more detailed mechanistic models as they become available.

The second objective is to improve independent NRC quantitative PA capabilities, which are considered to be a key element in the NRC ORS and PASP. In Phase 2, a system code was developed which will be incrementally improved during Phase 3. The major areas for improvement include: a new database design, a more modular structure, a more flexible structure, a more structured protocol for data input, and a more mathematically rigorous generation of the complementary cumulative distribution functions (CCDFs). It is anticipated that a new database design will more effectively control the flow of data between modules and increase modularity and flexibility. Similarly, a more standardized and uniform protocol for data input will improve the utility of the system code for a larger number of users. The treatment of CCDFs is also targeted for improvement in order to reflect the effects of the variability of parameters on the overall prediction of performance.

The third objective is to apply the NRC PA capability to evaluate the DOE PA activities, thereby contributing to the pre-LA review activities outlined in the ORS. Because PA is multidisciplinary, it offers a unique opportunity for both the DOE and the NRC to address high-order site suitability issues. In PA, discipline-specific evaluations would be considered in the context of the total system performance, which is based on a variety of data, assumptions, models, and analysis methods.

In earlier IPA activities, the TSPAs of the DOE were evaluated and critiqued. To date, these reviews have been considered screening reviews. In Phase 3, more in-depth quantitative evaluations are planned for the review of DOE TSPAs. In particular, reviews are being planned for the three-dimensional (3D) stratigraphic models, alternative models for matrix/fracture flow, dose assessment calculations, and transport of gaseous radionuclides. The suite of quantitative evaluations will be finalized after the most recent DOE TSPA is published (expected in late FY94).

In addition to the review of the DOE PA models, it is planned that IPA will contribute to the review and analysis of activities in the ESF design, test activities, and site investigations. It is anticipated that the DOE will soon be accelerating efforts in these areas; hence, IPA can contribute to the NRC pre-LA activities by performing reactive reviews of DOE plans in these areas. Subsequent to the release of DOE plans, IPA can also perform more in-depth quantitative evaluations that would guide the DOE activities.

The fourth objective is to apply NRC PA capabilities to development of the LARP. In particular, a number of KTUs have been identified in the Compliance Determination Strategy (CDS) development efforts. Currently, the LARP team is conducting an integration review of the KTUs. Shortly after the review is completed, it is anticipated that a quantitative assessment of selected KTUs be performed using the tools developed in IPA.

In addition, a number of KTUs have been identified that are specific to PA, including construction of the CCDF (which represents total system performance), PA model validation, formal expert elicitation practices, propagation and representation of uncertainties, and scenario analyses. In Phase 3, the issues of CCDF construction, validation, expert elicitation, and scenario analysis are being targeted as PA issues which potentially can be closed at the staff level. In particular, validation is currently being studied in conjunction with international organizations and is planned to continue to be studied. Similarly, work is currently being performed in the area of expert elicitation. Scenario analysis methods and CCDF construction are areas of recent and planned investigation.

3 STRUCTURE OF CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES CONTRIBUTION

The project structure of the CNWRA contribution to the IPA Phase 3 plan is similar to that used in the Phase 2 plan. In the Phase 2 plan, the TSPA was organized in the six components outlined in Figure 3-1. These components are described briefly below.

(i) System description—For the purposes of modeling, the repository system is described in terms of its component parts, which include the waste form, the engineered barrier, and site characteristics. Raw field and laboratory data are reduced to data sets suitable for input into mathematical models designed to describe the performance of the system. The system structure and the description of ongoing natural processes at the site are determined from both qualitative and quantitative data.

(ii) Scenario analysis—Scenario classes representing possible alternative future states of the repository system environment are identified and screened. Probabilities are estimated for those scenarios selected, possibly using results from expert elicitations.

(iii) Consequence analysis—The consequence in terms of cumulative release of radionuclides to the accessible environment over a specified period of time (usually 10,000 yr) is calculated for each scenario class, normally for numerous realizations of possible parameter values.

(iv) Performance measure calculation—The consequences for each scenario class are calculated and combined into a curve of consequences versus the probability that such consequences will be exceeded (i.e., a CCDF). Certain types of consequences might also be used to compare separately to standards for maximum doses to individuals and maximum concentration in groundwater.

(v) Sensitivity and uncertainty analysis—Sensitivity analyses investigate the change in performance measures caused by incremental changes in the values of input parameters and data. Uncertainty analyses attempt to quantify the uncertainty in performance estimates and to relate those uncertainties to modeling and data uncertainties.

(vi) Comparison to regulatory standards and documentation of results—Comparisons to regulatory standards must take into account both the estimated performance of the repository (obtained from predictive modeling) and the uncertainty inherent in such estimates (obtained from sensitivity and uncertainty analyses and other studies). The most effective documentation must make the assumptions used in the analysis and their bases clear and the implications of their use explicit.

Based on this description of the components required to perform a TSPA, six areas of work were identified in the Phase 2 plan and are recommended for continuation in Phase 3:

(i) System Code

(ii) Scenario Analysis

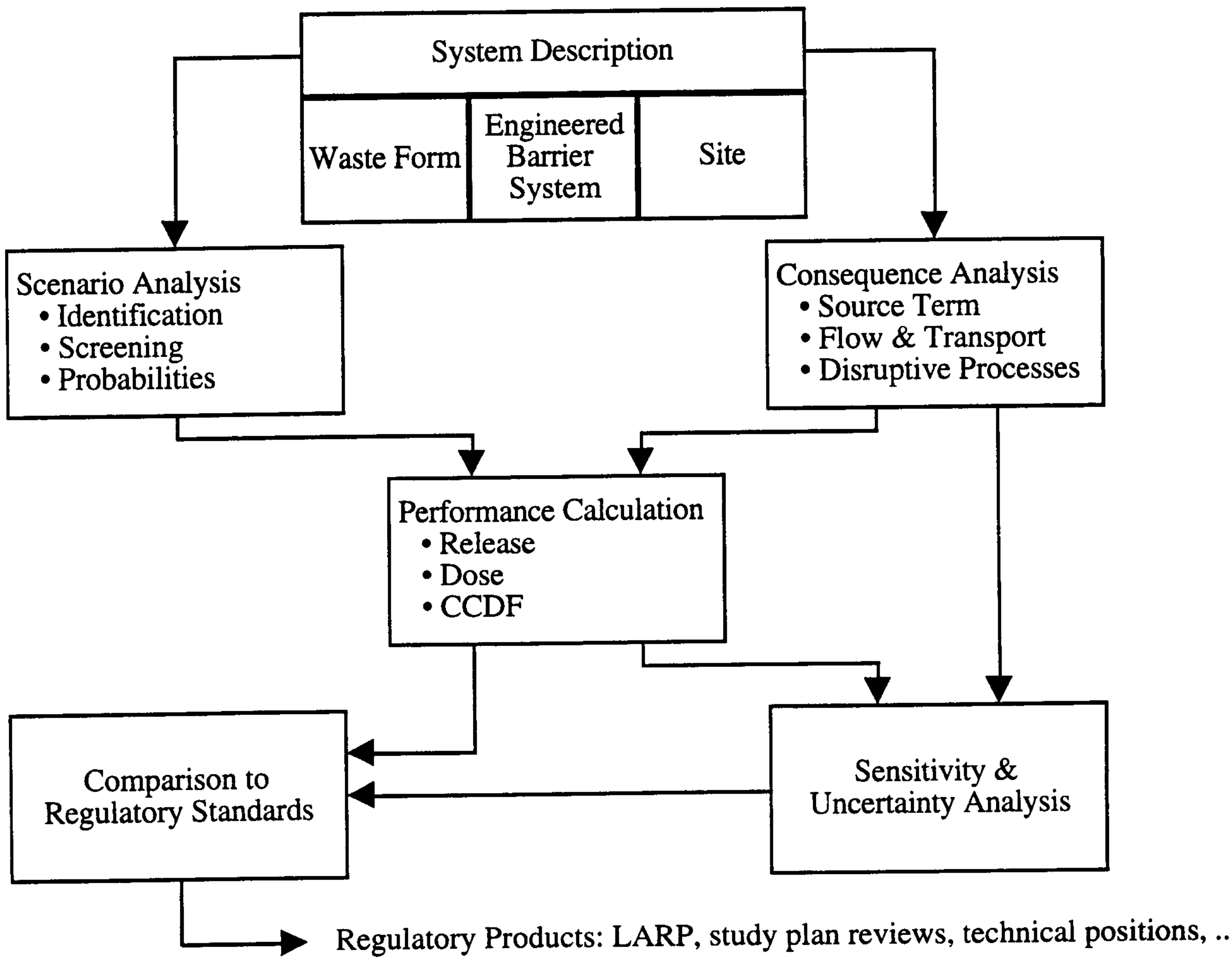

Figure 3-1. Components of a total system performance assessment

(iii) Flow and Transport

(iv) Source Term

(v) Disruptive Consequences

(vi) Sensitivity and Uncertainty

Based on anticipated regulatory changes, a seventh area is proposed for Phase 3:

(vii) Dose Assessment

Thus for Phase 3, a seven-task structure is proposed as shown in Figure 3-2. The work breakdown structure consists of seven main technical tasks:

Task 1: System Code—This activity will involve the improvement and maintenance of the system code developed in Phase 2. The system code is used to calculate a CCDF to estimate the performance of the repository. The system code will continue to be consistent with the overall concept and logic of repository PA. The system code will integrate the probabilistic information on scenario occurrence (Task 2), flow and transport (Task 3), source term (Task 4), disruptive consequences (Task 5), sensitivity and uncertainty analysis (Task 6), and dose assessment (Task 7).

Task 2: Scenario Analysis—This activity will enumerate potential scenarios for analysis and provide scenario descriptions and probability estimates for those scenarios to be included in the analysis.

Task 3: Flow and Transport—This activity will provide the computational modules used in the system code to estimate transport of radionuclides by fluids (groundwater and gas) through the geosphere. A prerequisite to the estimation of radionuclide transport will be the estimation of fluid movement.

Task 4: Source Term—This activity will provide the computational module used to estimate the flux of radionuclides moving from the repository (alternatively the EBS) into the geosphere for transport to the accessible environment. Calculation of this radionuclide flux will involve consideration of: (i) hydrologic, thermal, and geochemical conditions near the repository; (ii) waste package failure; (iii) waste form dissolution; and (iv) mass transfer of radionuclides from the repository to the geosphere.

Task 5: Disruptive Consequences—This activity will provide computational modules to estimate the movement of radionuclides from the repository to the accessible environment for certain types of disruptive scenarios involving, for example, volcanism, human intrusion, climate change, faulting, subsidence, and uplift.

Task 6: Sensitivity and Uncertainty Analyses—This activity will provide or enhance the methods to perform sensitivity and uncertainty analyses.

Task 7: Dose Assessment—This activity will provide or enhance the methods to calculate dose as a measure of repository performance.

Tasks 1, 2, and 6 correspond to components 1, 2 and 5 of the PA methodology described in Figure 3-1. Tasks 3, 4, 5, and 7 comprise the consequence analysis (component 3) in Figure 3-1. The system code is the integrated calculational means for conducting the entire process.

The organization of Phase 3 consists of four main tiers: (i) a Management Board, (ii) Technical Coordinators, (iii) Task Leaders, and (iv) Subtask Leaders. Both the management board and technical coordinators have one representative from each of the three participating organizations. In addition, it is planned that a single task leader be assigned to each of the seven tasks, and one subtask leader to each of the various subtasks. The current members of the management board are proposed to continue in Phase 3, namely:

M. Federline, NMSS
Representative, RES
B. Sagar, CNWRA

The management board is responsible for defining the goals of various activities and approving the schedule, allocation of resources, and deliverables. The management board can revise activities and scope of the IPA activities, subject to appropriate changes in the contractual (Operations Plans) commitments for the CNWRA.

Three technical coordinators will provide technical direction and integration for the various IPA activities. Each organization participating in this cooperative effort is represented by a technical coordinator. The current members are proposed to continue in Phase 3, namely:

R. Wescott, NMSS
T. McCartin, RES
R. Baca, CNWRA

The coordinators will: (i) conduct periodic management meetings between line managers and task leaders; (ii) provide periodic briefings on progress to upper management; (iii) be responsible for identifying any significant technical, scheduling, or staffing problems; and (iv) act as the organizational contacts for IPA activities.

The seven technical task leaders remain unspecified at this point.

Each task will consist of several subtasks and be led by a single technical person. The duties and responsibilities of each technical subtask leader are: (i) deciding the technical approach to achieve the goals of the subtask, (ii) developing and coordinating a team to successfully complete the work, (iii) functioning as the principal spokesperson for the subtask activities, and (iv) coordinating the subtask efforts to ensure its utility to other components of the IPA effort. At this point, subtask leaders are identified in the proposed subtask descriptions in the Appendix.

Within the tasks, auxiliary analyses may be performed to evaluate the uncertainty in the adequacy of the models, data, and computational tools used to estimate performance. In addition, IPA can perform reactive work in the seven-task structure. Reactive work includes those activities that are responsive to

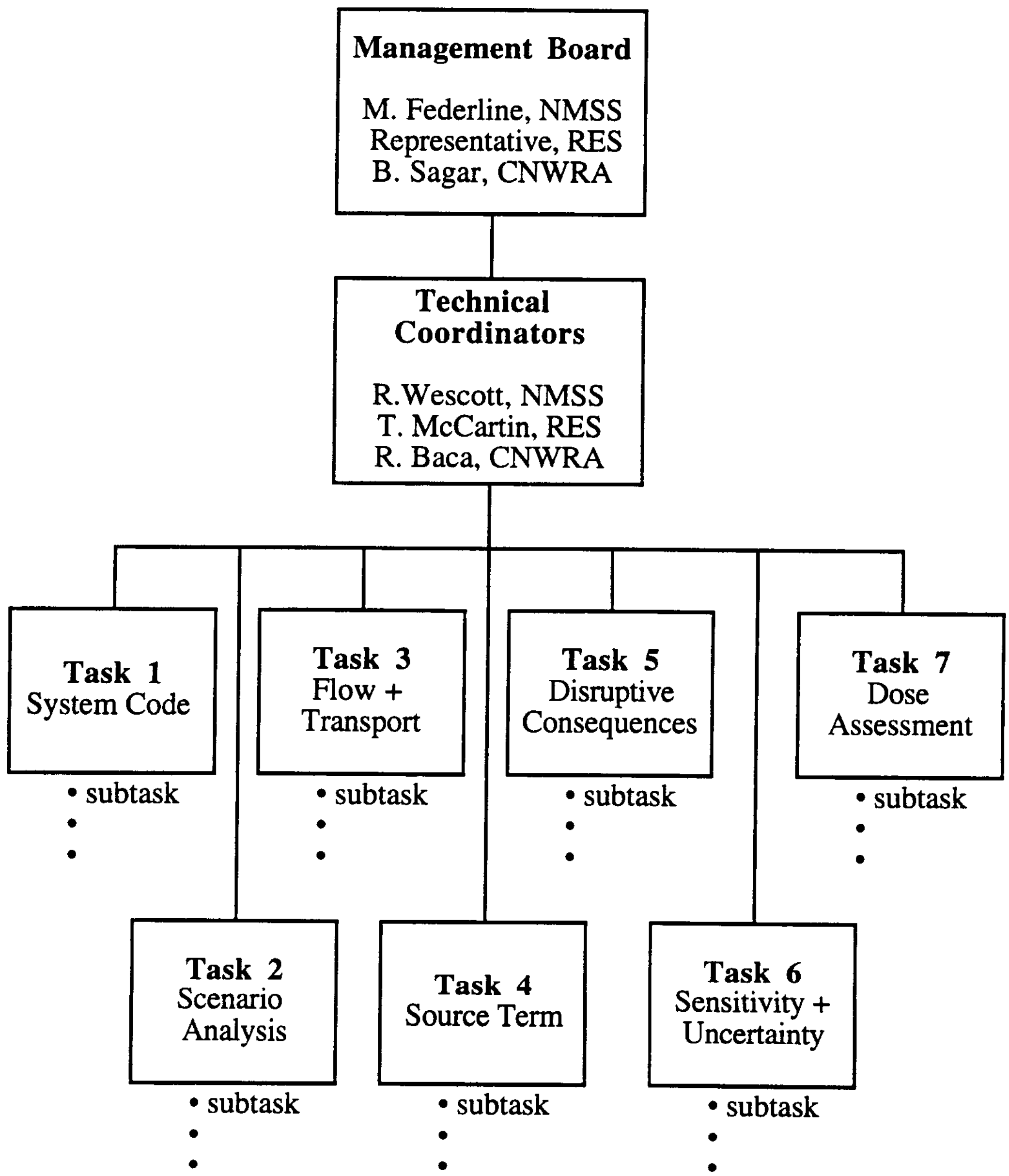

Figure 3-2. Organizational structure for IPA Phase 3

the DOE actions and includes document reviews (e.g., study plans, technical reports, topical reports), quality assurance reviews and audits, technical exchanges, and technical meetings. For the most part, reactive work is difficult to predict. However, a number of the subtask proposals focus on specific areas to review in Sandia National Laboratories TSPA-93 (in preparation).

Within each task, a number of subtasks are proposed by the CNWRA. These subtasks are provided in the Appendix. Based on the skills, capabilities, and interests within the CNWRA, the subtasks are not necessarily evenly distributed among the seven tasks. These proposals should be considered an initial contribution, to which additions and modifications should be made after contributions from other NMSS and RES staff are included. The entire set of recommendations for Phase 3 should then be evaluated, prioritized, and scheduled for (i) conduct during Phase 3, (ii) deferral to a subsequent phase of IPA, or (iii) deletion. It should be recognized that several of the proposals included in the Appendix are the subjects of ongoing FY94 work under IPA.

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APPENDIX

CONTRIBUTION TO THE PLAN FOR ITERATIVE PERFORMANCE ASSESSMENT PHASE 3

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CONTENTS (Cont'd)

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PROGRAMMER UTILITIES FOR TPA CODE

Overall Task:	1-System Code
Lead Person:	R. Janetzke
Key Personnel:	A. Lozano

Justification for Work:

The configuration control of a large number of modules in one system can be aided by the use of automated tools available to the programmer. This task will produce a set of generic tools enabling the code developer to adhere to the programming guidelines in an efficient manner. Also, utility libraries speed the development of the modules by permitting access to common code elements that may be used by more than one program.

Description of Work:

Appropriate components of FORTRAN code analyzers, formatters, and code listing utilities will be identified and acquired or adapted for use as code development tools. All should be compatible with the UNIX "makefile" utility. Frequently used library routines could handle such things as interpolation, operating system interface, dynamic memory allocation, and database access. These routines, as well as previously developed coding guidelines, will be described in a Total Performance Assessment (TPA) programmers manual and in training meetings.

Anticipated Effort:	R. Janetzke:	8 weeks
	A. Lozano:	4 weeks
Anticipated Schedule:	FY94	

CENTRALIZED DATABASE FOR TPA CODE

Overall Task:	1-System Code
Lead Person:	R. Janetzke
Key Personnel:	Computer Support

Justification for Work:

The TPA code for Phase 2 required over 100 input and output files to be managed by the executive. Although this requirement was manageable on the VAX and CRAY systems, it was unnecessary. A simple database approach for data access will eliminate the complexity of the many disk files. It is desirable to have the system accessible from many platforms, so the database will be implemented with the ORACLE database product.

Description of Work:

This task will require the development of a library of routines that could be called by the consequence modules to deposit data in the database. The modules will also be able to read the data submitted to the database by other modules. This capability will provide a standard means of communication for the modules including the executive. When all runs are completed, all data may reside in one file, which can be scanned by post-analysis routines.

Anticipated Effort:	R. Janetzke:	10 weeks
	Computer Support:	25 weeks
Anticipated Schedule:	FY94-95	

IMPROVED CCDF GENERATOR FOR TPA CODE

Overall Task: 1-System Code

Lead Person: R. Janetzke

Key Personnel: Computer Support

Justification for Work:

The generation of output plots from the database should be a separate process from the executive. In order to make changes to the statistical routines, the entire executive needed to be recompiled. The Complementary Cumulative Distribution Function (CCDF) plot generation should be treated as a subtask to the executive.

Description of Work:

This task would involve adding flexibility to the plot generator code which is an integral part of the TPA code for the analysis of the final CCDF data. The data plotted would be from the database which would contain all the necessary information to produce the plot. This work will have a significant impact on the contents of the database since not only the data values, but also their probabilities must be stored. The production of TECPLOT-compatible files will be expanded to include hair diagrams and general parameter plots of any data contained in the database. If possible, additional capabilities will be added to the system with the automatic generation of TECPLOT specific style files.

Anticipated Effort:	R. Janetzke:	2 weeks
	Computer Support:	7 weeks

Anticipated Schedule: FY95-96

GRAPHICAL USER INTERFACE (GUI) FOR TPA CODE

Overall Task: 1-System Code

Lead Person: R. Janetzke

Key Personnel: A. Lozano

Justification for Work:

In Phase 2, the TPA executive made a significant advancement in the input of commands, numeric data, and string data with the RDFREE library of routines for free format input. In addition to being free format, it was also keyword oriented, which allowed the development of context-sensitive constructs. However, there were no checks for completeness or out-of-range conditions at the time of entry by the analyst. This is a severe limitation for the widespread use of the software.

Description of Work:

This task would augment the batch mode of data input with the interactive window-oriented approach. Extensive use would be made of a window client module. This window would be developed using the GALAXY software to enable the porting of the system code to UNIX (CRAY) and PC platforms. The window client would deposit the input directly into the ORACLE database for use by all the modules. A new feature of the display could be an option that permits user-selectable units with automatic conversion to database units when stored. The client would handle most of the module input through an organized hierarchy of window displays.

Anticipated Effort:	R. Janetzke:	4 weeks
	A. Lozano:	33 weeks

Anticipated Schedule: FY94-95

HYDROGEOLOGIC FRAMEWORK MODEL FOR FLOW AND TRANSPORT SIMULATION

Overall Task: 3-Flow and Transport

Lead Person: S. Young

Key Personnel: B. Henderson

Justification for Work:

Improved simulation of flow and transport for IPA Phase 3 will require a comprehensive and integrated geological framework model of Yucca Mountain (YM). The framework model should be a true 3-dimensional (3D) model. Specifically, it should represent the current state of knowledge about the physical characteristics of the layered rock sequence (e.g., rock type, distribution, thickness, depositional architecture, diagenetic alteration), volume distribution of hydrogeologic properties (porosity, permeability), structural geometry (depth, dip), and characteristics of fault zones (volume extent, shape, dip, cutoff geometry of rock units). Perhaps most importantly, the model should represent heterogeneity and anisotropy due to rock fabric and geologic structures (faults and fractures). Using EarthVision software, such a model can benefit Iterative Performance Assessment (IPA) in several distinct ways: (i) it can be used as an evaluation and communication tool—to review and visualize the complex geologic framework of the subsurface, (ii) it can serve as an internally consistent database/archive of rock and hydrogeologic properties from which arbitrary two-dimensional (2D) and 3D sections can be extracted for iterative simulations, and (iii) it can be used as a template for direct comparison with equivalent models of YM produced by the U.S. Department of Energy (DOE) for Total System Performance Assessment (TSPA). Moreover, the model will likely have substantial heuristic value. Use of less abstract (i.e., more realistic) geological models will improve the ability to interpret simulation results and to develop new ideas and better approaches.

Description of Work:

The proposed work would be conducted as an integrated task in concert with an ongoing Geologic Setting (GS) element task (MM 20-5702-425-403) that includes development of a 3D geologic framework model. The IPA portion of this work will entail designing the model and compiling and entering rock and hydrogeologic properties to specifically support Phase 3 and later simulation work. Interpolation/extrapolation of property measurements from boreholes (logs and core analyses), outcrops (sample analyses and descriptions), and grid design (cell size, intersection of fault and layer grids, output grids, etc.) will constitute a significant part of the IPA contribution. Furthermore, methods for transferring general 3D and arbitrary 2D property grids from the model to simulation codes will be investigated. The GS contribution is primarily in constructing the faulted, layered rock sequence, and in entering the borehole trajectories and layer-intercept points. For FY94, deliverables for this project will consist of the model and a report that explains how the model was developed (MM 425-403 is due 09/30/94). It is proposed that MM 425-403 serve as a joint deliverable for the GS/IPA task.

Anticipated Effort:	S. Young:	8 weeks
	B. Henderson:	2 weeks
	G. Rice:	2 weeks

Anticipated Schedule: FY94

ASSIGNMENT OF REPRESENTATIVE HYDRAULIC PROPERTIES TO HYDROGEOLOGIC UNITS AT YUCCA MOUNTAIN

Overall Task: 3-Flow and Transport

Lead Person: S. Mohanty

Key Personnel: T. McCartin
S. Young
B. Sagar

Justification for Work:

Phase 1 recommendations specifically designated the need for improving hydrologic flow models from one-dimensional (1D) to 2D and/or 3D. The issue of using site hydrologic data for generating more realistic data set was also addressed.

Heterogeneity both in the matrix and fractures plays a very important role as it relates to the perching of groundwater and subsequent fracture flow, which would lead to shorter travel times. Modeling fluid flow in such spatially heterogeneous media using 2D or 3D grid requires a large number of grid blocks. When the contrast in hydraulic conductivities is large, discretization of the flow domain to an extremely fine scale is necessary. This fine scale, in turn, poses problems in terms of the availability of computer memory space as well as computational effort. Due to the large number of modules and associated computer memory requirements in the total system performance code, it is required that the grid discretization be minimal in the flow and transport module. It is therefore necessary to develop effective parameters that will retain sufficient information to provide insights on perched water while simultaneously allowing the code user to perform simulation in a reasonable amount of time and using less computer memory space.

Description of Work:

A methodology based on small-cell renormalization group approach was developed under Stochastic Flow and Transport Research Project (IM 20-5704-056-094) and was demonstrated to be up to 300 times faster than the numerical simulation in calculating effective saturated and unsaturated hydraulic conductivities. The method proved to be more accurate than other available approximate methods. A small-cell renormalization group, however, is not adequate when the heterogeneous field shows large geometric anisotropies or when the fractures are not aligned or orthogonal to the flow direction. Therefore, large-cell renormalization group and differential renormalization group methods will be explored for determining the effective properties for systems with such heterogeneities. The method initially will be implemented for saturated fluid flow and later will be extended to unsaturated fluid flow.

Before implementing the homogenization method to reduce the number of grid blocks, heterogeneous fields will be generated by using stochastic simulation methods. In order to obtain meaningful results, the fields will be conditioned to available site-specific hydrologic data. The conditioning procedure will utilize the geologic description of YM to be developed under a GS element task (MM 20-5702-425-403) and the 3D porosity map developed under the proposal title "Hydrogeologic Framework Model for Flow and Transport Simulation," led by S. Young. Additional information from the well logs and core plugs the sampled from various wells will be used to represent permeability heterogeneities at scales smaller than the geologic scale.

Anticipated Effort:	S. Mohanty:	12 weeks
	S. Young:	2 weeks
	B. Sagar:	1 week
	T. McCartin:	TBD
	Part-Time Student:	6 weeks

Anticipated Schedule: FY95

QUANTITATIVE EVALUATION OF HYDROGEOLOGIC MODELS IN SNL TSPA-93

Overall Task: 3-Flow and Transport

Lead Person: S. Young

Key Personnel: S. Mohanty
N. Coleman

Justification for Work:

This work is substantially dependent on, and would follow, work accomplished under the proposal entitled Hydrogeologic Framework Models for Flow and Transport Simulation. The proposed comparative analyses will indicate where substantial differences occur in the respective models, and will include a quantitative assessment of the implications, or importance, of these differences to Performance Assessment (PA).

Description of Work:

This work will entail a detailed comparison between the Center for Nuclear Waste Regulatory Analyses (CNWRA) hydrogeologic framework model and those used in IPA Phase 2 and in the Sandia National Laboratories (SNL) TSPA-93. Geological framework models and related data (especially hydrogeologic zones and properties, layer isopachs, and fault geometry) currently available from the Yucca Mountain Project (YMP) will be acquired for comparison. The scope and detail of the comparison are dependent on data available from the YMP, and will be adjusted as these data are reviewed. Sources of discrepancies can then be investigated, perhaps resolved, or noted as particular uncertainties that may require special attention.

Anticipated Effort:	S. Young	10 weeks
	S. Mohanty	3 weeks

Anticipated Schedule: FY95

PREDICTION OF pH-DEPENDENT Kds BASED ON SURFACE COMPLEXATION MODELS

Overall Task: 3-Flow and Transport

Lead Person: D. Turner

Key Personnel: R. Pabalan
P. Muller

Justification for Work:

One IPA Phase 2 recommendation is to improve chemistry models, particularly for speciation of elements released into water, and the contribution of minerals from both host rock and waste package materials.

Description of Work:

Surface complexation models (SCMs) can be used to quantitatively predict sorption behavior as a function of chemistry, particularly with respect to solution pH. The work proposed here will make use of results from the Sorption Modeling for (HLW) PA Research Project.

Computational requirements resulting from nonlinear geochemical relationships limit direct incorporation of SCMs in PA calculations. A possible bridge is using SCMs to calculate look-up K_d tables as a function of mineralogy and chemistry. SCMs would be used to calculate distribution between sorbed and aqueous phases; results are converted to K_d values for flow and transport calculations. For different radioelements, the K_d values could be presented at pH intervals. Due to lack of experimental data, the tables would not be exhaustive but could provide information for key radionuclides and minerals. Since most available data are for actinides, initial efforts will focus on these (U, Pu, Am, Th, Np). For example:

KAOLINITE	pH				
Element	5	6	7	8	9
U	K_d(ml/g)	K_d	K_d	K_d	K_d
Pu	K_d	...	...	...	...
Np	K_d	...	...	...	...
Am	K_d	...	...	...	...
Th	K_d	...	...	...	...

As determined using SCMs, K_ds are discrete values. For stochastic PA calculations, it may be possible to use uncertainties in the calculated SCM binding constants to generate a range in K_d values. It may also be possible to develop distribution functions for sorption by assuming a probability distribution function (pdf) and sampling a range in pH. Appropriate K_ds can be extracted from the tables and used in transport calculations.

Anticipated Effort: D. Turner: 5 weeks
R. Pabalan: 2 weeks
P. Muller: 5 weeks

Anticipated Schedule: FY94

ANALYSIS OF SHALLOW INFILTRATION AT YUCCA MOUNTAIN

Overall Task: 3-Flow and Transport

Lead Person: S. Stothoff

Key Personnel: A. Nedungadi
A. Bagtzoglou
A. DeWispelare

Justification for Work:

One recommendation of the IPA Phase 2 report is that the nature of infiltration at the YM site should be investigated. The imposed infiltration rate was observed to be one of the most sensitive parameters which affect the cumulative release to the accessible environment. This is consistently observed throughout the Nuclear Regulatory Commission (NRC) PA analyses, the DOE PA analyses, and the Electric Power Research Institute (EPRI) PA analyses. Despite this observation, there is large uncertainty regarding the magnitude, spatial variation, and temporal distribution of infiltration.

Description of Work:

The objective of this study is to estimate the time-dependent infiltration behavior for various surficial conditions representative of YM. A 1D numerical model will be created, incorporating physics appropriate to a generic column in the near-surface environment. Available meteorological data from nearby National Oceanic and Atmospheric Administration measurement sites will be synthesized into statistically equivalent input for the numerical model. Adjustments to current precipitation rates, representing various possible future climatological conditions, will be based on recommendations coming from the Expert Elicitation of Future Climate in the YM Vicinity.

Various factors play a role in infiltration, including meteorological conditions, soil, rock, fracture properties, site vegetation, and site topography. In this study, it will not be possible to sample all possible combinations of these properties; rather, a few representative combinations will be chosen. The numerical model will act as a nonlinear filter for these input sets, yielding information on the time variation of infiltration for the particular input combination. This information can guide the generation of synthetic infiltration histories for subsequent models without resorting to further extremely computationally intensive near-surface simulation. In particular, the results of this study are intended to guide representation of infiltration in TPA activities and other analyses considering flow of moisture in YM.

This work is intended to be coupled with the research and IPA work of A. Bagtzoglou, who will be considering the effects of focused recharge within YM. The near-surface numerical model will be interrogated for the time behavior of infiltration for matrix properties representative of the YM surface. A column can be considered a unit-area portion of the surface; by appropriately area-weighting the infiltration signal from various surface columns, representative input signals for the top boundary conditions of his model will be obtained.

Anticipated Effort:	S. Stothoff:	16 weeks
	A. Nedungadi:	2 weeks
	R. Bagtzoglou:	1 week
	A. DeWispelare:	1 week

Anticipated Schedule: FY94

ANALYSIS OF DEEP INFILTRATION AT YUCCA MOUNTAIN

Task:	3-Flow and Transport
Lead Person:	R. Bagtzoglou
Key Personnel:	M. Muller S. Stothoff T. McCartin

Justification for Work:

The majority of numerical modeling efforts related to the YMP assume that the net infiltration signal is uniformly distributed in space and time. The mean values used in these types of simulations do not take into account the more extreme rainfall rates that may occur due to either interannual or interseasonal fluctuations, or even individual storm events. It is hypothesized that concentrating or focusing (U.S. Geological Survey—U.S. Department of Energy Study Plan 8.3.1.2.2.9) the infiltration signal may have a significant effect on various measures related to performance. These measures include, but are not limited to: (i) Groundwater Travel Time (GWTT) estimate; (ii) flux of water, and its temporal variation at selected points in space (preferably at or around the repository horizon); and (iii) saturation levels at selected points. The effects of short transient events on performance-related measures may have to be addressed separately through the use of simplified modeling.

Description of Work:

This work will examine the effects of focusing infiltration in space and time so that the net infiltration rates remain at the 0.1 to 5 mm/yr levels. This focusing will ensure that the total mass of water entering the system is preserved, but allow the infiltration rates to locally become several orders of magnitude higher. The steps followed in this work will be: (i) solve the flow problem in a 3D domain with a simplified YM stratigraphy (horizontal layers with no faults present) for the case of uniform infiltration, q_o, (spatially, and temporally). This will constitute the reference case on which all subsequent comparisons will be based; (ii) gradually focus or concentrate the infiltration signal spatially. Solve the flow problem in a transient mode and present the dependence of the selected measure on the focusing parameter, defined as the ratio of areas where the infiltration is being applied to; and (iii) choose some spatial focusing level and perform an exercise analogous to (ii) by concentrating the signal temporally. A variety of options are available for such temporal focusing. This last analysis, however, will be conditioned on the temporal infiltration patterns obtained from a similar effort (see description below) slated toward the upper part of the mountain. Similar to the approach in (ii), a parameter defined as the ratio of $\max\{q(t)\}$ over the reference value q_o, and its influence on selected performance-related measures, will be investigated.

This work is coupled with the work S. Stothoff will be conducting for a relatively short length of strata (less than 50 to 70 m) near the surface of the mountain. The synergism between the two efforts exists in the theorized "smoothing" effect that the upper layers may have on the infiltration signal entering deeper layers. Indeed, the weighted flux output of the shallow column will be the reference input signal for this work. Therefore, it is anticipated that the attenuation of the input signal will make it possible for such focused fluxes of water to enter a domain that is relatively dry. Prior modeling experience has indicated that this type of boundary conditions is particularly difficult to be dealt with by numerical codes, such as the DCM3D code. The two studies are synergistic in that it would be unwise for this study to investigate the effects of unrealistically high focused signals. Tailoring, or constraining, the temporal patterns of infiltration to be analogous to the patterns observed in the upper layer infiltration effort would, therefore, eliminate a great deal of parameter space searching and save substantial time and resources. Finally, both studies will contribute to the understanding of the infiltration processes at a site scale that is going to be an issue addressed by the Subregional Hydrology Project.

The anticipated product of this effort is to help answer the following questions: (i) Are selected performance-related measures sensitive enough to the focusing of the net infiltration signal? (ii) How deep in the rock is the sensitivity becoming negligible if it becomes negligible at all? (iii) Does spatial or temporal averaging of infiltration affect the system more?

Anticipated Effort:	R. Bagtzoglou:	5 weeks
	M. Muller:	10 weeks
	S. Stothoff:	1 week
	T. McCartin:	TBD

Anticipated Schedule: FY95

ANALYSIS OF THE EFFECTS OF CLIMATIC CHANGES ON INFILTRATION AT YUCCA MOUNTAIN

Overall Task:	3-Flow and Transport
Lead Person:	B. Gureghian
Key Personnel:	R. Codell B. Sagar

Justification for Work:

Recent findings obtained from an expert elicitation of future climate conditions in the vicinity of YM, highlighted probabilistic perturbations of several key atmospheric parameters, including precipitation, temperature and cloud cover, for the next 10,000 years. In addition to deterministic predictions of the temporal variations of the infiltration rates, the sensitivity and uncertainty issues, associated with the infiltration problem, inherent to those predicted changes in climatic conditions at YM must also be addressed. A 1-D groundwater flow model designed for a variably saturated, layered geologic medium must be developed, in order to get an accurate representation of a typical performance measure (e.g., Darcy's flux), and subsequently be used to perform the auxiliary sensitivity and uncertainty analyses.

Description of Work:

The objective of this task is to develop an analytical model for the 1D isothermal flow of water in a variably saturated and multi-layered geologic medium assumed to extend to infinity. The analytical solution of the quasi-linear form of Richard's equation will be based on the Laplace's transformation technique. Initial conditions for each layer corresponding either to a constant pressure head or a spatially varying one would be considered. The surface boundary conditions associated with site relevant climatic conditions (i.e., precipitation and potential evaporation), will be simulated through time-dependent fluxes described by exponential and/or simple harmonic functions. Gardner's formulation of the unsaturated hydraulic conductivity will be adopted. The solution will yield the spatial and temporal variations of the pressure head, flux, time integrated flux, and water content. This work is ongoing and early results have been published in a paper at the International HLW Management Conference.

Anticipated Effort:	B. Gureghian:	8 weeks
	B. Sagar:	TBD
	R. Codell:	TBD

Anticipated Schedule: FY94

ANALYSIS OF CARBON-14 TRANSPORT AT YUCCA MOUNTAIN

Overall Task: 3-Flow and Transport

Lead Person: W. Murphy

Key Personnel: R. Codell
Computer Support

Justification for Work:

A planned accomplishment in IPA Phase 3 is a more direct treatment of radionuclide transport in an unsaturated medium. Multiphase radionuclide transport and retardation due to gas-liquid-solid interactions are special aspects of mass transport in an unsaturated medium. One Phase 1 recommendation that was not fully implemented in Phase 2 was to develop improved models for gaseous transport of volatile radionuclides, especially carbon-14. Carbon-14 release by gas phase transport consistently shows a potential to violate release standards in PAs for YM. An auxiliary analysis in Phase 2 illustrated the theoretical basis and demonstrated the feasibility of relatively realistic nonisothermal models for the evolution of the carbon geochemical system in a YM repository. However, this analysis employed highly schematic representations of gas flow in one dimension and variations in liquid saturation, and neglected liquid transport. Consequently, the results were too limited to provide quantitative predictions of carbon-14 release for repository performance modeling. In Phase 2, gaseous radionuclide release computations were based on independent heat and gas flow modeling and transport of carbon-14 using a retardation factor based in part on the auxiliary analysis of the carbon system geochemistry.

Description of Work:

A carbon system transport model will be developed and implemented for modeling system performance with regard to gaseous release of carbon-14. Maximum use will be made of results of heat and multi-phase fluid flow models and geochemical models developed independently either for IPA Phase 2 or research projects. In the past several years, models for heat and two-phase fluid flow have been generated with codes such as TOUGH, which provide temperature, gas and liquid flow, and liquid saturation as a function of location and time. Such results appear to be adequate to support carbon transport modeling, and the proposed work will take advantage of existing tools for thermohydrologic modeling. The first task of the proposed work is to develop a carbon system transport model analogous to that of the IPA Phase 2 auxiliary analysis. The improved model will use temperature and flow fields from thermohydrologic models to allow more accurate descriptions of the evolution of the carbon system for various manifestations of a YM repository. To limit the computational burden of the carbon system transport model, a radially symmetric system may be considered that neglects much geologic complexity. The geochemical system model will be highly simplified, but, nevertheless, it will account explicitly for the most significant chemistry of the carbon system. It may be the same as that employed in the Phase 2 auxiliary analysis (which contains seven equations), or it may contain one additional equation representing a hypothetical reaction to capture the main effects of silicate system reactions on the carbon system. The geochemical model will provide the distribution of carbon among gas, liquid, and solid phases at each point and for each time as a function of temperature, saturation, and mass transport (primarily gaseous) of carbon.

To avoid lengthy run times, the numerical model for gas flow and transport used in IPA Phase 2 should be replaced in the PA system code by a response surface describing carbon transport. This accomplishment would constitute the second task of this work. The response surface would be abstracted from more detailed coupled thermohydrologic and geochemical carbon system transport calculations for various repository scenarios. These computations would be performed externally from the TPA code using the carbon system transport model developed in the first task. Gaseous carbon-14 release in the TPA system model would depend on the source term for carbon-14 and carbon transport. Carbon-14 introduced in the system will be modeled to be transported as a trace component in proportion to transport of native carbon, with radioactive decay, and negligible isotopic fractionation. Liquid transport of carbon-14 in fracture flow would require a separate treatment.

Anticipated Effort:	W. Murphy:	10 weeks
	R. Codell:	TBD
	Computer Support:	12 weeks

Anticipated Schedule: FY95

QUANTITATIVE EVALUATION OF CARBON-14 MODELS IN SNL TSPA-93

Overall Task:	3-Flow and Transport
Lead Person:	B. Murphy
Key Personnel:	R. Codell Computer Support

Justification for Work:

DOE and SNL have indicated that models of carbon-14 release and transport are included in the recently completed SNL TSPA-93. Because IPA Phase 2 predictions of carbon-14 release and transport showed it to be a significant contributor to the overall release, a detailed analysis of DOE data, assumption, and models is appropriate.

Description of Work:

Review of models and analyses of carbon-14 in the SNL TSPA-93 will be performed through two activities. First, results will be compared qualitatively and quantitatively to results from NRC IPA Phase 2 and Phase 3 auxiliary analyses of carbon-14 source and transport and IPA Phase 2 release computations. Causes of identified differences will be examined. Second, a set of basic calculations/computations will be performed to check aspects of the TSPA-93 carbon-14 model such as initial source amount, radioactive decay, and conservation of mass in aqueous and gas (and solid?) phases.

Anticipated Effort:	W. Murphy:	2 weeks
	R. Codell:	2 weeks
	Computer Support:	2 weeks

Anticipated Schedule: FY95

ANALYSIS OF THE IMPORTANCE OF SEALS FOR SHAFTS, RAMPS, OR BOREHOLES IN AN UNSATURATED ENVIRONMENT

Overall Task: 3-Flow and Transport

Lead Person: M. Ahola

Key Personnel: G. Ofoegbu
B. Gureghian

Justification for Work:

During IPA Phase 2 activities related to hydrologic flow and transport, no effort was made to address the varying degree of uncertainty in issues related to the long-term performance of seals for shafts, ramps, and boreholes and the effect that their degradation would have on creating preferential pathways leading to accelerated radionuclide release rates.

Description of Work:

The objective of this proposed study for IPA Phase 3 is to conduct an auxiliary analysis to evaluate the role of seals under unsaturated environments. This analysis will be accomplished through use of the finite-element code ABAQUS, which is capable of conducting unsaturated liquid flow in a multilayered system. A model will be developed to investigate unsaturated hydrologic flow in a multilayered system in the presence of a vertical shaft or borehole. For simplicity, the problem geometry will be assumed to be axisymmetric with a shaft or borehole located in the center. Also, only steady-state, variably saturated conditions will be assumed. The analysis will be conducted in the absence of heat, however, if time permits, the thermal aspect will be incorporated. Comparisons will be made with cases run without the presence of a shaft or borehole. The mechanically induced changes in permeability will be estimated by appropriate deterministic or statistical means as a result of stress changes around the openings due to excavation and later thermal loading. The available literature will be reviewed to determine the unsaturated properties of representative rock matrix and seal materials, and any constitutive relations related to mechanically induced changes in permeabilities of such materials. Along the upper ground surface of the model, a mean value of precipitation/evaporation will be assigned, taking into account seasonal variations in climatic conditions (i.e., rainfall and evaporation) at the proposed repository site. A very simplified sensitivity analysis will be conducted to determine the impact on defined performance measures with respect to variations in input parameters (e.g., seal and rock parameters) to the finite-element model.

Anticipated Effort:	M. Ahola:	10 weeks
	G. Ofoegbu:	2 weeks
	B. Gureghian:	2 weeks

Anticipated Schedule: FY94

QUANTITATIVE EVALUATION OF THE FLOW MODELS USED IN SNL TSPA-93

Overall Task: 3-Flow and Transport

Lead Person: V. Kapoor

Key Personnel: V. Kapoor

Justification for work:

In the IPA Phase 2 report it is recommended that different conceptual models for matrix-fracture coupling be evaluated. Proposed here is an evaluation of two different conceptual flow models, and their impact on estimates of groundwater travel time (GWTT) and cumulative mass flux performance measures.

Description of Work:

In the current model of flow in IPA-2, all of the flux is carried by the matrix, unless the imposed infiltration rate is greater than the saturated hydraulic conductivity. When that happens, the additional flux of water is directed through the fracture. Conceptually, this is similar to the equivalent continuum-pressure equilibrium assumption of Peters and Klavetter (Water Resour Res. 24:416-430, 1988), which is called the composite porosity model in SNL TSPA-91. A contrasting model is the WEEPS model also used in SNL TSPA-91 that directs all the water through the fracture. It needs to be noted however, that if the flux on top of a porous column is specified, and the model assumes 1D steady state conditions, the cumulative water flux through the column is independent of its properties, or the presence of fractures. Proposed is an evaluation of the WEEPS and composite porosity model, and comparisons with the current IPA Phase 2 conceptual flow model. The different conceptual models and the role of the boundary condition on the top in determining the performance measures of groundwater travel time and the cumulative contaminant mass flux will be assessed. The extent to which these different models can a priori claim to be conservative (by underestimating the GWTT, or overestimating the cumulative mass flux) will be investigated. The focus will be on determining the spatial-temporal scales of movement of water in fractured porous medium that are pertinent to the performance measures, and relating them to basic constitutive properties of water and the porous medium. Analytical approximations and simple numerical approximations will be applied to calculate performance measures with different conceptual models.

Anticipated effort: V. Kapoor: 12 weeks

Anticipated Schedule: FY94

INVENT MODULE: IMPROVED CALCULATION OF RADIONUCLIDE INVENTORIES

Overall Task:	4-Source Term
Lead Person:	H. Karimi
Key Personnel:	A. Lozano R. Manteufel

Justification for Work:

Having uniform and tested values for radionuclide inventory as the input for different codes and module would assist module integration between the modules that require inventory information.

Description of Work:

Based on recommendations from IPA Phase 2 to improve transparency, accuracy, and robustness of the information utilized in different modules; CNWRA proposes to create an inventory generation program. This task will create pre- and post-processor software (using GALAXY) that will execute the ORIGEN software to tabulate radionuclides of interest and store them in a database (using ORACLE). The database could efficiently be interrogated for radionuclide inventories by the TPA execute code. The pre- and post-processor software could efficiently be executed for different fuels (e.g., PWR, BWR) for different burnup, for different fuel characteristics (which, for example, influence C-14 inventory), different radionuclides of interest, and different times of interest.

ORIGEN creates ASCII files containing the buildup, decay, and in-growth of radioactive materials results in tabular format. Results are time dependent concentration of radionuclides and include libraries for cross sections, fission product yields, decay data, and other data in accordance with users request. This code uses a matrix exponential method to solve a large system of coupled, linear, first-order ordinary differential equations with constant coefficients. The user can tailor the size of the executable module to the problem size or the available radionuclides.

For proper integration, CNWRA will determine the form in which the ORIGEN results are desired and provide reasonable default values for some of the parameters to facilitate the use of this code. Finally, the software will extract the information from the output files and provide the information to a controlled database so that the other codes can quickly determine the radionuclides inventory at different times.

Anticipated Effort:	H. Karimi:	6 weeks
	A. Lozano:	4 weeks
	R. Manteufel:	1 week

Anticipated Schedule: FY94

ANALYTIC ANALYSIS OF THERMALLY-DRIVEN NEAR-FIELD FLOW

Overall Task: 4-Source Term

Lead Person: R. Manteufel

Key Personnel: J. Firth

Justification for Work:

During the last 2-3 yr, theories have been developed within the DOE YM program about the potential benefits of high thermal loading. It has been hypothesized by Lawrence Livermore National Laboratory (LLNL) staff that a high thermal load will lead to a prolonged dry-out period around waste packages. In a dry environment, corrosion of the waste packages is significantly reduced and waste package lifetime is significantly extended. The thermal loading that could create a dry environment may also contribute to other phenomena that may be detrimental to the overall or long-term performance of the repository. Recently, EPRI and M&O/Intera have evaluated the impact of different thermal loadings and the resulting near-field hydrologic environment on repository performance for three cases: low loading (~28 kW/Ac), Site Characterization Plan (SCP) loading (~57 kW/Ac), high loading (~114 kW/Ac). It appears that the DOE will soon be making a decision about the thermal loading strategy, hence it is timely for the NRC/CNWRA to perform an independent assessment of the effects of thermal loading on near-field flow and repository performance. The evaluation of the DOE decision will require knowledge about the thermodynamic, hydrologic, and heat transfer phenomena established by different thermal loading conditions.

Description of Work:

The work will build on work already completed at the CNWRA [especially Thermohydrology Research Project and engineered barrier system (EBS) element], and will be conducted in three phases: (i) identification of simple thermohydrologic models that describe thermally-driven near-field flow; (ii) identification of different thermal flow regimes where different phenomena are dominant (e.g., boiling, vapor driven, buoyancy driven); and (iii) the anticipated impact of the thermal loading strategy on the thermal flow regime (only simplified calculations will be performed). Results from this work include the identification of important thermal and flow processes. It is also anticipated that alternative conceptual models will be identified similar to those identified by EPRI: conduction-dominated heat transfer, conduction/convection heat transfer, boiling/condensation-dominated heat transfer, dry-out zone, condensate dripping in fractures, pressure-driven vapor flow, matrix/fracture assumptions. Key parameters may be items such as: bulk permeability, funneling factor for condensate dripping, criteria for dry out (temperature or saturation value), magnitude of thermal load. Appropriate performance measures may be items such as the duration of dry-out, degree of saturation, and the dominant mode of vapor transfer. It is anticipated that the thermal hydrologic regimes of the near-field can be characterized in order to evaluate some of the thermal loading options currently being considered by the DOE.

Anticipated Effort: R. Manteufel: 5 weeks
J. Firth: 5 weeks (staff exchange)

Anticipated Schedule: FY94

NUMERICAL ANALYSIS OF NEAR-FIELD FLOW AND COMPARISON WITH SEMI-ANALYTIC SOLUTIONS

Overall Task:	4-Source Term
Lead Person:	P. Lichtner
Key Personnel:	J. Walton M. Seth

Justification for Work:

In a partially saturated repository for HLW, the presence and movement of water are controlled by a combination of effects due to a temperature gradient, flow and diffusion of water vapor away from the waste package, and liquid flow of water in small capillaries toward the waste package. The dynamics of water plays an essential role in determining corrosion of the waste container and release of radionuclides. Although the most dramatic effect of thermal loading is boiling of water near the waste package, the effects of thermal loading on water movement can also be significant below the boiling point of water. The period of lower temperatures is a prime consideration in waste package design since water availability for corrosion and radionuclide transport is greater during this period.

The computer code V-TOUGH, a two-phase liquid-gas transport model, uses Fick's law combined with Darcy's law to describe vapor diffusion. This treatment may be too simplistic, however, especially at low permeabilities where it is to be expected that Knudsen diffusion becomes competitive with Fickian diffusion. Therefore, it is important to evaluate the possible limitations of V-TOUGH in describing vapor transport.

Description of Work:

In this work, a semi-analytic solution is used to predict thermo-hydrology near the waste package for the case in which either a heat pipe does not develop or when the heat pipe is away from the waste container. The solution considers water vapor transport by diffusion and diffusion-caused advection, and advection of liquid in small capillaries in a heterogeneous 1D geometry. The results of the dusty gas model that incorporates the transition to Knudsen diffusion at small pore sizes, or equivalently low permeability, are compared with combined Fick and Darcian flow of vapor. The solution predicts vapor and liquid compositions and fluxes as a function of distance from the waste package. Heat transfer is assumed to be conduction dominated. A series of simulations are presented relating vapor pressure lowering around the waste package to design parameters such as packing material and thermal loading. The results of the simplified model will be compared with V-TOUGH, and modified to include calculation of the rates of evaporation and condensation. The methodology should provide a rapid method of assessing the influence of waste package design parameters such as use of packing material on the near-field environment.

Anticipated Effort:	P. Lichtner:	8 weeks
	J. Walton:	4 weeks
	M. Seth:	3 weeks

Anticipated Schedule: FY94

A MODULE FOR EVALUATING THE CORROSION PERFORMANCE OF CONTAINERS

Overall Task:	4-Source Term
Lead Person:	P. Lichtner
Key Personnel:	G. Cragnolino N. Sridhar

Justification for Work:

The recently evolving repository design of the DOE involves the use of high thermal loading to create a dry-out zone around the waste packages for an extended period in order to minimize corrosion and aqueous radionuclide transport. However, there are many uncertainties in predicting the effect of high thermal loading on the near-field environment, and a conservative approach dictates that the aqueous as well as vapor phase corrosion of the waste package components be evaluated. The waste package corrosion models in the SOTEC code of IPA Phase 2 did not consider corrosion to be significant under dry oxidation. Once aqueous conditions prevail, a generic power-law relationship for general corrosion rate with time was adopted. However, the power-law relationship for general corrosion does not have a fundamental justification, especially for passive metals, and other types of relationships need to be considered. The onset of localized corrosion was determined in IPA Phase 2 by the corrosion potential and critical potential. These potentials were considered to be dependent only on temperature. A more detailed consideration in terms of their dependence on other environmental and design parameters is necessary. A more realistic treatment of localized corrosion propagation rate is also necessary.

Description of Work:

The detailed analyses and modeling are being performed in the Engineered Barrier System Performance Assessment Codes (EBSPAC) program. Some of the corrosion models have already been considered in the Substantially Complete Containment Example (SCCEX) problem code. In the first phase, these models will be simplified in the SOTEC in the form of parametric equations. The corrosion and critical potentials depend upon the environmental chemistry. The parametric equations for critical potentials used in SCCEX code will be adopted with further literature database to augment the derived empirical parameters. In this analysis, as in SCCEX code, the critical potential for stress corrosion cracking will be assumed to be the same as for localized corrosion. For the first phase of the analysis, a saturated NaCl solution will be assumed as the composition of the last aqueous phase that will remain on the waste packages as a result of evaporative concentration. The time to wetting will be assumed to be dictated as in SOTEC by the waste package surface temperature and the boiling point of the saturated NaCl solution. However, this overly conservative assumption may not be justifiable. A detailed model for the evolution of near-field environmental chemistry and water stability will be performed in the EBSPAC program, the results of which may be incorporated into the SOTEC code at later phases. The corrosion potential will be evaluated for both a single-wall container design and a double-wall container, in which a hole in the outer steel wall will be assumed. The rate of general corrosion for the passive metals will be dictated by the passive current density. Empirical results justified by mechanistic considerations will be used for determining the passive current density as in the case of SCCEX code. For the corrosion allowance type materials, the general corrosion rate will be dictated by the corrosion potential and active corrosion current. Under repository conditions, the active current density will be controlled by the transport of cathodic species such as oxygen to the surface. A diffusion controlled relationship is used in the SCCEX code, which will be reviewed and updated. The rate of propagation of localized corrosion will be assumed from empirically derived equations (e.g., rate of growth proportional to $t^{-1/2}$) that have been justified on the basis of the diffusion-controlled dissolution. In the second phase of the project, the empirical relations of the oxidation rates, especially at low temperatures of the repository, will be reviewed, and appropriate relationships will be used in the SOTEC code.

Anticipated Efforts:	N. Sridhar:	4 weeks
	G. Cragnolino:	2 weeks
	P. Lichtner:	4 weeks

Anticipated Schedule: FY95-96

A MODULE FOR EVALUATING THE RELEASE RATE OF RADIONUCLIDES IN THE AQUEOUS PHASE

Overall Task: 4-Source Term

Lead Person: P. Lichtner

Key Personnel: H. Manaktala
N. Sridhar

Justification for Work:

The version of SOTEC in IPA Phase 2 considers radionuclide release in the form of dissolved ions for all species except ^{14}C, which is considered to be released as a gaseous species. The aqueous release rate is calculated by a solubility limited transport model, assuming congruent dissolution and a fixed solubility limit for all radionuclides. This model is based on the assumption that the dissolution rate of UO_{2+x} is rapid compared to the transport of dissolved species away from the spent fuel surface. The solubility of UO_{2+x} is dependent on the environmental parameters such as pH, redox potential, and bicarbonate concentration. The redox potential in the environment close to the breached spent fuel can be very high due to α-radiolysis. The pH may be determined locally by dissolution of container materials. Additionally, the influence of the spatial variability of the spent fuel, microstructurally and chemically, is not considered.

Description of Work:

The majority of this activity will be performed in the EBSPAC development project. The aqueous release rate calculations will be performed in a separate module from the gaseous release rate since the species involved are different. The calculation of the concentrations of various radionuclides as functions of space and time may be performed separately and an input in the form of a flux at any specific location of all the radionuclides can be provided as input to the SOTEC code, perhaps as functions of temperature, time, and other specific environmental parameters. This will reduce the total computation time of the SOTEC code. The aqueous release rate calculations will be performed in several phases. In the first phase, a fixed solubility limit condition will be assumed with a more rigorous calculation of the solubility as a function of environmental conditions. In the second phase, the electrochemical dissolution kinetics of the spent fuel will be considered, assuming that the stoichiometry of the UO_{2+x} has evolved to a specific value as a result of prior oxidation. The dissolution rate will be coupled to transport of species to and away from the spent fuel. These calculations will again be performed in a separate module. In the third phase, the spatial variability effect of spent fuel will be evaluated as an auxiliary analysis in order to determine its impact on the release rate.

Anticipated Effort:	P. Lichtner:	5 weeks
	Temporary Staff:	5 weeks
	N. Sridhar:	2 weeks
	H. Manaktala:	1 week

Anticipated Schedule: FY95-96

MATHEMATICAL MODELS FOR RELEASE OF RADIONUCLIDES FROM VITRIFIED (GLASS) WASTEFORM

Overall Task:	4-Source Term
Lead Person:	H. Manaktala
Key Personnel:	H. Karimi

Justification for Work:

About 40 percent of the waste packages are expected to contain vitrified wasteforms, with the remaining 60 percent contain spent fuel). However, the radionuclide inventory of vitrified wasteforms is expected to be only 5 to 10 percent of the total HLW that will be emplaced in the geologic repository. Based on this fact, it is often argued that fractional contribution of radionuclides released from waste packages upon loss of containment would be extremely small. Hence, modeling of the performance of vitrified wasteforms is considered relatively unimportant and was not attempted in IPA Phase 2. However, some experimental evidence indicates that radionuclide release (leaching) rates of vitrified wasteforms could be significantly higher than the release rates of the spent fuel under some anticipated repository conditions. Therefore, the relative contribution of radionuclide release from vitrified wasteforms could be much higher than assumed on the basis of the initial inventory. A definitive quantitative answer is not available at this time.

Description of Work:

The work will be conducted in three phases: (i) identifying the range of environmental conditions credible in an unsaturated repository, (ii) generating initial and time-dependent inventory of radionuclides utilizing the ORIGEN computer code utilizing the INVENT module being proposed by H. Karimi, and (iii) calculating the release rates of selected radionuclides from vitrified wasteform and spent fuel under those conditions. These release rates then can be incorporated into the "Module for Evaluating the Release Rate of Radionuclides in the Aqueous Phase" led by P. Lichtner. This work is based on the information generated and those parameters that influence vitrified wasteform degradation that have been previously identified in work performed in the EBS and Repository Design, Construction and Operation (RDCO) elements. Most of the new effort under this proposal will be devoted to calculations of releases based on calculated inventory and range of plausible environmental conditions and leaching/degradation mechanisms. If the results indicate that releases from vitrified wasteforms are much higher than the proportion assumed based on the initial inventory of radionuclides, there may be a justification for incorporating vitrified wasteform leaching model(s) in IPA Phase 3 so as to perform quantitative evaluations of the effect of vitrified wastes on the NRC release rate performance measure.

Anticipated Effort:	H. Manaktala:	8 weeks
	H. Karimi:	4 weeks
	R. Neel:	1 week
Anticipated Schedule:	FY95-96	

MATHEMATICAL ABSTRACTION OF DETAILED CALCULATIONS INTO THE TPA CODE USING THE RESPONSE SURFACE METHOD

Overall Task: 4-Source Term

Lead Person: P. Nair

Key Personnel: J. Wu
T. Torng

Justification for Work:

The IPA Phase 2 report has identified several areas for enhanced mechanistic models. However, computer costs restrict the incorporation of complex models into TPA, and encourage the abstraction from complex to simple models. A mechanistic mathematical abstraction would ease the integration of more detailed models and codes being developed and/or enhanced in other NRC-funded activities.

Description of Work:

Because of the need to model a large number of possible conditions, it is impractical to integrate detailed mechanistic codes directly with the system PA code. The proposed approach is to generate response surfaces from other codes (e.g., SCCEX), that can be integrated into the system PA code through an interface. Based on the fast probabilistic performance assessment concept (discussed in the IPA Phase 2 report), piecewise response surface models can be generated to approximate the true response from detailed calculations in the important regions of the input. The work will involve post-processing the results from detailed calculations to generate simplified models for the system performance assessment code.

The proposed approach has several advantages:

(i) It allows the state-of-the-art codes and models to be integrated into the system PA code

(ii) The generated response surface models will generally involve a smaller set of parameters and failure modes, therefore the computational efficiency can be significantly improved

Anticipated Effort:	P. Nair:	6 weeks
	J. Wu:	5 weeks
	T. Torng:	10 weeks

Anticipated Schedule: FY94-95

CANT2 MODULE: IMPROVED TEMPERATURE PREDICTIONS

Overall Task:	4-Source Term
Lead Person:	R. Manteufel
Key Personnel:	R. Codell Computer Support

Justification for Work:

In IPA Phase 3, it will be advantageous to model the temperature field for an in-drift design, as well as the SCP design and for variable thermal loads. The current IPA Phase 2 code has the CANT2 module, which can be updated.

Description of Work:

A model for calculating the temperature field will be developed and implemented in a computer module. The model will be an extension and enhancement of the existing CANT2 module and will be integrated with the GUI software implemented in GALAXY and the database software implemented in ORACLE. The model will be structured to allow the user to designate those key design features (e.g., thermal load strategy) that influence the evolution of the temperature field.

Anticipated Effort:	R. Manteufel:	6 weeks
	Computer Support:	8 weeks
	R. Codell:	TBD

Anticipated Schedule: FY95

MATHEMATICAL MODELS FOR THE RELEASE OF COLLOIDS FROM VITRIFIED WASTE AND SPENT FUEL

Overall Task: 4-Source Term

Lead Person: H. Manaktala

Key Personnel: R. Baca

Justification for Work:

The results of a recent study on vitrified wasteforms, using a simulated unsaturated repository environment, indicate that 70 percent of Np can be considered truly dissolved. On the other hand, greater than 99 percent of Am and Pu were retained as colloidal solids. The ratio of radioactivity of the filtered to the dissolved fraction was observed to be greater than 1000:1 for a number of low-solubility radionuclides. These results indicate that repository performance models that assume maximum release of actinides to be controlled by the solubility limit in groundwaters, particularly for Pu, Am, and Cm isotopes, would grossly underestimate the potential for radionuclide release into the environment. For the time period after 1,000 yr, Pu and Am will be the dominant radionuclides based on curie content of the waste. Therefore, resolution of their contribution to the source term is needed to increase the accuracy of repository performance estimates. Currently, the low-solubility radionuclides are either ignored or their contribution underestimated as a consequence of ignoring their release in colloidal form.

Description of Work:

The work will be focused on calculating release rates of selected low-solubility radionuclides, identified in IPA Phase 2 as the radionuclides with significant contribution to the repository inventory curie content, from both vitrified wasteform and spent fuel under repository-relevant conditions. Work performed as a joint project between the CNWRA and the NRC on the role of colloids in the release of radionuclides in a geologic repository (currently in progress and expected to be completed in FY94) will be used to provide background information for this task. The majority of the new effort will be devoted to developing/using appropriate mathematical algorithms for the calculations of releases based on a range of plausible environmental conditions. The mathematical models exercised in this task will be based on (or be a modification of) the currently available models described in the referenced CNWRA/NRC colloids report.

Anticipated Effort:	H. Manaktala:	10 weeks
	R. Baca:	6 weeks

Anticipated Schedule: FY95

SOLUBILITY ESTIMATES OF KEY RADIONUCLIDES BASED ON KNOWLEDGE OF FUEL DEGRADATION AND NEAR-FIELD CHEMISTRY

Overall Task: 4-Source Term

Lead Person: H. Manaktala

Key Personnel: H. Karimi

Justification for Work:

A number of radionuclides in spent fuel have a high solubility in aqueous solutions (e.g., radioisotopes of Iodine and Americium). Many such high-solubility radionuclides also have very long half-lives and significantly contribute to the repository inventory in terms of curie content. Since such elements are soluble in aqueous solutions, they are potentially highly mobile in repository groundwaters. Calculations related to the PA of the repository require that accurate values for their solubility limit be used to assess the compliance of the repository with the regulatory requirements. The data related to high-solubility radionuclides are available in literature. However, most data were not generated specifically for the HLW repository program and considerable uncertainties about their appropriateness for use in repository PA exist. To some extent, this uncertainty arises from the influence repository variables such as temperature, radiation level, and radionuclide synergistic effects on solubility limits of specific radionuclides.

Description of Work:

The work will be based on results of earlier reviews conducted in the EBS element. Appropriate conservative temperature and other near-field parameters such as radiation level or concentration of radiolysis products in the groundwater for radionuclides with high solubilities identified in IPA Phase 2 will be taken into account. Where experimental data are unavailable, calculation or estimates of appropriate range of values will be made. The results generated in the proposed task will form bases for conducting auxiliary analyses for releases of high-solubility species from spent fuel and vitrified wasteforms in IPA Phase 3. The thrust of this task will be quantification of solubility estimates of key radionuclides.

Anticipated Effort:	H. Manaktala:	10 weeks
	H. Karimi:	2 weeks

Anticipated Schedule: FY94-FY95

VOLCANO MODULE: IMPROVED CONSEQUENCE ANALYSIS FOR VOLCANIC PROCESSES

Overall Task:	5-Disruptive Consequences
Lead Person:	C. Connor
Key Personnel:	R. Manteufel Software Expert

Justification for Work:

The IPA Phase 2 Volcano Module fails to capture many fundamental aspects of volcanism, including the probability of volcanic disruption, the area of likely disruption, and the area affected indirectly by volcanic activity, due to, for example, flow of volatile magmatic gases through the unsaturated zone. Based on IPA Phase 2 recommendations, the Volcano Module needs to be improved to better reflect geological realities.

Description of Work:

The Volcano Module can be quickly and significantly improved simply by incorporating current volcanological information about cinder cone volcanism into the model. This information includes current probability and consequence models. Specific areas that will be improved for IPA Phase 3 include the estimation of probability of disruption, the effect of volcanic degassing, and the range of explosivity of volcanic eruptions.

The Volcano Module will be improved by:

- (i) Elimination of the 12×12 km assessment zone about the repository block
- (ii) Use of nonhomogeneous Poisson and / or Markov process models to estimate probability
- (iii) Including more reasonable dike parameters, including dike sets
- (iv) Including area terms to account for the indirect effects of volcanism
- (v) Including probability distribution functions for the explosivity of volcanic events, including area affected, ash effusion rate, and ash column height

Anticipated Effort:	C. Connor:	3 weeks
	R. Manteufel:	3 weeks
	Software Expert:	8 weeks

Anticipated Schedule: FY94-95

EFFECTS OF MAGMATIC DEGASSING ON REPOSITORY PERFORMANCE

Overall Task:	5-Disruptive Consequences
Lead Person:	C. Connor
Key Personnel:	R. Manteufel W. Murphy P. Lichtner Software Expert

Justification for Work:

One recommendation resulting from IPA Phase 2 is that indirect effects of volcanism, especially the impact of magmatic degassing, on repository performance should be considered in disruptive consequence models.

Description of Work:

The purpose of this auxiliary PA project will be to fully assess the consequences of magmatic degassing on repository performance. This assessment will be done through:

(i) Development of conceptual models for cinder cone degassing and cooling, primarily through interpretation of data collected as part of the Field Volcanism Research Project

(ii) Development of heat and mass transfer models for cooling and degassing cinder cones, primarily using the VTOUGH code

(iii) Investigation of the consequences of volcanic degassing on the geochemical setting of the repository, primarily through the use of the EQ3/6 code

The result of this investigation will be a set of model parameters that can be incorporated into the volcano module that summarize this complex geologic process using probability distributions.

Anticipated effort:	C. Connor:	8 weeks
	R. Manteufel:	2 weeks
	B. Murphy:	1 weeks
	P. Lichtner:	1 weeks
	Computer Support/Student:	10 weeks

Anticipated Schedule: FY95-96

CLIMBI MODULE: INFILTRATION AT YUCCA MOUNTAIN USING EXPERT ELICITATION OF FUTURE CLIMATE

Overall Task: 5-Disruptive Consequences

Lead Person: M. Miklas, Jr.

Key Personnel: B. Gureghian
A. DeWispelare

Justification for Work:

The IPA Phase 2 activity did not attempt to evaluate future climate/infiltration but rather used an arbitrary increase in infiltration to exercise the PA code. Phase 3 should use a more realistic evaluation of reasonably likely future climate/infiltration to condition the appropriate segments of the PA. The use of expert-derived precipitation and temperature values to define likely infiltration for the next 10,000 yr should be made a part of the aspects of the performance codes that require such hydrologic information.

Description of Work:

The purpose of this effort is to develop a climate-biased infiltration model and code (CLIMBI—CLIMATE BIASED INFILTRATION) for the YM proposed repository that utilizes the future climate states developed by the expert elicitation process in IPA Phase 2.5 to generate likely future infiltration at YM. Precipitation and temperature, as predicted by the experts, will be used in conjunction with an appropriate evapotranspiration model to develop a conditioned infiltration model. The effort will provide reasonable infiltration rates for the 10,000 yr future at the site based on probabilities of occurrence and expected likelihood and duration of extreme precipitation/infiltration events.

Staff will develop a series of likely scenarios of climate change utilizing the information derived from the expert elicitation for climate recently conducted as part of IPA Phase 2.5. The climate scenarios will be further refined into an existing evapotranspiration model (to be selected), and infiltration rates for the 10,000 yr future will be generated stochastically based on current understanding of the relationship of infiltration to physical constraints (particularly evapotranspiration and runoff) at the YM proposed site and similar arid environments. The product would be a code that uses probabilities of climate change as provided by the expert panel to generate a time oriented infiltration predictor (stochastically conditioned with the expertly assigned likelihood of occurrence). The actual relationship of infiltration and climate is not well known at the YM site, however, this research effort would provide a reasonable approach to generating future states of infiltration that might occur given current knowledge of both future climate and physical constraints on infiltration. Literature would be surveyed to assist in the definition of infiltration at the site and to acquire an up-to-date infiltration model. The effects of precipitation and temperature on evapotranspiration would be discussed and documented. A letter report detailing the results of a similar infiltration analysis and the evapotranspiration/runoff evaluation would be produced. Finally, a model that provides infiltration rates for the next 10,000 yr as conditioned by probabilities of occurrence arising from the melding of the climate elicitation results and the evapotranspiration/runoff relationship to infiltration would be produced.

Anticipated Effort:	M. Miklas:	7 weeks
	B. Gureghian:	5 weeks
	A. DeWispelare:	4 weeks
Anticipated Schedule:	FY94-95	

DRILLO MODULE: IMPROVED CONSEQUENCE ANALYSIS FOR HUMAN INTRUSION

Overall Task:	5-Disruptive Consequences
Lead Person:	D. Ferrill
Key Personnel:	C. Freitas J. Russell

Justification for Work:

The Phase 2 realization of the DRILLO consequence module of the TPA code used simplified models to represent the human intrusion scenario. These simplified models, for example, used a control volume formulation in which spatially-dependent quantities were assumed constant over the control volume (i.e., a volumetric average). The current implementation uses 92 random numbers. The random numbers are used in sensitivity studies, and the large number have been found to make sensitivity studies difficult to interpret. A recommendation of IPA Phase 2 was to revise the logic of DRILLO to make more efficient use of random numbers.

Description of Work:

The objective is to update the logic of DRILLO. The update will include a review of the current implementation to reduce the number of random variables and revise/concur with the basic philosophy behind DRILLO. In particular, the treatment of probabilities, location, size, depths, etc., of boreholes will be evaluated in light of previous CNWRA work on natural resources and other literature.

Anticipated Effort:	D. Ferrill	4 weeks
	C. Freitas:	4 weeks
	J. Russell	1 week

Anticipated Schedule: FY95

TECHNICAL DESIGN OF AN UPDATED SEISMO MODULE: ANALYSIS OF DRIFT STABILITY LEADING TO ROCK-INDUCED WASTE PACKAGE FAILURE

Overall Task:	5-Disruptive Consequenes
Lead Person:	M. Ahola
Key Personnel:	T. Torng S. Hsiung

Justification for Work:

Previous work on the mechanical failure models for the waste packages focused only on the vertical borehole waste emplacement scheme as well as very simple analytical expressions for the failure of canisters, including buckling and yielding. More recently, DOE has decided to consider a more robust multi purpose cannister (MPC) for horizontal in-drift emplacement. Consequently, the mechanical loads on the canister as a result of stress-fatigue phenomena, repetitive seismicity, and thermal expansion could be fundamentally different than those of the vertical borehole emplacement scheme, and new investigation in this area is warranted.

Description of Work:

Numerical studies will be performed in FY95 to substantiate or develop simple models for the prediction of rock falls or collapse of the emplacement drifts due to thermal and repetitive seismic effects, and their impact on failure of the waste canisters. As a conservative estimate, the work will focus only on the unbackfilled emplacement drift. Through the numerical studies using 2D and/or 3D discrete element programs (e.g., UDEC) and/or finite element programs (e.g., ABAQUS), those key parameters will be identified that have the greatest impact on causing instability of the emplacement drift and subsequent waste package failure. Such parameters could include the pattern and frequency of joint sets including their strength properties, and thermal loads, as well as the amplitude, frequency, and duration of seismic events. Models will then be developed relating the key parameters to rock collapse induced failure time of the waste packages. The models developed under this proposal will input into the proposal for enhancement of the SEISMO Module led by S. Hsiung and to be conducted in FY95-96.

Anticipated Effort:	M. Ahola:	10 weeks
	T. Torng:	4 weeks
	S. Hsiung:	5 weeks

Anticipated Schedule: FY95

SEISMO MODULE: IMPROVED CONSEQUENCE ANALYSIS FOR SEISMIC PROCESSES

Overall Task: 5-Disruptive Consequences

Lead Person: S. Hsiung

Key Personnel: M. Ahola
A. Chowdhury
R. Manteufel
Computer Support

Justification for Work:

The IPA Phase 2 SEISMO Module included two potential failure modes of a vertically emplaced waste package. However, it did not include the potential effects of instability of emplacement boreholes (for vertical emplacement) or of emplacement drifts (for in-drift emplacement using MPCs) due to long-term deterioration of these excavations induced by stress-fatigue phenomenon, repetitive seismic, and thermal loads. At the time of preparing this proposal, the DOE has decided to use multi purpose canisters for in-drift emplacement. Therefore, modifying the SEISMO Module to include the new emplacement scheme is justified. Toward this end, collapse of the emplacement drifts due to repetitive seismic events is a plausible scenario that may affect the integrity of the waste packages. Based on the IPA Phase 2 recommendations, the SEISMO Module needs to be improved to enable the evaluation of the importance of seismic events to total system performance using more realistic geological information.

Description of Work:

The SEISMO Module can be enhanced by incorporating thermal and repetitive seismic effects on long-term stability of emplacement excavations (perhaps through estimation of the extent of rock falls) into the module. For a more realistic improvement to the SEISMO Module, key parameters that need to be considered should include joint patterns and strength properties; thermal loads; and amplitude, frequency, and duration of seismic events. In the IPA Phase 3, the effects of several of the above mentioned parameters will be analyzed and determined in FY94 in a separate proposal: "Technical Design of an Updated SEISMO Module:Analysis of Drift Stability Leading to Rock-Induced Waste package Failure" led by M. Ahola. In this proposed activity, the model developed in Ahola's IPA Phase 3 work will be included in FY95 in the SEISMO Module.

The SEISMO Module in IPA Phase 3 will be enhanced by:

- Including reasonable mechanical parameters of rock mass surrounding emplacement excavations
- Including some earthquake characteristics
- Adding probability distribution functions for long-term stability of emplacement excavations by considering rock mass strength and the amplitude, frequency, duration, and recurrence number of seismic events

Anticipated Effort:	S. Hsiung:	7 weeks
	M. Ahola:	5 weeks
	A. Chowdhury:	1 week
	R. Manteufel:	1 week
	Computer Support:	5 weeks
Anticipated Schedule:	FY95-96	

TECHNICAL DESIGN OF A NEW FAULT MODULE: ANALYSIS OF THE EFFECTS OF FAULTING, UPLIFT, AND SUBSIDENCE

Overall Task: 5-Disruptive Consequences

Lead Person: G. Stirewalt

Key Personnel: J. Park

Justification for Work:

Acquisition of input from geoscientists to ensure an adequate analysis of tectonic processes and events related to faulting (and also subsidence/uplift) at YM was an IPA Phase 1 recommendation that was not implemented in the IPA Phase 2 work. Based on review comments on the draft IPA Phase 2 report (NUREG 1464) by NRC geologists, it was recognized that tectonic processes and events and their possible disruptive consequences had not been given suitable treatment in the analysis of total system performance. Hence, faulting (both seismic and aseismic slip) is to be more rigorously assessed and included in IPA Phase 3 auxiliary analyses in light of potential disruptive consequences related to this tectonic process.

Description of Work:

After determining how tectonic processes and events are currently included in assessment of repository performance by the DOE, the main focus of the auxiliary analysis will be to examine the existing EPRI methodology for assessing probability of seismic and aseismic slip (i.e., earthquakes and fault displacement) at YM. This examination will be conducted with consideration for any new data on faulting at YM and the potential effects of those data on earlier published results derived from use of the EPRI methodology. It is anticipated that the auxiliary analysis will result in preliminary calculations of probability of occurrence of earthquakes (seismic slip) and fault displacement (aseismic slip) at YM and the chance to address the likelihood of different faults of variable length and displacement disrupting the repository. Results of the auxiliary analysis will be factored into technical design of the FAULT Module in FY95 for considering probability of occurrence of faulting and potential disruptive consequences of faulting on the repository.

Site-specific and regional geologic data in the CNWRA database related to characteristics and frequency of occurrence of seismic and aseismic fault slip at YM will be used in this project. In addition, subsurface geologic framework models derived in connection with Office of Nuclear Materials Safety and Safeguards (NMSS) and research activities at the CNWRA (e.g., balanced 2D structural cross-sections and 2D/3D models developed using existing software) will also be used, as required, for considering tectonic processes and events and potential effects on repository performance. Any comparisons with models developed by the DOE using LYNX or EarthVision software will be done as necessary, if not already accomplished in other activities at the CNWRA.

Anticipated Effort:	G. Stirewalt	4 weeks
	J. Park	TBD

Anticipated Schedule: FY94

FAULT MODULE: CONSEQUENCE ANALYSIS OF SEISMIC/ASEISMIC FAULT DISPLACEMENT

Overall Task: 5-Disruptive Consequences

Lead Person: G. Stirewalt

Key Personnel: J. Park
Computer Support

Justification for Work:

Tectonic processes and events related to faulting, subsidence, and uplift at YM were identified in IPA Phase 1 recommendations as fundamental topics to be considered further in defining scenario classes for assessment of repository performance. Based on review comments on the draft IPA Phase 2 document (NUREG 1464) by NRC geologists, it was recognized that tectonic processes and events and their possible disruptive consequences were not considered in IPA Phase 2 analysis of total system performance. Hence, development of a FAULT module for analyzing the probability of seismic and aseismic fault displacement is to be undertaken in IPA Phase 3 so that potentially disruptive consequences related to earthquakes and fault slip can be included in the assessment of repository performance. Consideration of both seismic and aseismic slip is important because both types of fault displacements occur in the area, Holocene slip has occurred on fault systems at YM, and the Ghost Dance fault zone cuts the repository block.

Description of Work:

The FAULT module will be comprised of an occurrence module and a consequence module. Initial efforts will focus on developing reasonable probabilities for occurrence of earthquakes (seismic slip) and fault displacement (aseismic slip) at YM. Alternative models of faulting are to be included based on the geologic framework model(s) derived from the IPA Phase 3 auxiliary analysis of faulting so that realistic fault geometries can be considered in construction of the module. The risk-based EPRI methodology, or others as deemed appropriate, may be used in development of these probabilities for what can be considered the occurrence component of the FAULT module.

As a secondary goal of this effort, time permitting and in coordination with engineering staff, the FAULT module could be developed to incorporate the ability to assess repository performance in light of potential disruptive consequences of waste package failure resulting from seismic and aseismic fault displacement. The geologic framework model(s) derived from the IPA Phase 3 auxiliary analysis of faulting would be used in developing this disruptive consequence component of the FAULT module.

Other performance issues for future consideration related to fault displacement include possible effects on groundwater flow and transport due to faulting and related fracturing and possible changes in elevation of the groundwater table due to effects from subsidence, uplift, or earthquakes. These issues would be included in the disruptive consequence component of the FAULT module in coordination with hydrology staff.

Anticipated Effort:	G. Stirewalt:	10 weeks
	J. Park:	TBD
	Computer Support:	10 weeks
Anticipated Schedule:	FY95-96	

SENSITIVITY AND UNCERTAINTY ANALYSIS OF INFILTRATION DUE TO CLIMATIC CHANGES IN A VARIABLY SATURATED GEOLOGIC MEDIUM

Overall Task:	6-Sensitivity and Uncertainty
Lead Person:	B. Gureghian
Key Personnel:	R. Codell A. DeWispelare B. Sagar

Justification for Work:

Recent findings obtained from an expert elicitation of future climate conditions in the vicinity of YM, highlighted probabilistic perturbations of several key atmospheric parameters, including precipitation, temperature, and cloud cover, for the next 10,000 yr. Alternative sensitivity and uncertainty analysis methods applied to the infiltration problem must be evaluated and compared with that using the stepwise regression analysis method, in order to gain a better insight as to the efficiency of the methods and reliability of the results.

Description of Work:

The 1D analytical model that will be developed under the subtask "Analysis of the Effects of Climate Changes on Infiltration at Yucca Mountain" led by B. Gureghian, will be used to generate the data required to perform the evaluation of alternative methods for sensitivity and uncertainty analyses. The alternative methods will include: the mean value first order second moment (MVFOSM) the first order reliability method (FORM). Both of these methods will be applied to a 1D groundwater flow model in a variably saturated and layered geologic medium, in order to estimate the uncertainty in the infiltration rate, and assess the probabilistic sensitivity of the performance measure due to changes in climatic conditions. Optimization techniques may offer efficiencies in determining these sensitivities, especially in the case of constrained performance measures (the limit state case). The expert elicitation of future climate conditions will be used in conjunction with hydrogeologic data relevant to the YM site. The deliverable of this task will be a report on the evaluation of the various sensitivity and uncertainty methods from the viewpoints of assumptions, limitations, accuracy, and efficiency.

Anticipated Effort:	B. Gureghian:	8 weeks
	R. Codell:	TBD
	A. DeWispelare:	2 weeks

Anticipated Schedule: FY95

APPLICATION OF REGRESSION MODELING TECHNIQUES FOR ACCURATE CCDF SENSITIVITY ANALYSIS

Overall Task:	6-Sensitivity and Uncertainty Analysis
Lead Person:	V. Colten-Bradley
Key Personnel:	R. Mason J. Wu

Justification for Work:

The IPA Phase 2 report identified the potential usefulness of regression models in abstracting the full TSPA model, predicting model releases, and studying the sensitivities associated with performance assessment models. However, only simple procedures were applied and implemented. The report suggests that the approach be evaluated further to determine which techniques will be most useful to the development of robust methods for evaluating system sensitivity for a probabilistic performance measure.

Description of Work:

The objective of the proposed task is to apply a global regression approach to constructing a full repository system model to provide efficient and accurate CCDF and CCDF sensitivity analysis. The results will be used to provide input variables for the proposed local Limit State (LS) approach being applied in another area of the IPA Phase 3 work.

The LS approach has been identified as a potential method for efficiently computing CCDF and CCDF sensitivity for problems associated with a reasonably small number of random variables (e.g., less than 50). The full repository system model, however, has several hundred random variables. Thus, initial screening will be necessary to reduce the number of random variables to be included in the LS analysis. The focus in this final stage will be on the (say, 15) random variables identified as important in a local important region of the CCDF. Regression modeling is to be used as the primary tool in the reduction of the number of random variables to a size that will be manageable for application of the LS approach. However, such modeling has many different facets and includes a variety of decisions. For example, consideration must be given to correct model specification, the functional form of the chosen random variables, the proper use of stepwise regression techniques, the identification of the correct variables to delete, the validity of the model assumptions, and the determination of what constitutes a correct model. The CNWRA proposes devising a regression methodology for determining the optimal subset of the available random variables. It will include the use of modern regression techniques to arrive at a correct model in circumstances where hundreds of candidate random variables are available. In essence, the CNWRA will determine the best approach for doing the exploratory work needed to arrive at the correct model for input to the LS approach.

Anticipated Effort:	V. Colten-Bradley:	TBD
	R. Mason:	10 weeks
	J. Wu:	2 weeks

Anticipated Schedule: FY94

APPLICATION OF THE LIMIT STATE APPROACH FOR EFFICIENT CCDF AND CCDF SENSITIVITY ANALYSIS

Overall Task: 6-Sensitivity and Uncertainty Analysis

Lead Person: R. Codell

Key Personnel: V. Colten-Bradley
J. Wu

Justification for Work:

The IPA Phase 2 report has identified that the LS approach (also known as Fast Probabilistic Performance Assessment) has the potential for easing the computational burden experienced in the Phase 2 study by reducing the number of vectors needed to construct the CCDFs and perform the sensitivity analysis. The report suggests that the approach be evaluated further on the full repository system model.

The report also recommends that some effort be directed at developing a robust method for evaluating system sensitivity for a probabilistic performance measure.

Description of Work:

The objective of the proposed task is to apply a global/local LS approach to a full repository system model to provide efficient and accurate CCDF and CCDF sensitivity analysis. The results based on the LS approach will be compared with other approaches already implemented in the IPA Phase 2 study.

Based on a previous study, the LS approach has been identified to be a potential method for efficiently computing CCDF and CCDF sensitivity for problems associated with a reasonably small number of random variables (e.g., less than 50). The full repository system model, however, has 200 to 300 random variables. To apply the LS approach, initial screening will be necessary to reduce the number of random variables to be included in the analysis. It is proposed that a rough LHS-based stepwise regression analysis be conducted on a global scale to identify those random variables that can be neglected and focus the analysis in a local, tail region of CCDF (i.e. the low-probability, high-consequence region) based on a smaller set of important random variables.

In addition, an adaptive importance sampling method will be used to check the LS approach at one or two selected critical CCDF levels. In this approach, the sampling space will be adaptively increased to cover the region of importance in computing a CCDF. Further, the final importance sampling points can be used to compute the sensitivity of the CCDF with respect to the expected values and the standard deviations of the input random variables. These probabilistic sensitivities are useful because many input random variable distributions in the system model are uncertain due to lack of data.

Anticipated Effort:	R. Codell:	TBD
	V. Colten-Bradley:	TBD
	J. Wu:	8 weeks

Anticipated Schedule: FY95

IDENTIFICATION OF SITE-SPECIFIC DOSE PARAMETERS FOR YUCCA MOUNTAIN

Overall Task:	7-Dose Assessment
Lead Person:	J. Hageman
Key Personnel:	P. LaPlante B. Neel

Justification for Work:

One of the goals in Phase 3 is further evaluation of appropriate dose calculations for repository PA. Dose assessment appears important in view of recent Congressional directives to the National Academy of Sciences (NAS), recent NAS meetings, and pending changes to the Environmental Protection Agency (EPA) regulations for radioactive waste disposal at YM. Assuring that the dose calculations are reasonable for the potential YM site will require further identification of the factors or parameters used to convert the amounts or concentration of radionuclides released into doses.

Description of Work:

Identify site-specific parameters used in the YM PA that impact dose calculations. Identify those parameters that may require potential adjustments or documented concurrence for continued use. Typical parameters to be examined will include:

(i) Transfer factors related to possible treatment of drinking water to remove radionuclides (should it be assumed water is taken from a surface well without any treatment, i.e., a treatment factor of one)

(ii) Where data is available, identify other site-specific factors, such as food transfer factors; the number, type, and amount of harvests per year for YM; and other parameters that may be unique to YM

Anticipated Effort:	J. Hageman:	5 weeks
	P. LaPlante:	2 weeks
	B. Neel:	TBD
	Consultant:	2 weeks

Anticipated Schedule: FY95

LITERATURE SEARCH FOR ANALOGOUS HISTORICAL RELEASE AND DOSE DATA

Overall Task: 7-Dose Assessment

Lead Person: P. LaPlante

Key Personnel: J. Hageman

Justification for Work:

One of the goals in Phase 3 is incorporation of appropriate dose calculations for repository PA. Dose assessment appears essential in view of recent and pending changes to the EPA regulations for radioactive waste disposal. While the dose assessment codes used in PA (i.e., DITTY, GENII) may incorporate commonly used methods and calculations it is important to demonstrate the applicability of these models to real life situations in which radioactive materials have been released and measurements of dispersion have been documented. While there is general knowledge of potentially relevant historical release events (e.g., Three-Mile Island incident, Chernobyl), specific knowledge of the content, availability, and form of available data and its applicability to the dose model inputs is uncertain. As a result, a limited but useful search of available sources of information would provide the necessary information to determine if there is sufficient and applicable data to support a comparison of PA dose model results with a real-world radionuclide release event.

Description of Work:

Pertinent data input needs for DITTY code will be identified and likely sources of information on known radionuclide release events will be investigated to determine if applicable release and dispersion data exist. Attention will focus on recent revelations regarding previously classified United States government experiments involving measured releases of radioactive materials, assessments of the Three Mile Island incident, and any literature characterizing local impacts of the Chernobyl incident. A letter report will be produced describing the sources investigated and whether applicable data sources were identified. The report will include a recommendation as to whether sufficient data were identified to establish a baseline for potential future work involving DITTY code output comparisons.

Anticipated Effort:	P. LaPlante:	5 weeks
	J. Hageman:	2 weeks

Anticipated Schedule: FY94-95

QUANTITATIVE EVALUATION OF DOSE ASSESSMENT MODELS IN SNL TSPA-93

Overall Task: 7-Dose Assessment

Lead Person: J. Hageman

Key Personnel: P. LaPlante
B. Neel

Justification for Work:

DOE and SNL have indicated they are including dose assessments in TSPA-93. Ensuring that the DOE dose calculations are reasonable for the potential YM site will involve a quantitative evaluation of the dose calculations.

Description of Work:

Identify and compare the input, output, and dose conversion and model parameters and calculational methods of TSPA-93 and IPA Phase 2 that are related to dose calculations. This will identify quantitative differences in such parameters as:

- (i) Organ dose weighting factors
- (ii) Dose pathways
- (iii) Individual or collective dose calculations
- (iv) Annual, committed, or cumulative dose calculations
- (v) Specified populations

A letter report will be prepared for this subtask, that will describe the differences and the potential impacts on dose calculational results.

Anticipated Effort:		
	J. Hageman:	4 weeks
	P. LaPlante:	3 weeks
	B. Neel:	TBD
	Consultant:	2 weeks
	Computer Programmer:	2 weeks

Anticipated Schedule: FY95