

## SECTION 2.3 REPOSITORY OVERVIEW

### 2.3.1 Geomechanical Analyses (SCP Section 8.3.2.1.4.1)

The objective of this work is to develop, evaluate, document, verify and validate material models, analysis methods, and computer codes for use in preclosure performance analyses of a repository. Rock mass properties for use in design activities are also developed under this work.

A series of laboratory tests was conducted over the reporting period that is designed to provide data for mechanical computer code validation efforts and to help develop laboratory testing techniques that could be used with jointed rock simulates and, in the future, jointed rock. In these tests, models of jointed rock structures were constructed and loaded mechanically. The models consisted of 1/4-in-thick, layered polycarbonate plates with a hole drilled in the center of the lay-up. The hole creates a nonuniform stress field in which local slip of the joints can occur. A Moiré technique was used to measure the slip and deformations in the model. A data reduction technique was developed, and several tests were conducted and analyzed. The tests consisted of: (1) a far-field view of loading normal to the plate, (2) a close-up view of loading normal to the plate, (3) a far-field view of loading at ten degrees to the plate, and (4) a close-up view of loading at ten degrees to the plate. For the first two experiments, the displacements around the hole were nearly symmetrical. The experiments detected joints that exhibited two to three  $\mu\text{m}$  of uniform slip. Although these experiments will be very helpful for the code validation efforts, the data reduction process for these tests is extremely time consuming. Sandia National Laboratories (SNL) will be exploring ways of either speeding up the data reduction or modifying the tests to obtain the information necessary for code validation. The report documenting the experiments is being drafted and will be ready for review near the end of September 1993.

A series of experiments designed to study the effects of a nonstandard loading condition on the mechanical properties of joints was conducted at the University of Colorado in 1992. During fiscal year (FY) 1993, the data were analyzed and reports were written to put the data in usable form. This work generated a wealth of information about joint behavior that can be used for model development and to help the design effort. Of particular interest were the data gathered on joint dilation. There appeared to be significant dilation in the tuffs tested. This behavior is not usually accounted for in the design analyses. If it were, it could result in higher safety factors (predict more stable rock masses) than previously calculated. This work will be documented in a number of reports that are in the final approval stages.

A study was conducted of the surface characteristics of natural fractures and how to relate these to the frictional data gathered on replicas on the surfaces. This study will place special emphasis on determining whether or not the fitting parameters in the Barton Model for frictional behavior have physical significance. This is being accomplished by investigating the effect on fracture shear strength and dilation with variation in three parameters: normal stress, roughness, and the strength of the rock material. This work is essentially complete, with the report to be published early in FY 1994.

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A number of thermal-mechanical analyses were conducted to support experiments planned for the Exploratory Studies Facility (ESF). These experiments include the Heated Room Experiment, the Thermal Stress test, and the Canister Scale Heater test. These analyses were conducted and designed to determine the required separation between tests so that they do not interfere with other tests. This work is essentially complete and the report documenting the results will be issued in the next few months.

A report entitled "Rock Mass Mechanical Property Estimations for the Yucca Mountain Site Characterization Project" (Lin et al., 1993) that compiled and synthesized the available data on the mechanical properties of the rock mass in Yucca Mountain was completed and issued.

An important component of this work involved the development and application of constitutive models capable of analyzing the response of jointed rock masses. State-of-the-art analysis capabilities in which the composite behavior of the intact rock and joints are modeled are represented by SNL's current continuum jointed rock constitutive models. In this reporting period, there were ongoing efforts to improve both the capabilities and efficiency of the models. This work began with a critical review of the models to identify where improvements can be made. The possible improvements include adding more joint sets, the inclusion of joint dilation, and increased model robustness. Particular attention is being paid to develop techniques that are applicable in two dimensions but can be easily extended to three dimensions. Progress was made in developing a simple three-dimensional jointed rock model in the latter part of the year; however, the bulk of the actual testing and coding of this model will take place in FY 1994.

Work at the University of Colorado in developing joint constitutive models was completed. This work began by the University conducting a literature search to identify the "best" available joint constitutive model in the literature. Experimental data developed in related efforts were fitted to Plesha's joint constitutive model. The University and SNL are disappointed that, although the Plesha joint constitutive model originally appeared to have the features that were needed, working with the model showed a number of deficiencies that the original developers were apparently unaware of. Therefore, further work with this model will not be pursued.

In other work at the University of Colorado, modifications to the discrete element code, DDA, are being performed to implement an augmented Lagrangian approach for enforcing the contact constraints and a sub-block concept. A classical Lagrangian approach to explore the sub-blocking concept in a two-dimensional research code was implemented by SNL. The classical Lagrangian approach needed to be explored in order to have a basis to compare the augmented approach. The sub-blocking concept appears to be workable, although the particular numerical implementation of it needs some refinement. The objective of this work is to develop the needed refinements and include them into a discrete block code that can be used support the design and performance assessment efforts.

Notable progress was also made in developing methods which couple finite element and boundary element techniques. This capability will be particularly useful for repository

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scale analyses. By combining the nonlinear capabilities of finite elements with the efficiency of boundary elements for modeling large linear regions (far-field), repository scale analyses become technically and economically feasible. The main idea is for finite elements to represent the near-field solution and for boundary elements to capture the far-field effects. Not only has SNL been able to couple linear finite elements with linear boundary elements (Koterakos, 1993), but in the last part of FY 1993, SNL was able to perform problems in which nonlinear finite elements were coupled to linear boundary elements. The test cases involved pressurizing a cavity in an infinite media.

Documentation for the JAC2D finite element code was essentially completed this year. JAC2D is the primary nonlinear finite element code used for the Yucca Mountain thermal-mechanical analyses.

**Forecast:** An objective of the work in FY 1994 is to evaluate the significance of rock mass creep on the stability of underground openings affiliated with the ESF and repository. The work in FY 1994 will analyze site-specific data and published information and interface with external experts to incorporate specific concerns into ESF/repository analyses and testing programs or to document that no further work is required.

Recent laboratory tests indicate that there are significant changes in the thermal expansion coefficients of rock samples that contain significant amounts of tridymite and cristobalite. This work is designed to evaluate the potential impacts of these silica phase transformations on the rock mass and repository drifts. Two- and three-dimensional thermal-mechanical analyses will be conducted to evaluate the effect of changes in the thermal expansion coefficients on the rock mass stability associated with the ESF/repository. The impacts may be reflected in the repository thermal goals or drift designs.

This activity will provide thermal and structural analysis support of planned ESF experiments. Field tests will be analyzed to develop and evaluate techniques for determining rock mass response to thermomechanical loading. The analysis methods developed here will be used in the pretest evaluation and analysis of the proposed underground experiments. The analysis results will help define the space requirements of each experiment so that the experiments do not interfere with each other.

Laboratory-scale experiments on rock joints and simulated rock masses will be performed for development, verification, and validation of ESF rock-mass design models. These ongoing tests are conducted under controlled conditions to obtain the quality of data necessary to properly validate analysis models. With laboratory-scale experiments researchers can control critical properties such as joint geometries and roughness, and to obtain higher quality full-field data.

Mechanical properties data will be consolidated and placed into the Reference Information Base so that they are readily available to all Project Participants. These data may include, but not be limited to, intact mechanical and thermal properties and estimated rock mass properties.

More general and robust continuum jointed rock models will be developed from existing models. This work will begin with two-dimensional models and extended as quickly as possible into three-dimensional models.

Coupled finite element-boundary element technology will be incorporated into production two-dimensional codes and three-dimensional work will be initiated.

### **2.3.2 Seismic Analyses (SCP Section 8.3.2.1.4.2)**

Dynamic and quasi-static seismic loading analyses of the North Ramp were performed. Of the in situ, thermal, and seismic loading components on the upper portion of the North Ramp, the seismic loading components are clearly the dominate loading. For this work, quasi-static and dynamic analyses for a 0.4g ground acceleration were conducted using a variety of codes, including JAC2D, UDEC, and DYNA3D. These analyses were used to estimate if the planned ground support would be sufficient. Although there is a potential for significant damage of the Tiva Canyon welded unit at a collapse loading of 0.67g, the 4.88 m rock bolts and fibre-reinforced shotcrete planned for support appear to be sufficient to resist the fallout rock potentially loosened by the seismic event.

**Forecast:** It is anticipated that similar analyses will be conducted for Design Packages 1B (to the Bow Ridge fault) and 2C (the remainder of the North Ramp).

### **2.3.3 Ventilation Analyses (SCP Section 8.3.2.1.4.3)**

An initial study was performed to develop and evaluate preliminary concepts and requirements for the repository underground ventilation system as a part of the repository Advanced Conceptual Design studies. The analysis used an ESF/repository design layout currently under consideration to evaluate the underground ventilation system. Emphasis was on the requirements of air-volume flow rates and concepts of ventilating air distribution.

Ventilation requirements for repository development were evaluated by considering the air flow requirements for underground personnel, dilution of diesel emission, air velocity, air cooling, and special mining operations and equipment. Preliminary results show that the air flow quantity requirement for the development of the repository is anticipated to be within the common range of the ventilation requirement for conventional underground mines.

Emplacement air quantities were investigated based on the air flow requirements for control of drift temperature during the emplacement activities, as well as other standard requirements for underground operations. Analysis of heat transfer between the waste packages and the surrounding air and rock was performed using the in-drift emplacement mode to represent the worst case scenario for control of drift temperature during the emplacement operations. It is anticipated that the forced convection in the drift will predominate the overall heat transfer process and remove most heat generated by the waste packages during the emplacement operations, if adequate ventilation is provided. Effects of



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ventilation on the air temperature in the drift were demonstrated through typical numerical calculations using the overall energy balance relation. The calculated results showed that the temperature of the operating emplacement drift can be controlled within an acceptable level for the range of thermal loadings evaluated.

Air flow requirements for retrieval of emplaced waste were also addressed. Heat transfer during the cooling period was analyzed using traditional methods for thermal fluids. The numerical results indicate that it is possible to regain access to an emplacement drift sealed for an extended time such as 50 years, by ventilating the drift with a fairly large air flow rate, for the range of thermal loadings evaluated. It is also possible to maintain the accessibility to an emplacement drift for an extended period of time by providing ventilation continuously.

**Forecast:** Engineering studies and evaluations will continue during FY 1994 to better define the subsurface ventilation system including fan, filter, and network requirements for various subsurface design options. Analytical solution of the heat transfer process from the waste packages to the rock mass will be performed for various thermal loadings and lengths and dimensions of drifts to support the repository/ESF interface design development.

### **2.3.4 Safety Analyses (SCP Section 8.3.2.1.4.4)**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

## SECTION 2.4 REPOSITORY DESIGN

### **2.4.1 Configuration of Underground Facilities (Postclosure) (SCP Section 8.3.2.2)**

#### **2.4.1.1 Design Activity 1.11.1.1 - Compile a Comprehensive List of All the Information Required From Site Characterization to Resolve This Issue**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for fiscal year (FY) 1994.

#### **2.4.1.2 Design Activity 1.11.1.2 - Determine Adequacy of Existing Site Data**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

#### **2.4.1.3 Design Activity 1.11.1.3 - Document Reference Three-Dimensional Thermal/Mechanical Stratigraphy of Yucca Mountain**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

#### **2.4.1.4 Design Activity 1.11.1.4 - Preparation of Reference Properties for the Reference Information Base**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

#### **2.4.1.5 Design Activity 1.11.2.1 - Compile Waste Package Information Needed for Repository Design**

The waste package information needed for repository design has been tentatively identified as physical dimensions, mass, handling requirements, closure method, package heat and radiation output, throughput, environment requirements. While the information needed has been identified, the information is not yet available. Work continued in this area to support systems engineering studies that are aimed at defining waste package performance allocation for various waste package emplacement modes, thermal loads, and waste package designs so that the information needs can be met.

**Forecast:** Work will continue throughout FY 1994.

#### **2.4.1.6 Design Activity 1.11.3.1 - Area Needed Determination**

Work continued in this area to understand the need for area required to accommodate different thermal loads.

**Forecast:** Work will continue throughout FY 1994.

#### **2.4.1.7 Design Activity 1.11.3.2 - Useable Area and Flexibility Evaluation**

Work in this area continued. Several areas beyond the repository block shown in the Site Characterization Plan-Conceptual Design Report (SCP-CDR) (SNL, 1987) that may be suitable for waste disposal have been preliminarily identified. The influence of faults, overburden thickness, and Exploratory Studies Facility (ESF) features is being considered.

**Forecast:** Work will continue throughout FY 1994.

#### **2.4.1.8 Design Activity 1.11.3.3 - Vertical and Horizontal Emplacement Orientation Decision**

This activity was previously expanded to include in-drift emplacement. Advanced Conceptual Design work continues toward determining the emplacement mode, which is intimately related to thermal load and waste package size and type. These have a strong influence on repository layout and waste package handling equipment. Preliminary layouts to accommodate the three emplacement modes and a variety of thermal loads were made. Some of the layouts involve a split-level repository and permit flatter gradients than in the SCP-CDR layout. The flatter gradients allow the use of rail transport as a viable option.

The emplacement mode selection will depend on a number of factors including: repository layout, thermal load, operational considerations, waste package size, worker safety, and cost. The following studies, performed during this reporting period, examined several of these factors.

A study was performed to investigate various types of equipment and shielding that may be used in the transportation of waste packages from the repository surface facilities to their final underground emplacement areas. The type and number of fuel assemblies in the canister and the type of overpack influences the ultimate size and weight of the waste package to be transported. These factors in turn affect the selection of the transport vehicle and emplacement mode that can physically be achieved using currently available technology. The waste package used in the study varied from 2-3 pressurized-water reactor assemblies and 66 cm diameter to 21 pressurized-water reactor assemblies and over 2 m diameter.

The study considered transportation equipment for use in horizontal and vertical borehole emplacement, as well as in-drift emplacement. The range of equipment investigated

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included rubber tired, crawler tractor drive and rail, powered by alternative sources involving diesel and electric schemes. Rail systems included both conventional ground mounted rails and overhead monorail configurations.

The size of the emplacement drift is a function of various factors including equipment characteristics and operating envelopes, emplacement mode, and waste package dimension. For example, smaller drift profiles can be used with rail and monorail systems, and larger profiles are necessary for the trackless haulage transporter.

Generally, diesel power provides a safe and reliable means of propulsion, but may be limited in both track and trackless application because of potential impacts to waste isolation. At this time, definitive results are not available on the effects of carbon-based residue on the transport of radionuclides through the rock medium. Alternately, electric power is available in either battery or trolley configurations, and mitigates the undesirable effects of diesel exhaust. The electric systems, however, tend to reduce flexibility of movement while providing a cleaner atmosphere.

The study concluded that transportation for all three emplacement modes can be accommodated by currently available technology.

A study was performed to initiate Advanced Conceptual Design of the subsurface repository related to operations and maintenance. Its scope was to advance the definitions of operating concepts and modes for repository systems and equipment. Included in these activities were engineering studies and evaluations of operating concepts for waste package emplacement, waste package retrieval, and backfill emplacement. Waste package dimensions and thermal outputs currently being considered impact features of the repository design and emplacement operations. The findings of the study are summarized below.

1. The large multibarrier and multipurpose canister waste package concepts impose changes to the Site Characterization Plan (SCP) (DOE, 1988c) conceptual designs. Major changes to the waste package conceptual designs that influence emplacement and retrieval modes include greatly increased waste package exterior dimensions and much higher thermal output. Vertical emplacement of these very large waste packages in boreholes may be shown to be impractical under the SCP-CDR concept. Horizontal long borehole emplacement of the large waste packages requires an opening with a cross sectional dimension approaching that of a drift. In-drift emplacement of large waste packages may have operating advantages over boreholes in accommodating the very large transport vehicles and the option of accommodating an in-drift rail system.
2. Waste package retrieval is conceptually the reverse of emplacement, however, this functional activity may follow emplacement by as much as 84 years. The ability to retrieve must be maintained in all waste package emplacement modes and operating systems. The effects of retrieval on total repository layout features, ventilation system design, backfill specifications and requirements, and the whole area of subsurface maintenance are being studied.

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3. Backfilling of the completed repository is an integral part of the total subsurface Advanced Conceptual Design effort. Design and management of the surface stockpile so that mined rock can be used as backfilling material without violation of specifications must be understood. Another concern is the fact that filled inverts of underground openings essentially become early backfilling operations. The quality of those invert fills should be in accordance with the end-product backfills at closure. Evaluation of these concerns has begun.

An Emplacement Mode System Study (CRWMS M&O, 1993f) provides an initial look at a range of potential emplacement modes associated with possible waste package designs and repository thermal loadings. This study evaluated several emplacement modes in terms of human health and safety, and repository cost. Preliminary recommendations, depending on the waste package configuration, were provided for various emplacement modes. Further work will include the effects of emplacement mode on thermal-loading-related ventilation requirements, handling requirements, costs, and postclosure performance. The Emplacement Mode System Study was submitted to the Yucca Mountain Site Characterization Project Office (YMPO) on September 30, 1993.

**Forecast:** Work will continue throughout FY 1994 and later years.

### **2.4.1.9 Design Activity 1.11.3.4 - Drainage and Moisture Control Plan**

No progress during the reporting period; this was an unfunded activity.

**Forecast:** No activity is planned for FY 1994.

### **2.4.1.10 Design Activity 1.11.3.5 - Criteria for Contingency Plan**

No progress during the reporting period; this was an unfunded activity.

**Forecast:** No activity is planned for FY 1994.

### **2.4.1.11 Design Activity 1.11.4.1 - Chemical Changes Resulting From the Use of Construction Materials**

Identification of materials to be left by ESF construction activities which could potentially impact the waste package were coordinated. This led to more detailed analyses of the amount of diesel exhaust which could be left on ESF drift walls, the amount of Tunnel Boring Machine fluids which could be left on the ESF drift floor, and the amount of conveyor belt covering which could be left in the ESF drift.

The residual diesel exhaust was determined to be potentially significant. The residual Tunnel Boring Machine fluids were determined to be likely insignificant, while the residual conveyor belt covering was determined to be definitely insignificant.

#### **2.4.1.12 Design Activity 1.11.4.2 - Material Inventory Criteria**

No progress during the reporting period; this was an unfunded activity.

**Forecast:** No activity is planned for FY 1994.

#### **2.4.1.13 Design Activity 1.11.4.3 - Water Management Criteria**

A report entitled "Estimations of the Extent of Migration of Surficially-Applied Water for Various Surface Conditions Near the Potential Repository Perimeter" (Sobolik) (ESF Performance Assessment Analysis Number 12) was approved by YMPO and sent for publication.

A report entitled "Evaluation of the Effects of Underground Water Usage and Spillage in the Exploratory Studies Facility" (Dunn and Sobolik) (ESF Performance Assessment Analysis Number 13) completed technical review. This report addresses concerns regarding underground water usage for dust control during excavation and fire fighting in the ESF North Ramp, South Ramp, and Main Test Level tunnels. This analysis evaluated the effects of large quantities of water in the tunnel on spatial and temporal variations in situ moisture content, as well as the potential amount of water that may evaporate from the rock walls due to moving air required for ventilation in the tunnels. Recommendations for inclusion in Appendix I of the Exploratory Studies Facility Design Requirements completed Sandia National Laboratories (SNL) technical and management reviews and were transmitted to YMPO. Additional calculations assuming a higher fracture permeability have been performed to assess water imbibition in the densely welded devitrified lithophysal-poor tuff, Topopah Spring Member sections of the North Ramp and Main Test Level of the ESF. The results of all of these calculations are included in Analysis Number 13; a preliminary draft of this report completed SNL technical, management, and editorial reviews in September 1993. This work is also reported under SCP Section 8.3.2.5.7, Design Activity 1.2.1.6 (Mining ventilation).

**Forecast:** Activities in support of the M&O studies of test-to-test interference and waste isolation impacts for surface-based and ESF testing will be conducted. These activities include performing performance assessment analyses, and using performance assessment analyses to make recommendations for the appropriate design documents (e.g., Exploratory Studies Facility Design Requirements). The following activities have been identified as potential requirements for the M&O for FY 1994 in support of ESF construction and testing activities and surface-based activities. They are listed in expected order of priority. Other Project Participants, such as the M&O, Lawrence Livermore National Laboratory (LLNL), and Los Alamos National Laboratory may be involved in any or all of these activities.

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1. Determine the sensitivity of the results of previous performance assessment analyses on a variety of parameters. The purpose of these activities would be to evaluate the sensitivity of the expected changes in in situ saturation, and the resulting potential impact on waste isolation. Identify, test, and compare different models for rock drying due to ventilation, particularly as it relates to fracture flow of water and fracture/matrix interaction, and the potential effects of ventilation on in situ saturation, and thus on waste isolation and site characterization. This activity is related to the current activity (Analysis Number 13) evaluating the effects of water used underground for ESF construction and testing activities. Determine the sensitivity of the results of previous performance assessment analyses on the computational and conceptual models used for the analysis. Previous hydrologic performance assessment analyses have employed the equivalent continuum approach for matrix and fracture flow, and have usually modeled flow as single phase (liquid) and isothermal. Would the effect on saturation be different if a dual porosity or discrete fracture flow model were used? Can recent laboratory results on fracture/matrix interaction be integrated into performance assessment analyses? Would they differ if multi-phase water/air flow were considered? What about the effects of heat? Determine the sensitivity of the results of previous performance assessment analyses on the assumptions made regarding heterogeneity and isotropy of hydraulic parameters. This activity was initiated in FY 1993 by SNL (ESF Analysis Number 14) by beginning a study of the sensitivity of the results of previous performance assessment analyses on the material properties used for the Paintbrush Tuff nonwelded unit. How discretely must certain stratigraphic units be divided into homogeneous media? What are the effects on the calculations of heterogeneity within each unit? This activity would require integration with soil and rock properties, statistical simulation work.
2. Evaluate the effect of a given local or global change in saturation on aqueous or gaseous flux, and on chemical transport into/out of the emplacement area. This analysis would require the integration of total systems performance assessment, waste isolation performance assessment, and other gaseous flow work.

### **2.4.1.14 Design Activity 1.11.5.1 - Excavation Methods Criteria**

No progress during the reporting period; this was an unfunded activity.

**Forecast:** No activity is planned for FY 1994.

### **2.4.1.15 Design Activity 1.11.5.2 - Long-Term Subsidence Control Strategy**

No progress during the reporting period; this was an unfunded activity.

**Forecast:** No activity is planned for FY 1994.

#### **2.4.1.16 Design Activity 1.11.6.1 - Thermal Loading for Underground Facility**

The M&O systems analysis group conducted systems studies and analyses in support of the Advanced Conceptual Design effort. Two related studies pertinent to this activity and conducted during this reporting period were: the Thermal Loading System Study and the Emplacement Mode System Study (CRWMS M&O, 1993f). The Emplacement Mode System Study progress is presented in Section 2.4.1.8 of this report.

##### Thermal Loading System Study

This study was performed with the intention of integrating the activities pertaining to the Mined Geologic Disposal System (MGDS) thermal loading decision, focusing the thermal loading activities and potentially determining what is "too hot," identifying a range of thermal loading options that are believed to meet licensing requirements, and identifying further analyses, code development, and/or testing required to reduce thermal loading issue uncertainties. A product of this study was the "Site Characterization Plan Thermal Goals Reevaluation" report (CRWMS M&O, 1993g) which was delivered to YMPO on September 22, 1993. The SCP (DOE, 1988a) developed a set of repository thermal goals which were used to estimate the "goodness" of design concepts on the basis of preliminary data and immature predictive models. These goals emphasized the SCP reference emplacement mode, a vertical borehole, and, for the most part, emphasized postclosure performance related to a thermal loading of 141 kW/ha (57 kW/acre). During the Advanced Conceptual Design phase, new emplacement modes and thermal loadings are being considered and improved performance prediction models have been developed, making it necessary to reevaluate the original SCP thermal goals. The results of this activity are reported in the SCP Thermal Goals Reevaluation report.

In support of this study, the conclusions of the Operations and Safety Team were compiled into a summary memorandum submitted to the U.S. Department of Energy (DOE) and the SCP Thermal Goals Reevaluation Working Group. In addition to researching the original intent behind established SCP thermal goals, preliminary work investigating the importance on structural predictions of recently measured changes in thermal expansion due to polymorph silica phase transformations was completed and incorporated into the reevaluation effort. The reevaluation report is currently being reviewed.

The SNL role in the development of the thermal loading systems study was to investigate a series of thermal loading scenarios with emphasis on preclosure performance. Numerous interactions with the M&O narrowed the FY 1993 focus of this effort to 17 combinations of two in-drift emplacement scenarios, three waste package designs, and five areal mass loadings. Three-dimensional, near-field calculations are currently being carried out to assess thermal environments that can be associated with these scenarios.

##### Extended Hot Evaluation

The SNL participation in the Project's evaluation of the "extended hot" concept was completed. Translations of the LLNL VTOUGH input decks used in the "extended hot"



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scenarios were provided to the Project by SNL. In addition, a preliminary assessment of addressing such issues as the importance of multiple material property designations (layering), functional property designations, and general repository layout on the prediction of host-rock thermal response was completed. Based on the work performed on this effort, SNL staff participated in a briefing to DOE on June 29, 1993, in Las Vegas, Nevada, and gave a presentation to the Nuclear Waste Technical Review Board on July 13, 1993, in Denver, Colorado.

### Total System Performance Assessment 1993

As SNL input into the Total System Performance Assessment (TSPA) 1993, four thermal loading scenarios were investigated. Specifically, the induced thermal responses for two in-drift emplacement and two vertical borehole emplacement cases were modeled using a three-dimensional analytical and two- and three-dimensional finite element models. Areal power densities of 141 kW/ha (57 kW/acre) and 282 kW/ha (114 kW/acre) were investigated for a levelized waste stream. The results of the models were reduced to designations of the number of waste packages that would be "protected" at 5 m by a 96°C isotherm, estimates of dry-out volumes, and representative waste package temperature histories. The waste package temperature histories were also provided to LLNL and the M&O's waste package design team for use as boundary conditions in determining waste form temperature histories. This information is currently being used as input into the SNL TSPA calculations.

### Non-Isothermal Flow Modeling and Experiments

Lab-scale experiments were performed to determine the effects of saturation variations on nonisothermal flow in sand enclosed within a square test cell with bottom heating. Totally saturated, half saturated, and residually saturated cases were examined for constant temperature boundary conditions at the top and bottom of the cell. Results showed that in all three cases, two counter-rotating convective cells developed in the saturated region of sand, but no bulk liquid movement was evident in the unsaturated regions. Preliminary numerical simulations using the TOUGH2 code provided consistent results with regard to flow patterns and temperature fields during simulations of the natural convection in a saturated, two-dimensional, porous media. Qualitative agreement of flow patterns between the numerical simulations and the experiment was achieved. Sensitivity analyses using TOUGH2 showed nonisothermal flow behavior to be very sensitive to boundary conditions. More rigorous experiments are planned so that boundary conditions can be monitored and stipulated in future numerical simulations. The results of the experimental and numerical modeling efforts for FY 1993 have been documented in a report entitled "Experimental and Numerical Investigations of Non-Isothermal Flow in Saturated and Partially Saturated Porous Media" (Ho et al., 1993).

**Forecast:** Further work on emplacement mode will include the effects on thermal-loading-related ventilation requirements, handling requirements, costs, and postclosure performance.

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The review process associated with the report documenting the review of current thermal design goals is expected to continue into FY 1994. Future changes to the final report and, hence, to the thermal goals is considered an evolutionary process to be made as new information becomes available. The Thermal Loading System Study report will be provided to YMPO in December 1993.

Work in the area of scenario evaluation is planned to continue in FY 1994. Evaluations will consist of thermal and thermal-mechanical simulations to establish predictions of the near-field response to various options of waste emplacement.

Documentation of the thermal loading scenarios investigated as part of TSPA 1993 will be completed early in FY 1994. In addition, sensitivity studies will be performed as necessary during FY 1994.

Experimental and numerical work in the nonisothermal area will continue in FY 1994. The primary emphasis in the FY 1994 work will be in evaluating the agreement between experimental and numerical results as well as establishing criteria for use in simplifying geostatistical simulations in a physically meaningful manner.

### **2.4.1.17 Design Activity 1.11.6.2 - Borehole Spacing Strategy**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

### **2.4.1.18 Design Activity 1.11.6.3 - Sensitivity Studies**

No progress during the reporting period; this was an unfunded activity.

**Forecast:** No activity is planned for FY 1994.

### **2.4.1.19 Design Activity 1.11.6.4 - Strategy for Containment Enhancement**

Due to the prioritization of analysis directly supporting the design of the ESF North Ramp, work in this area was discontinued in FY 1993.

**Forecast:** No activity is planned for FY 1994.

### **2.4.1.20 Design Activity 1.11.6.5 - Reference Calculations**

No information generated in this reporting period.

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### **2.4.1.21 Design Activity 1.11.7.1 - Reference Postclosure Repository Design**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

### **2.4.1.22 Design Activity 1.11.7.2 - Documentation of Compliance**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

### **2.4.2 Repository Design Criteria for Radiological Safety (SCP 8.3.2.3)**

#### **2.4.2.1 Design Activity 2.7.1.1 - Design Evaluation for Compliance with Radiological Safety Design Criteria and Performance Goals**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

### **2.4.3 Nonradiological Health and Safety (SCP Section 8.3.2.4)**

#### **2.4.3.1 Design Activity 8.3.2.4.1.1 - Design Activity to Verify Access and Drift Usability**

In February 1993, SNL was requested to provide the M&O with design analyses required to support the 90% Design Review of the North Ramp. These analyses were originally defined to support the entire North Ramp connecting the surface with the potential repository horizon. In response to this request, SNL formulated and ran three-dimensional thermal calculations for use in determining the thermally induced boundary conditions (e.g., stress) for use in two-dimensional structural models of a series of North Ramp cross-sections.

Alterations in the alignment of the North Ramp and changes in schedule due to site-specific information from the North Ramp Geologic drilling program resulted in a change in the basic repository layout that made the original thermal studies of the North Ramp no longer applicable. Because of the changes in schedule, however, this did not have a major impact other than in the area of budget. Specifically, the only package that was due in FY 1993 was that for the first 200 ft of the Starter Tunnel (Package 1A). Due to the near-surface emphasis of this package, thermal and in situ loads are negligible. Seismic analyses were completed for this design package and were transmitted to the M&O design team. A memo report, "Static Analysis of a Representative North Ramp Cross-Section in Tiva Canyon" (Shephard to Dyer, September 7, 1993), was transmitted to YMPO for approval. It

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is noted that FY 1994 calculations will require a reformulation of thermal and seismic analyses for use in supporting Design Packages 1B (to the Bow Ridge fault) and 2C (the remainder of the North Ramp connecting to the repository horizon).

**Forecast:** It is anticipated that thermal/structural/seismic analyses will be conducted in FY 1994 for North Ramp Design Packages 1B (to the Bow Ridge fault) and 2C (the remainder of the North Ramp).

### **2.4.3.2 Design Activity 8.3.2.4.1.2 - Design Activity to Verify Air Quality and Ventilation**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

### **2.4.4 Preclosure Design and Technical Feasibility (SCP Section 8.3.2.5)**

#### **2.4.4.1 Design Activity 4.4.3.1 - Operations Plan to Accompany the Advanced Conceptual Design**

An initial version of the "Mined Geologic Disposal System Systems Engineering Decision List" (CRWMS M&O, 1993h) was delivered to YMPO. This list provided a first draft of MGDS-related design decisions required to support the Yucca Mountain site characterization activities. The list was compiled from a review of the SCP and baselined technical requirements and management documents.

**Forecast:** This decision list will be used as a tool to prioritize design and analysis efforts in support of Advanced Conceptual Design and site characterization.

#### **2.4.4.2 Design Activity 4.4.3.2 - Operations Plan to Accompany the License Application Design**

No information generated in this reporting period.

#### **2.4.4.3 Design Activity 4.4.4.1 - Repository Design Requirements for License Application Design**

No information generated in this reporting period.

**SECTION 2.5 SEALS SYSTEM DESIGN**

**2.5.1 Shaft and Borehole Seals Characteristics (SCP Section 8.3.3.2)**

**2.5.1.1 Study 1.12.2.1 - Seal Material Properties Development**

Activities 1.12.2.1.1 and 1.12.2.1.2. No progress during the reporting period; these were unfunded activities.

**Forecast:** No activity is planned for fiscal year (FY) 1994.

**2.5.1.2 Design Activity 1.12.2.2 - A Degradation Model for Cementitious Materials Emplaced in a Tuffaceous Environment**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

**2.5.1.3 Study 1.12.2.3 - In Situ Testing of Seal Components**

A report entitled "Initial Seal Test Definition of Subsurface Sealing and Backfilling Tests in Unsaturated Tuff" (Fernandez et al., 1993) was published. An extended abstract was also prepared for the upcoming rock mechanics symposium. The abstract entitled "An Overview of the Yucca Mountain Site Characterization Project, Field-Test Program for Evaluating Seal Performance" (Fernandez and Case, 1993) was approved by the Yucca Mountain Site Characterization Project Office (YMPO).

**Forecast:** Field-scale tests to validate borehole sealing concepts and strategy will be initiated. Activities include conducting limited field and laboratory testing and evaluations of borehole sealing concepts. Verification of these borehole sealing concepts is vital to the continued progress of the various drilling programs at Yucca Mountain. Simple tests to evaluate the performance of suggested cementitious sealing materials along with evaluations of the adequacy of standard emplacement techniques will be performed.

**2.5.1.4 Design Activity 1.12.4.1 - Development of the Advanced Conceptual Design for Sealing**

Design Subactivity 1.12.4.1.1 - Define subsystem design requirements. A report entitled "A Strategy to Seal Exploratory Boreholes in Unsaturated Tuff" (Fernandez et al.) was completed and submitted to YMPO for review. The report describes the proposed strategy for sealing boreholes and develops a strategy for sealing boreholes based on evaluations of the current and planned borehole system, the potential impacts on performance that the borehole system could have, and the available technologies to seal boreholes.

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Sandia National Laboratories provided extensive evaluation and information to YMPO regarding the potential impacts of testing in UE-25 UZ#16 on the ability to seal the boreholes. As a result, special grout mixes are being evaluated for use in UE-25 UZ#16 that would have minimal impact on eventual sealing.

Design Subactivity 1.12.4.1.2 - Perform trade-off studies to support advanced design development. No progress during the reporting period. The emphasis in this reporting period was in support of Design Subactivity 1.12.4.1.1.

**Forecast:** "Proof-of-Concept" laboratory and in situ demonstration tests of cementitious exploratory borehole sealing systems will be defined and started. These tests will evaluate the exploratory borehole sealing design concepts defined in "A Strategy to Seal Exploratory Boreholes in Tuff" (Fernandez et al.) to be published in FY 1994.

A sealing design strategy for sealing the Exploratory Studies Facility (ESF)/repository openings will be developed for supporting the ESF design and construction process. This strategy will include design and performance analyses to address various sealing issues and requirements and will entail close cooperation with ESF design engineers using an iterative process. These ESF sealing strategies are necessary to ensure that portions of the ESF can be incorporated into the repository, if constructed.

### **2.5.1.5 Design Activity 1.12.4.2 - Development of the License Application Design for Sealing**

Design Subactivities 1.12.4.2.1 through 1.12.4.2.3. No progress during the reporting period; these were out-year activities.

**Forecast:** No activity is planned for FY 1994.

## SECTION 2.6 WASTE PACKAGE

The waste package consists of the waste form and the container in which the waste form is placed. The waste package design program includes the development of waste package design bases, design analysis, container materials testing, the development of a reference design, waste form testing, and characterization of the waste package emplacement environment. Status of the waste package program is provided in this section.

### **2.6.1 Waste Package Design (SCP Section 8.3.4.2)**

#### **2.6.1.1 Design Activity 1.10.2.1 - Concept Development**

During this reporting period, a report entitled "Waste Package Design Status Report, Fiscal Year 1993" (CRWMS M&O, 1993i) was issued. The report provides a detailed review of the analytical activities performed by the Waste Package Development staff. On October 1, 1992, Waste Package Development moved into the Advanced Conceptual Design phase of the three-phase design effort. The results presented in the status report are in support of the "Waste Package Implementation Plan," (DOE, 1992b). The evaluations and results support the goals of the waste package design process defined in the plan.

Advanced Conceptual Design is a four-year effort to provide the basis for License Application Design. During Advanced Conceptual Design a number of waste package/engineered barrier system design options are to be evaluated for applicability to the component design, performance and Mined Geologic Disposal System (MGDS) design requirements.

The "Waste Package Performance Allocation Study" (CRWMS M&O, 1993j) began the process of providing a technical basis for the design lifetime of the waste package. This study report described the regulatory background related to the issue of waste package performance allocation, provided initial estimates of the impact of waste package thickness on postdevelopment and evaluation repository costs, and related waste package thickness to preliminary estimates of corrosion time periods. The Waste Package Performance Allocation Study Report was delivered to the Yucca Mountain Site Characterization Project Office (YMPO) on September 30, 1993.

In September 1993, the "Multi-Purpose Canister (MPC) Implementation Program Conceptual Design Phase Report" (CRWMS M&O, 1993k) was completed. This report will assist the Department in making a decision on whether to proceed with further development of the multipurpose canister for the Civilian Radioactive Waste Management System.

During this period, the "Waste Package Engineering Interface Plan" (CRWMS M&O, 1993m) was also issued. The document first presents the purpose and requirements followed by a description of the waste package conceptual design and waste package performance requirements. The purpose of the plan is to outline the interface requirements between the Waste Package Design Section and other affected organizations.

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Interface Drawings and Specifications which will be derived from the Interface Plan will ensure the functional and physical compatibility of the waste package and other elements of the MGDS by documenting and controlling the design characteristics. As the waste package interfacing design features are developed and become more definitive, the Interface Drawings and Specifications will be modified to incorporate the latest interface design requirements.

Work during this reporting period, the early part of the Advanced Conceptual Design phase, was based on the ten years of data generated during preconceptual design. The scientific and engineering data gathered over the past years were the basis from which the Advanced Conceptual Design concepts were identified. The major goal for the first year of engineering evaluations was to develop a parametric data base from which specific design concepts could be evaluated in detail. The parametric evaluations performed included thermal response of the waste package and repository with respect to a number of variables including: age of spent nuclear fuel; stored energy (burnup); initial  $^{235}\text{U}$  enrichment; repository thermal mass loading (areal mass loading and areal power density); drift spacing; waste package spacing; material properties of the waste package and repository; and spent nuclear fuel receipt rate. Included in the parametric evaluation was the understanding of long-term criticality behavior. The parametric evaluations explored many different initial enrichments and configurations. The results of the evaluation were a major contributor to the understanding of long-term disposal requirements.

Calculating the analytical evaluation of the multipurpose canister was the second major effort for the waste package design staff. Waste package concepts included a waste package (or disposal overpack) for the multipurpose canister. Much of the waste package design effort has been focused on the design of the waste package/multipurpose canister and the response of the repository to the multipurpose canister. For the multipurpose canister to be economical for the waste management system, its capacity should be as high as practical. Maximizing the capacity will cause the thermal output of the device to be relatively high. The thermal output will cause the multipurpose canister to be compatible with the "hot" or "extended hot" repository thermal load scenarios, but may not be compatible with the low thermal load scenario as it is presently defined. Various loading strategies are being considered which may allow a large package to be compatible with a low thermal loading. The thermal output of a single large multipurpose canister will be high enough to ensure above-boiling conditions into the near field. The large capacity multipurpose canister is suitable for in-drift emplacement only.

In addition to the parametric thermal and criticality evaluations, a number of engineering calculations and bases were developed (i.e., the design basis spent nuclear fuel for thermal and criticality evaluations was defined; shielding requirements were developed and evaluated; internal thermal variance due to different spent nuclear fuel was explored; initial cost estimates for a range of waste package sizes were developed; material selection criteria development was initiated; fuel rod cladding performance evaluation was initiated; evaluation of structural response over time was initiated; data and information for three system studies were provided; and performance assessment was supported). The analytical topics included in the report are summarized in the activity discussions below.



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**Forecast:** Total system performance analyses relating the waste package period of containment to the overall containment performance of the geologic setting will be conducted as part of the fiscal year (FY) 1994 emplacement mode/waste package performance allocation study.

Activity 1.10.2.1.1 - Advanced Conceptual Design concepts. This section provides a description of the waste package options being evaluated during Advanced Conceptual Design. During Advanced Conceptual Design a range of concepts are being investigated, from the thin-walled small capacity pre-Advanced Conceptual Design concepts to a variety of sizes and capacity multibarrier design concepts, including different levels of radiation shielding and spent fuel capacities. Included in the concepts are metallic and nonmetallic/ceramic barrier concepts. Depending on the repository environment and operational restrictions, the options will be combined as necessary to ensure a licensable waste package.

A matrix of waste package design options has been compiled, as shown in Table 2.6-1. The purpose of this section will be to define the seven basic spent nuclear fuel and defense high level waste Advanced Conceptual Design waste package design options that will receive further evaluation.

Activity 1.10.2.1.2 - Design basis fuel. This section describes the process by which a design basis fuel is systematically selected. The goal is to provide a source term for thermal and neutronic evaluations. The selection of the design basis fuel is the key to the design of the waste package. The design basis fuel will determine the capacity (thermal output of the waste package), criticality behavior, and shielding needs. It is also understood that not all of the spent nuclear fuel can be accommodated with just one waste package design. It is logical to provide at least two basic waste package designs: one design that can accept the majority of the spent nuclear fuel, and the other to accept off-normal or failed spent nuclear fuel assemblies. This method prevents over-designing the waste package for relatively few spent nuclear fuel assemblies.

### Analysis Methodology

To determine the range of likely values for the 'enrichment' and 'burnup' parameters, statistics of the Energy Information Administration forecast data base have been tabulated: both for all 86,000 MTU expected to be discharged; and for only those discharges expected before 2003 (which will be the fuel available for pickup in the first ten years of waste acceptance). The latter is more relevant for design of the first phase multipurpose canister while the former is closer to what can be expected for the entire repository.

The statistics on criticality cannot be characterized by a single parameter, since criticality is a function of age, burnup, and initial enrichment. The situation is further complicated by the fact that burnup and initial enrichment are strongly correlated for most of the fuel. To determine parameters for criticality, a formula developed by Cerne et al. (1987) has been used. This formula gives  $k_{\infty}$  as a function of age, burnup, and initial enrichment, based upon a curve fit to a set of 210 SCALE runs which actually computed  $k_{\infty}$  for representative range of values for age, burnup, and initial enrichment. The formula developed by

Table 2.6-1. Advanced Conceptual Design Waste Package Design Concepts

Descriptions	Borehole Emplaced	Drift Emplaced	Metallic Barriers	Non-Metallic Barrier	Single Container	Multi-Barrier	Totally Shielded	Partially Shielded	Fillers	Backfill Credit	Storage/Transport/Disposal	Storage/Transport
Metallic Multibarrier		X	X			X		X	X	X		
Metallic Shielded		X	X			X	X		X	X		
Small, Metallic Multibarrier Borehole	X	X	X			X	X	X	X	X		
Nonmetallic Multibarrier	X	X	X	X		X	X	X	X	X		
Multipurpose Canister		X	X	X		X	X	X	X	X		X
Universal Cask (Multipurpose Unit)		X	X			X	X	X		X	X	
SCP-CDR (Single Container)	X		X		X				X			

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The Cerne et al. (1987) curve has a constant term, the three possible linear terms, the three squared terms, the three quadratic product terms, and an additional cubic term having the product of all three variables. Of course, it is recognized that any criticality analysis must consider the specific geometry of the fuel assembly and its environment, as represented by  $k_{eff}$ . However, it is assumed that the burnup-enrichment pairs which make up the lines of constant  $k_{\infty}$  corresponding to a specified percentile of all  $k_{\infty}$  values, will be the same burnup-enrichment pairs which would make up a constant  $k_{eff}$  line if the detailed, geometry-dependant values were calculated for all the batch points in the data base.

This formula was then applied to every batch in the Energy Information Administration data base and the resulting values of  $k_{\infty}$  were statistically tabulated. To be conservative, an age of five years was assumed for all the fuel (although it is known that over half the fuel will be older than five years by the time it can be emplaced in a repository).

### Design Basis Spent Nuclear Fuel Results

The results can best be presented as two sets of recommendations, one for the waste package, using all the fuel; and the other for the multipurpose canister in the first ten years of waste acceptance, using the fuel discharged before 2003.

By examining the statistical tabulation of all expected spent fuel, it is found that the 25 percent lines for burnup and  $k_{\infty}$  intersect at the point burnup = 49 GWd/MTU, and enrichment = 5.05 percent. This means that 75 percent of the fuel will be less stressing from both a burnup (thermal and shielding) and a criticality standpoint. Similarly, from the pre-2003 discharges, there is an intersection of the 20 percent lines at the point 42.5 GWd/MTU, 4.35 percent enrichment. (Once again, the particular value of  $k_{\infty}$  is unimportant. The only purpose of calculating it is to obtain statistics on forecast fuel according to a parameter which will be proportional to any ultimate criticality analysis.)

It is, therefore, recommended that the following design points, as illustrated in Table 2.6-2, be used.

Table 2.6-2. Design Basis Spent Nuclear Fuel

<b>Application</b>	<b>Burnup</b>	<b>Enrichment</b>	<b>SNF Covered</b>
Multipurpose Canister	42.5 GWd/MTU	4.35%	80%
Waste Package	49 GWd/MTU	5.05%	75%

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There are two problems with this single point definition of design basis fuel: (1) it might be desirable to have the primary waste package design capture/represent a larger fraction of the fuel than 75 or 80 percent; and (2) this design point would represent a very unlikely fuel assembly, having too low a burnup for this enrichment.

### Design Basis Spent Nuclear Fuel for Shielding and Thermal Evaluations

It may be useful to abandon the concept that the design basis fuel should be expressed as a combination of parameters likely to be found in the same assembly, and use instead one set of parameters for shielding/thermal and another set for criticality. From a tabulation of all spent fuel, it can be shown that a more conservative design, covering 90 percent of all fuel, would have a burnup of 55.5 GWd/MTU. Similarly, from a pre-2003 tabulation, the 90 percentile for burnup for all discharges prior to 2003 would be 45 GWd/MTU. These results are summarized in Table 2.6-3. The design point enrichments are taken at the lower end of the range of initial enrichments corresponding to these burnups because neutron flux (and hence shielding requirements) increases with decreasing enrichment, for fixed burnup since the lower initial enrichment corresponds to a higher residual Pu.

Table 2.6-3. Design Basis Spent Nuclear Fuel for Shielding/Thermal

<b>Application</b>	<b>Burnup</b>	<b>Enrichment</b>	<b>SNF Covered</b>
Multipurpose Canister	45 GWd/MTU	3.25%	90%
Waste Package	55.5 GWd/MTU	3.85%	90%

### Design Basis Spent Nuclear Fuel for Criticality Evaluations

The other half of the dual design basis fuel would be for criticality. For either waste package or multipurpose canister, one could pick any point on the 10 percent  $k_{\infty}$  line, but it would be most meaningful to pick a value of burnup such that the constant burnup line intersects the constant  $k_{\infty}$  line at the midpoint of the burnup line, so that the enrichment most represents the average enrichment for that burnup. The results are shown in Table 2.6-4.

Table 2.6-4. Design Basis Spent Nuclear Fuel for Criticality

<b>Application</b>	<b>Burnup</b>	<b>Enrichment</b>	<b>SNF Covered</b>
Multipurpose Canister	25 GWd/MTU	2.75%	90%
Waste Package	22 GWd/MTU	2.40%	90%

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The age of the spent fuel being emplaced will depend on the utility receipt rate. For any reasonable scenarios the average age will be upwards of 20 years, but as much as 50 percent could be as young as ten years. Accordingly, it would be more conservative to use a design basis fuel age of 10 years. The repository Mission Plan notes that five-year-old spent nuclear fuel will also be accepted at the repository. As part of the MGDS parametric evaluation, five-year-old spent nuclear fuel will be considered as a limit.

### **2.6.1.2 Design Activity 1.10.2.2 - Design Tools**

No information generated in this reporting period.

### **2.6.1.3 Design Activity 1.10.2.3 - Design Evaluations**

Activity 1.10.2.3.1 - Thermal. Many factors contribute to the thermal response of the waste package/engineered barrier system. Design-basis fuel characteristics and waste package capacity determine the heat produced; materials of construction, basket design (flux trap or burnup credit), emplacement mode, and tunnel diameter determine the waste package ability to expel its heat; and thermal loading of the repository determines the environment around the waste package.

The waste package/engineered barrier system thermal evaluation can be divided into two parts. The first is an analysis of the far-field repository thermal behavior, and the second is an analysis of the near-field waste package thermal behavior with boundary conditions from the repository analysis. Two finite element models were generated representing the repository and the waste package. Both systems exhibit highly time dependent behavior and must be modeled by a transient analysis unlike a spent fuel storage or transportation analysis where steady state conditions can be assumed.

Long-term thermal behavior of the repository rock is primarily a function of the areal mass loading in MTU/ha (or MTU/acre). The repository response is determined more by the integrated heat from the emplaced spent nuclear fuel and less by the initial heat of the individual waste packages. Thus, specifying an initial areal power density in kW/ha (or kW/acre) without specifying the fuel type will not determine the thermal response because the areal power density will change with time differently depending on the average fuel characteristics. For a given areal mass loading and assuming average fuel characteristics, the long-term repository thermal response is fixed and the average host rock temperatures can be determined and applied as the environment for a detailed thermal analysis of the waste package and near field.

The designs of the waste package must be sufficiently conservative to ensure that they will meet regulatory requirements when loaded. It is most efficient to design to the most stressing values of the parameters (age, burnup, and enrichment) which are likely to be encountered when loading the waste package. The most stressing parameter values are used to characterize the design basis fuel. The relevant regulatory requirements can be efficiently

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satisfied by designing shielding, package size, and neutron absorber material to accommodate the set of design basis fuel types. The relatively few assemblies having more stressing parameter values may be handled by de-rating the standard package and/or by designing and utilizing a more conservative (and, consequently more expensive) waste package. The design basis is currently expressed in terms of pressurized-water reactor fuel, since it is the more stressing with respect to age, burnup, and initial enrichment.

Several different waste package capacities have been evaluated, but recent interest has centered on the large multibarrier drift emplaced waste package with capacities up to 21 pressurized-water reactor assemblies or 40 boiling water reactor assemblies, (pressurized-water reactor assemblies are considered limiting because of their higher decay heat output compared to boiling water reactor assemblies). Higher capacity waste packages are more likely to exceed thermal goals than smaller ones in the same repository thermal environment. The choice of a design basis fuel is important because it will directly limit the number of assemblies that can be loaded and still meet thermal goals. The limiting thermal goal for large waste packages is 350°C at the spent nuclear fuel cladding. For the multipurpose canister conceptual design basis fuel characteristics of ten years aged with 40 GWd/MTU burnup, the 21 pressurized-water reactor capacity is considered at or above the maximum allowable temperature for a metallic multibarrier waste package such as the multipurpose canister with disposal container.

All these factors affect the timing of peak temperatures as well as the magnitude. Host rock temperatures will peak between 20 to 500 years depending on the thermal loading but peak rock temperature will be largely independent of the individual waste package design. The waste package will experience its peak temperature between initial emplacement and the repository peak depending on the design basis fuel and the basket/container design. For the large waste package, higher conductivity spent nuclear fuel baskets will lower and delay the peak temperatures experienced. The choice of the design basis fuel is of key importance to the timing of peak temperatures. Younger fuel types produce high peak temperatures within the first few years which then drop off quickly. Older fuel (at the same areal power density) produces lower temperatures and later peaks with more stable and higher long-term temperatures.

Although the parameters of a "cold repository" have not been defined, the large waste package most likely will preclude such a scenario because of the localized high temperatures immediately surrounding the 21 pressurized-water reactor capacity waste package. Preliminary analyses show that even at low thermal loads such as 87 kW/ha (35 kW/acre), near-field temperatures can exceed the boiling point. In any case, it would not be possible to emplace 63,000 MTU of spent nuclear fuel in Yucca Mountain without introducing significant thermal perturbations in the host rock.

Activity 1.10.2.3.2 - Structural. This section presents the structural evaluations that have been performed in the first year of Advanced Conceptual Design. Thermal and neutron concerns dominated the effort; only limited structural evaluations were performed. One of the concerns for drift emplacement is the size and weight of a rock that would breach the waste package. For a waste package with about a 12 cm wall thickness, a structural evaluation

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indicated that a 1.2-m-diameter rock weighing 2.26 metric tons falling from the ceiling would plastically deform the waste package but not fail it. Next fiscal year a plastic deformation evaluation will be performed to define the failure point. Additional evaluations will be performed for each waste package design concept—end load, slap down, lifting loads, and drop test—to note a few.

Activity 1.10.2.3.3 - Criticality. A number of important results were gathered during this reporting period. The criticality safety evaluations confirmed the viability of the high capacity burnup credit designs. In the area of long-term criticality safety for a waste package in the MGDS, two important points were found. The first point is that the criticality potential of spent nuclear fuel initially decreases (100 to 200 years) but then increases to a local maximum (10,000 to 20,000 years) before decreasing again. Waste packages must be designed for this increase in criticality potential.

The second important point investigated during the criticality safety evaluations is that neutron absorber materials will be partially depleted over the long time periods. To maintain criticality control in a disposal waste package, extra neutron absorber material must be included initially to control criticality in the out years. This may require the use of  $^{10}\text{B}$  enriched boron, an expensive material, in the current waste package designs. Up to an additional 25 percent of  $^{10}\text{B}$  is recommended for final disposal to compensate for the depletion process.

Two concepts were evaluated for radiation shielding in the MGDS, the 'shielding outer barrier' and the 'shielded waste package emplacement transporter.' The evaluation demonstrated that the reusable shielded waste package emplacement transporter is more efficient and cost effective than a shielding outer barrier for each waste package.

Other calculations and evaluations are needed, such as validation of criticality and shielding models against other codes. Evaluations needed include the amount of water in the waste package necessary for criticality, the effect of varying axial burnups, mixing of spent nuclear fuel assemblies with different spent nuclear fuel characteristics in a waste package, the depletion of the materials in the fuel over the long time period, and the total reevaluation of the new waste package design with the new criticality design-basis spent nuclear fuel characteristics.

Detailed two- or three-dimensional evaluations of each waste package design are required as well as evaluations of neutron activation of the waste package components and engineered barriers in the MGDS by the subcritical neutron flux over the time of operation. The neutron activation of Co impurities found in the stainless steel of the new baseline design is especially important due to the high strength gamma dose from the activated  $^{60}\text{Co}$ . An evaluation of the new multipurpose canister waste package design (or disposal overpack) for the multipurpose canister is also needed.

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Activity 1.10.2.3.4 - Cost Estimation. This section describes an initial cost estimate of the multipurpose canister and large multibarrier waste package. The cost estimate takes into consideration the 1989 total life cycle cost estimate and expands to include additional cost and fabrication methods for larger containers.

Estimated costs for selected multipurpose disposal overpack and waste packages are presented in Table 2.6-5. The design cases which consider fuel burnup credit allowance are indicated by the footnotes. Taking a fuel burnup credit allowance results in a less bulky spent nuclear fuel basket design, reducing size and weight of the basket and concurrently reducing size and weight of the multipurpose canister overpack or waste package as well. On the basis of burnup credit, the 21 pressurized-water reactor cases in Table 2.6-5 are generally comparable, whereas the 12 pressurized-water reactor cases are less so. However, note that at present the multipurpose canister design and the waste package design do not have common spent nuclear fuel basket designs and sizes, which result in the multipurpose canister and waste package having slightly different inside diameters. Multipurpose canister disposal overpack and waste package costs are presently based on a single vendor budgetary estimate.

The baseline multipurpose canister material is 316L stainless steel, whereas Alloy 825 is considered an alternate material. Should the multipurpose canister be made of Alloy 825, the multipurpose canister would then qualify as the inner corrosion barrier, and the multipurpose canister overpack would be reduced to a single layer of carbon steel. The cost of materials places Alloy 825 at nearly three times the cost of 316L (\$9.37/kg versus \$3.20/kg, or \$4.25/lb versus \$1.45/lb). Whether made of stainless steel or Alloy 825, the multipurpose canister wall thickness would be essentially the same in either case because the thickness is driven by container stresses in the fully loaded condition.

### **2.6.1.4 Design Activity 1.10.2.4 - Material Selection Design Support**

This section presents the method by which materials will be selected in support of the waste package/engineered barrier system. The selection process is a systematic approach based on component functions, performance and design requirements. The process is equally adapted to the multipurpose canister as well as the design concepts that include overpacks. Multipurpose canisters, which are relatively thin-walled containers, may be a part of an onsite dry storage device, then loaded into a transportation overpack and shipped to the MGDS. While the engineering evaluations of this design concept will include structural, thermal, shielding and nuclear criticality studies, this section will be concerned with the selection of materials for different components of the multipurpose canister.

Activity 1.10.2.4.1 - Materials selection process. The materials selection process, illustrated in Figure 2.6-1, includes the following items.

1. Definition of component functions, performance/design requirements and environments.



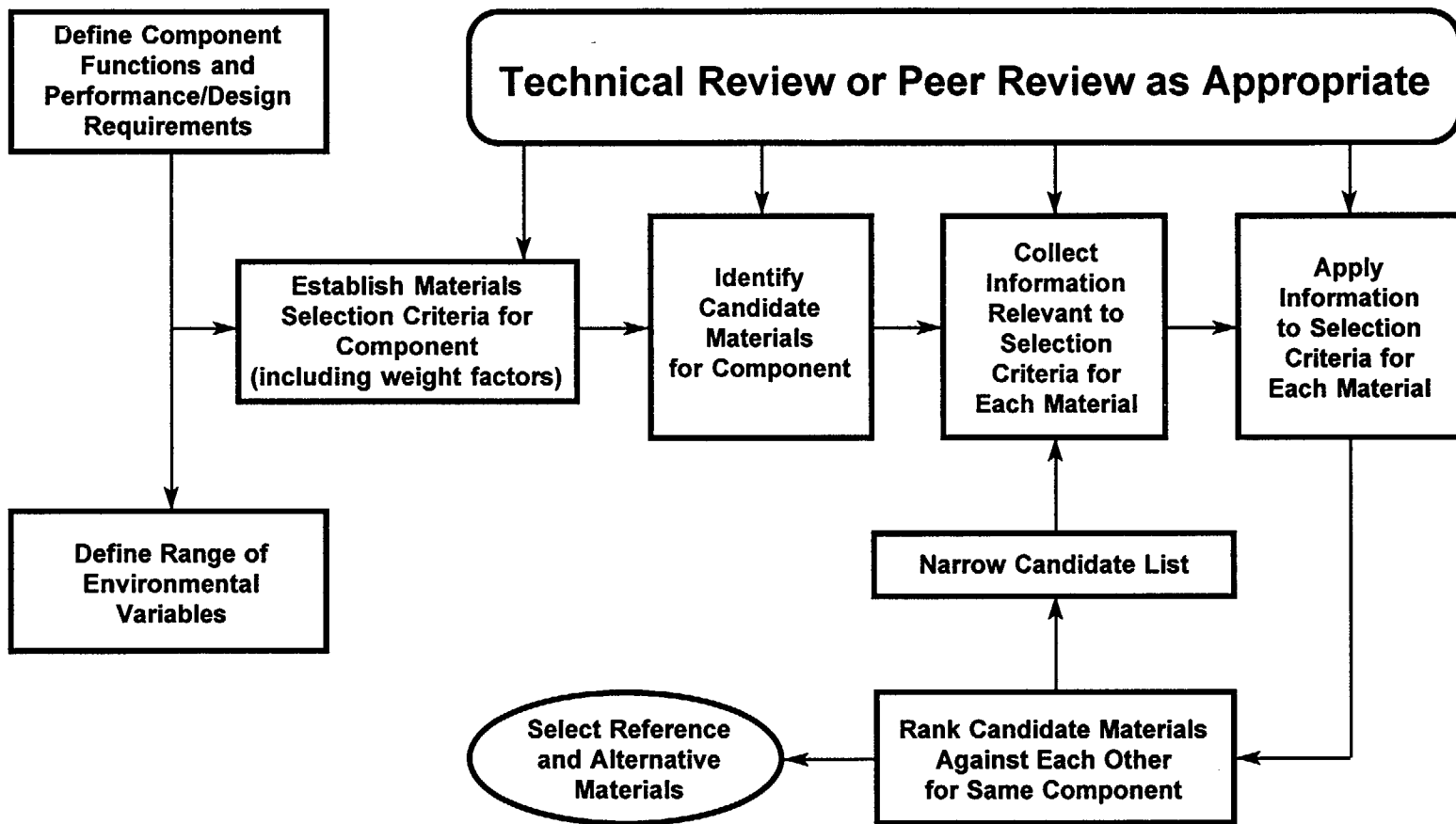
Table 2.6-5. Multipurpose Canister Implementation Study Waste Package Cost Estimate Comparison

Costs based on 1993 material costs

First Barrier (cm) = 0.95 Alloy 825  
 Second Barrier (cm) = 10 Carbon Steel

Type	Number of PWRs	Number of BWRs	Inside Diameter (cm)	Internal Support PWR (kg)	First Barrier (kg)	Second Barrier (kg)	Estimated Cost
Multi-Barrier Waste Package, SNF (note 1)	21	40	152.09	9540	2104	24537	\$367,835
Multi-Barrier Waste Package, SNF (note 1)	12	21	117.52	5900	1562	18849	\$247,098
Multi-Barrier Waste Package, DHLW (4)	--	--	156.04	790	1562	18582	\$ 111,009
MPC Overpack, Multi-Layer (note 1)	21	--	154.4/157.5	--	2260	26216	\$151,590
MPC Overpack, Single Layer (note 1)	21	--	154.4	--	0	25463	\$ 82,755
MPC Overpack, Multi-Layer (note 2)	12	--	127.3/130.4	--	1802	21429	\$122,578
MPC Overpack, Single Layer (note 2)	12	--	127.3	--	0	20729	\$ 67,369

Note 1: With burnup credit allowance  
 Note 2: No burnup credit allowance



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Figure 2.6-1. Waste Package Materials Selection Process

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2. Selection criteria and weighting factors.
3. Identification of candidate materials.
4. Collection of information/data.
5. Application of selection criteria and ranking.

The initial step in selecting a material for a waste package component is to define the functions required of that component. Specific functions will be assigned to each individual component of the waste package based on the need to satisfy federal as well as other regulatory requirements. For each identified component function, performance measures and quantitative performance requirements will be identified. Quantification will be achieved through use of models to be developed to predict each performance measure. Furthermore, the expected environmental conditions (including parameters and ranges) surrounding each component will be identified and defined as a function of service time.

Selection criteria are determined based on the performance and design requirements for each component. The selection criteria can typically be classified into two major categories: (1) those related to the performance of the candidate material in the anticipated repository environment; and (2) nonperformance-related aspects dealing with cost, engineering experience, and practical considerations of fabrication, closure, and material availability. Each selection criterion may consist of several topical areas such as mechanical and chemical performance, performance predictability, and compatibility with other materials, etc. Weighting factors will be assigned to the selection criteria so that eventually an overall score or figure of merit can be determined for each candidate material. Since there exists no universally accepted way of balancing the selection criteria against each other, the assignment of these weighting factors will be unique to each component and will require the application of engineering judgment.

The identification of candidate materials for a specific component will be based on a literature review of the anticipated degradation modes that may occur under the expected environmental conditions, information relevant to each selection criterion, and the results of preliminary tests. These preliminary tests will be focused on evaluating the selection criteria-related corrosion and mechanical properties of potential materials. Engineering judgment will be used to identify materials that have the desired properties and generally favorable attributes relative to the selection criteria.

Data and information will be developed to allow an assessment of how well the candidate materials will satisfy the selection criteria. Pertinent information related to the cost, engineering experience and fabricability of each identified material will be collected. Other information relevant to performance selection criteria will be generated, as appropriate. These collected data/information will eventually be applied in selecting material for each component.

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A quantitative rating will be given to each candidate material for each selection criterion. This rating will be based on the gathered information/data in both performance-related and nonperformance-related categories. The weighting factor for each criterion will be multiplied by these ratings and the results summed for each material to establish an overall material rating. These quantitative ratings will then be used to rank the candidate materials for each component. The information gathering and testing will be continued on fewer materials followed by reapplication of selection criteria and rating/ranking to provide sufficient basis for final materials selection near the beginning of the License Application Design.

Activity 1.10.2.4.2 - Container shell. The disposal waste package (or disposal overpack for the multipurpose canister) will contain a set of spent nuclear fuel assemblies inside a shell. These containers are to be designed to contain the radionuclides, and to provide contamination control from the possible reactor service crud build-up on some spent nuclear fuel assemblies. Furthermore, the shell will be designed to provide thermal coupling between the spent nuclear fuel basket and waste package overpack and will have to withstand a normal operating temperature of  $<350^{\circ}\text{C}$  for a prolonged containment period.

Since the primary function of the shell is to contain the radionuclides, the metallic material to be used for the shell should be highly corrosion resistant. The fact that the potential repository will be located in an unsaturated zone suggests that the oxidation will probably be the dominant degradation mode of the shell. However, it seems prudent to allow for the possibility that the shell may be in contact with some bulk water for some period of time. Under this condition, the shell would be subjected to various modes of corrosion damage such as general corrosion, crevice corrosion, pitting attack, stress corrosion cracking, and other forms of environment-induced embrittlement. Thus, the selected material for the shell should possess sufficient resistance to these types of degradation modes.

From a design point of view, the shell material should be compatible with the spent nuclear fuel basket and disposal overpack. In addition, it should be capable of withstanding normal and off-normal handling loads. Deformation and failure of the shell may occur differently depending on the candidate material, and its processing and fabrication history. The fabrication process and the welding or other closure process may have a significant influence on the mechanical and microstructural properties that can influence the performance of the shell. The selected material should also possess high thermal conductivity so as to transmit heat away from the spent nuclear fuel.

In view of the above-mentioned functions, and the desired performance and design requirements of the shell, Alloy 825 has been recommended as the primary shell material. Alloy 825, which is a high-nickel austenitic alloy, is readily formable and weldable; reasonably priced for a sufficiently corrosion resistant material; and exhibits superior resistance to both general and localized corrosion compared to other ASME boiler and pressure vessel code materials. Titanium Grade 12 and Hastelloy C-4, which are also very corrosion resistant, have been recommended as back-up materials for the shell. However, the Titanium Grade 12 requires a greater degree of care in fabrication/welding, and the Hastelloy C-4 is more expensive than the Alloy 825.

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Activity 1.10.2.4.3 - Shield plug. The function of this component is to reduce the radiation dose so that the radiation workers can install the remote multipurpose canister lid closure device, namely the automatic welding apparatus. Thus, the plug material should be effective in shielding both the gamma and neutron radiations. From a design perspective, the plug material should be capable of withstanding normal and accident temperatures of up to 350°C for an extended time period, in hundreds of years. Furthermore, it has to be compatible with the spent nuclear fuel basket material and the outer shell.

Since the shield plug has no specific function relative to the waste package postclosure performance, degradation of this component during service is only a concern should retrieval of the spent fuel become necessary. Therefore, some degree of corrosion protection during the preclosure period may be desirable. This can be accomplished by using either stainless steel sheathing or a nickel plating. Since corrosion protection is unnecessary, either an unprotected iron based material or depleted uranium can be used as secondary materials for the multipurpose canister shield plug.

Activity 1.10.2.4.4 - Spent nuclear fuel basket (structural). The function of the basket is to provide structural separation of the spent nuclear fuel assemblies and to ensure that they remain in their original positions without interference as emplaced. The basket material is designed to withstand sufficient transportation loads (i.e., 9-m drop), and to withstand normal and accident temperatures of up to 350°C for a prolonged duration upon emplacement. Thus, the basket material should maintain structural integrity, and be capable of conducting heat away from the waste. In addition, it should be compatible with the basket criticality material and waste form.

In view of the above functional and design requirements, the basket material should possess sufficient strength and toughness, high thermal conductivity, superior fabricability/weldability, and excellent corrosion resistance. The fabrication process and the closure technique may exert a significant influence on the mechanical, microstructural and corrosion properties of this component. These requirements can most effectively be accomplished by using a corrosion resistant, American Society of Mechanical Engineers boiler and pressure vessel code material. The relatively corrosion resistant 316L stainless steel has been recommended as a primary choice due to its lower cost and satisfactory resistance to both general and localized corrosion.

Activity 1.10.2.4.5 - Spent nuclear fuel basket (criticality). The function of the criticality control component of the basket is to provide neutron absorption for a prolonged time period. Thus, the basket material should contain sufficient quantities of neutron absorbing element. This material should possess high strength, high toughness, and high thermal conductivity to enhance heat transfer from the spent fuel. In addition, the basket material should maintain its microstructural stability at temperatures of up to 350°C while in contact with the spent nuclear fuel assemblies.

It is necessary that the criticality control material remain intact for as long as possible, particularly after containment barriers breach. The addition of boron, a neutron absorber, to a relatively corrosion resistant material such as austenitic stainless steel can accomplish this

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goal. Therefore, the use of borated stainless steel has been recommended for the criticality control component of the spent nuclear fuel basket. The borated aluminum alloy has been identified as a secondary choice of material. However, aluminum alloys are susceptible to pitting corrosion and the possibility of galvanic corrosion due to its contact with the structural component material of the spent nuclear fuel basket.

Activity 1.10.2.4.6 - Filler material. A filler material may be required to provide enhanced heat transfer, criticality control, and chemical buffering for radionuclides. The material under consideration is a size graded iron shot. This material is designed to fill a substantial part of the space in and around the spent nuclear fuel assemblies to aid in transferring heat from the fuel rods. In addition, the use of filler material will eliminate the need for assuming complete water flooding in criticality calculations, and will provide chemical buffering of any water that may enter the waste package.

Activity 1.10.2.4.7 - Fill gas. The function of the fill gas is to provide an inert internal environment, thus minimizing the tendency for corrosion-related damage of internal components of the waste package prior to breach of the shell. Furthermore, it should act as a short-term thermal conductivity enhancer, and be compatible with construction materials for different components of the waste package. The primary choice of fill gas has been argon since it does not diffuse through the metallic containment barriers, is inert and inexpensive, and will not react in a moisture-containing gamma field to form deleterious radiolysis products. Helium has been identified as a secondary choice since it also exhibits the positive attributes of argon but does have the potential for diffusion through the shell wall over a period of time.

### 2.6.1.5 Design Activity 1.10.2.5 - Performance Evaluations

This section includes the progress made during the reporting period on performance of the container and the spent fuel waste form.

Activity 1.10.2.5.1 - Container oxidation and corrosion. Dry oxidation and aqueous corrosion of the outer corrosion-allowance containers were evaluated.

Dry oxidation data for iron-based materials in the 100° - 250°C range are almost nonexistent. Most of the data on dry oxidation are from atmospheric exposures over long periods in various environments including rural, semi-industrial, industrial, and marine. Data are available for many materials exposed for up to 20 years. The data, with the exception of those for marine environments, tend to fit an exponential equation with corrosion rates decreasing with time, suggesting the establishment of a protective film. (The chloride present in the mist in marine environments tends to inhibit the formation of protective films.) The time exponent usually falls between 0.3 and 0.6. Previously, this time effect was neglected in that a constant oxidation rate (20 µm/year) was provided. From the environmental data given in the American Society for Materials Handbook for carbon steels, an exponent of 0.57 was obtained. This would yield an expression for penetration,  $P = 1.156 t^{0.57}$ , where  $t$  is in days. Thus, the penetration for one year is 33 µm, for two years it is 50 µm, and for ten years it is

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124  $\mu\text{m}$ , which agrees with the data. The average penetration rates are then 33, 25 and 12  $\mu\text{m}/\text{year}$ , for one, two and ten years, respectively. The variation is on the order of  $\pm 25$  percent.

The American Society for Materials Handbook provides one set of data at elevated temperature, 454°C (850°F) and 538°C (1000°F), for air oxidation of carbon steels for about one year. (Similar data also are provided for a steam atmosphere.) The time exponent was about 0.3, suggesting that a more tenacious oxide film is developing at the higher temperatures than at the ambient temperatures discussed above. The penetration equations from the data provided are  $P = 2.01 t^{0.33}$  for 454°C and  $P = 5.35 t^{0.33}$  for 538°C. For one year, the penetrations would be 14 and 38  $\mu\text{m}$ , respectively.

If the same process can be extrapolated to lower temperatures, then the penetration equation would follow the same form with the same exponent, but with a different coefficient. The coefficient can be estimated by using an Arrhenius approach (where the temperature effect is proportional to  $e^{-Q/RT}$ ) by plotting the data vs  $1/T$ , where  $T$  is the absolute temperature, ( $Q$  is the activation energy, and  $R$  is the gas constant). The coefficients for 300°C and 200°C are 0.2 and 0.02, respectively. The activation energy for this process, which is presumably due to diffusion of oxygen through the oxide film, was calculated to be 57.1 kJ/mol. This compares favorably to data provided in a review by R. Freer, which gives the activation energy for the diffusion of oxygen in FeO as 83.6 kJ/mol and in  $\text{Fe}_3\text{O}_4$  as 71 kJ/mol. The value of  $Q$  (57.1 kJ/mol), when divided by  $R$ , which is 8.3143 J/K-mol, yields a value of  $Q/R$  of 6870. Thus, the entire equation for penetration (in  $\mu\text{m}$ ) can now be written as  $P = 25,500 t^{0.33} e^{-6870/T}$ . If an expression for penetration is needed in years, the equation becomes  $P = 178,700 t(y)^{0.33} e^{-6870/T}$ .

This approach provides much smaller penetration values for temperatures in the range of repository interest. For example, the penetration at 200°C would be 0.09, 0.19, 0.40, 0.86, and 1.84  $\mu\text{m}$ , after 1, 10, 100, 1000, and 10,000 years, respectively. The error is likely to be larger because of the method of extrapolation. However, even at 100 percent error, these values are very low, which would make degradation by dry oxidation negligible.

The available data for corrosion of carbon steels in aqueous environments were also reviewed. Most of the data are for flowing river waters. These data follow a time dependency with an exponent ranging from 0.5 to 0.8. One set of data relate to static exposure in Gatun Lake for up to 16 years. This set of data was used by Westinghouse as their basis for design of waste packages in tuff. The time dependency was found to have an exponent of 0.47. From these data an equation was generated for penetration,  $P = 200 t(y)^{0.47}$ , with  $P$  in  $\mu\text{m}$ .

The Westinghouse (1982) report also estimates the effect of temperature using a very limited data set for corrosion rate of cast steel and iron in brine and seawater. A value was found of  $Q/R$  of 2850k. From a very sparse data set in a report by S. Pednekar (1987), a value of  $Q/R$  of 2300k was calculated. Thus the temperature effect from Westinghouse may represent conditions adequately for carbon steels in static waters. This report provides a combined penetration equation,  $P = 2,525 t^{0.47} e^{-2850/T}$ , where  $P$  is the penetration in mm,  $t$  is

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the time in years, and T is the temperature in degrees Kelvin. They estimated an error band of about +/- 25 percent. The penetration at 100°C would be 1.2, 3.6, 10.6, 31.2, and 92.0 mm for 1, 10, 100, 1000, and 10,000 years, respectively. The corrosion rate for these periods would then be 1.2, 0.36, 0.11, 0.03, and 0.01 mm/year (or 48, 14.4, 4.4, 1.2, and 0.37 mils/year). The calculated penetrations at 50°C would be 30 percent of those calculated at 100°C. The Westinghouse report also evaluates a pitting factor which is the ratio of pitting attack to general corrosion. The Gatun Lake data set yields a range from 2.6-3.4. (They then use a value of 4.0 for conservatism.) This is roughly consistent with values obtained for pitting factor by D. McCright of about 0.9-3.2. The pitting factor would be used as a multiple of the penetrations calculated using the above equation.

The recommended penetration equations can then be summarized as follows:

$$\text{For high-temperature oxidation, } P = 178 t^{0.33} e^{-6870/T}.$$

$$\text{For general corrosion, } P = 2,525 t^{0.47} e^{-2850/T}.$$

$$\text{For general corrosion with a pitting factor, } P = 10,100 t^{0.47} e^{-2850/T}.$$

Activity 1.10.2.5.2 - Waste package degradation by mechanical stress. Waste packages, especially degraded ones, may be damaged or breached by mechanical stresses. To guide future calculations, we have assessed possible sources of mechanical stress and their effects on waste packages.

Five sources of mechanical stress are considered:

1. A fault that intersects a waste package may slip and shear the package.
2. An earthquake or underground nuclear event may cause ground shaking, imposing acceleration loads on the package.
3. A large rock may fall on the package.
4. Lithostatic pressure may collapse the package.
5. Products of corrosion, which are larger than the original metal, may press against the backfill, imposing compressive forces on the package.

Analysis of these sources shows that the most important is forces due to products of corrosion. Fault shear and ground shaking are dismissed as being unlikely to cause failure because of their relatively small displacements and accelerations. Rock fall for a drift without backfill is being evaluated by the Waste Package Design group; it is thought to be unimportant for a backfilled drift because of the protection provided by the backfill. Lithostatic forces are smaller than those due to products of corrosion.



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It has been found that the robust containers currently under consideration must be seriously degraded before mechanical stress can cause failure. Buckling of the side of a container is predicted to occur at a wall thickness of 11.4 to 5.3 mm, depending on the effectiveness of the basket as a stiffener. The ends of the container will not buckle but must sustain tensile stresses of up to 153 to 710 MPa. If the container thins uniformly as a result of general corrosion, the ends of the container will probably fail before the side unless additional thickness is provided there.

Current designs for a metallic multibarrier waste package call for at least 9.5 mm of corrosion resistant material. This material alone has roughly enough thickness to sustain the expected mechanical stresses. Since this layer is expected to fail by localized and not general corrosion, failure as a direct result of mechanical stress will not significantly reduce the life of a waste package.

### Fault Shear

Fault shear could severely damage a waste package. In a report entitled "Preliminary Near-Field Environment Report, Volume I: Technical Bases for EBS Design" (Wilder, 1993a), Wilder suggests such damage can be avoided by not placing waste packages in a fault zone. Damage by fault shear will thus occur only if waste packages are placed on an unrecognized fault. Even if this should happen, the waste packages are not in immediate danger. According to Wilder, the design basis underground nuclear explosion or earthquake allows for displacements of up to 50 mm horizontally and 20 mm vertically. These displacements are small enough that even borehole-emplaced packages would not be sheared by a single event. Drift emplacement provides large clearances around a waste package and thus allow large displacements. The most important fault in the vicinity of Yucca Mountain (as defined by Wilder), the Bare Mountain fault, has a slip rate of only 0.15 mm/year, so shearing of a drift emplaced waste package would take a long time.

### Ground Shaking

Ground shaking is not expected to be intense enough to damage an undegraded waste package. The design basis earthquake has a vertical acceleration of 0.2g and an acceleration of 0.1g in each horizontal direction. These accelerations are smaller than those expected from handling incidents such as tipping. Shaking of a badly degraded package may produce damage, but dynamic calculations are necessary.

### Rock Fall

The importance of falling rocks depends on whether the emplacement drift has been backfilled. Backfill will protect the waste packages by only allowing rocks to fall a short distance, distributing force, and absorbing energy. These effects greatly reduce the effects of falling rocks. Rock falls onto unprotected waste packages are under study by the Waste Package Design group. However, little degradation is expected before the drifts are backfilled, and the robust waste packages under consideration should be able to survive large rock falls without damage.

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### Lithostatic Force

Lithostatic forces will be present only after the drift is backfilled. Tuff shows no tendency to creep under expected repository conditions (Wilder, 1993a), so the lithostatic pressure will be due only to the backfill and any fallen rock. However, the lithostatic pressure will be smaller than the pressure from products of corrosion, so we may consider only the latter.

### Forces Due to Products of Corrosion

Several of the proposed designs for waste packages include a thick disposal container of carbon steel or cast iron. These materials expand significantly upon oxidation; oxidizing iron to  $\text{Fe}_2\text{O}_3$  produces a 114 percent increase in volume. Some volume increase can be accommodated if the products of corrosion move into the interstices in the backfill. Especially for fine or densely packed backfill, however, the available volume is small and the backfill must be displaced.

The stress state in the backfill at the surface of the container may be approximated by a hydrostatic stress from the backfill plus a uniaxial compressive stress from the products of corrosion:  $\sigma_{xx} = \sigma_{yy} = p_3$ ,  $\sigma_{zz} = p_1$ ,  $p_1 > p_3$ , where the  $x$  and  $y$  directions are parallel to the surface of the waste package and the  $z$  direction is normal to the surface. All off-diagonal components are zero. The stress state is equivalent to that used in standard triaxial tests of the strength of soil, in which  $p_3$  is the confining or all-around pressure and  $p_1$  is the vertical pressure. In dry sand or gravel, shear failure occurs when

$$\frac{p_1}{p_3} = \frac{1 + \sin\phi}{1 - \sin\phi} \quad (2.6.1.5-1)$$

A value of  $\phi = 35^\circ$ , which is appropriate for a sandy gravel (Peck, 1974) was used. The confining pressure will be the lithostatic pressure, which is approximately  $h\rho fg$ , where  $h$  is the height of the overlying layer,  $\rho$  is the density of pore-free backfill material,  $f$  is the packing fraction, and  $g$  is the acceleration due to gravity. For waste packages 1.5 m in diameter, a 7.5 m drift, 1.5 m of invert, and 0.5 m of unfilled space at the top of the drift, there is 4.0 m of backfill on top of the packages. This is taken to be crushed tuff with a packing fraction of 0.74. (This is the packing fraction for close packing of spheres.) There may also be loads from fallen rock. Rocks of up to half the drift diameter may fall, so the load from a 3.75-m high block of solid rock is added. With  $\rho = 2300 \text{ kg/m}^3$  (Wilder, 1993b) and  $g = 9.806 \text{ m/s}^2$  (Weast, 1980),  $p_3 = 150 \text{ kPa}$  and  $p_1 = 560 \text{ kPa}$ . To provide a safety factor,  $p_1$  was doubled. The waste package must thus withstand pressures up to  $q = 1.12 \text{ MPa}$ .

As general corrosion thins the container, pressure from the products of corrosion may cause buckling of the cylindrical wall. The container was approximated as a thin-walled elastic cylinder. Such a cylinder will buckle (Roark and Young, 1975) at a pressure  $q$ , where

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$$q = \frac{Et/r}{1 + (\pi r/nl)^2/2} \left[ \frac{1}{n^2 [1 + (nl/\pi r)^2]^2} + \frac{n^2 t^2 [1 + (\pi r/nl)^2]^2}{12 r^2 (1 - \nu^2)} \right] \quad (2.6.1.5-2)$$

Here  $E$  is Young's modulus,  $\nu$  is Poisson's ratio,  $t$  is the wall thickness,  $r$  is the radius,  $l$  is the length, and  $n$  is the number of lobes for collapse. The equation applies only for  $n \geq 2$ . The actual buckling mode is expected to be that with the smallest  $q$ . It is assumed that  $r = 0.75$  m,  $l = 4$  m,  $E = 210$  GPa, and  $\nu = 0.3$  and found that, for  $q = 1.12$  MPa, buckling occurs at  $t = 11.4$  mm. The corresponding hoop stress is  $-qr/t = -73$  MPa.

No credit is taken in Equation 2.6.1.5-2 for the basket, which will support the cylindrical shell along lines of contact. The area between supports may be approximated as a long, curved panel with hinged straight edges and free curved edges. The pressure for buckling is (Roark and Young, 1975)

$$q = \frac{Et^3 (\pi^2/\alpha^2 - 1)}{12 r^3 (1 - \nu^3)} \quad (2.6.1.5-3)$$

where  $2\alpha$  is the central angle of the panel. For a 21 pressurized-water reactor package, the widest span between contacts has  $2\alpha = \text{Arctan}(5/3) - \text{Arctan}(3/5)$ . The panel buckles at  $t = 5.3$  mm and a hoop stress of  $-158$  MPa. However, if there is a clearance between the basket and the container, buckling should be described by Equation 2.6.1.5-2. The extent of buckling will be limited by contact of the container with the basket, but the effective values of  $r$  and  $\alpha$  may be changed so that Equation 2.6.1.5-3 is no longer conservative.

Force on the supports for the waste package may affect the thickness for buckling, but the change is expected to be small for three reasons. First, the total force on the panel discussed in the previous paragraph is 1.6 MN, but the weight of the waste, basket, and 9.5 mm inner barrier is only 0.27 MN for a 21 pressurized-water reactor package. Second, products of corrosion will tend to fill any available space under the package, thus transferring load from the supports. Third, the thickness required to prevent buckling is not linear as pressure varies only with its cube root.

The ends of the waste package will not buckle, but the stresses there are still of interest. The end is a continuous member, supported by the walls of the basket as well as the cylindrical outer wall, so the square part covering one opening in the basket was approximated by a plate with fixed edges. The maximum stress is

$$\sigma = Cqa^2/t^2 \quad (2.6.1.5-4)$$

where  $C = 0.3078$  and  $a$  is the spacing between basket walls. It has been assumed that  $a = 240$  mm and that the thickness of the ends is the same as that of the side. For  $t = 11.4$  mm,  $\sigma = 153$  MPa; and for  $t = 5.3$  mm,  $\sigma = 710$  MPa. Membrane effects will reduce these stresses somewhat. The lower of these stresses is comparable to the yield strength of the materials under consideration.

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Activity 1.10.2.5.3 - Thermal degradation of fuel cladding. It is generally desirable to take credit for all available containment barriers because additional barriers tend to delay release and to distribute it over a longer time. For spent fuel, potential containment barriers include the fuel cladding. But if cladding credit is to be taken, the thermal exposure must not destroy the integrity of the cladding. To predict the effects of thermal exposure we modeled the durability of the cladding.

Disposal of spent fuel is much like dry storage, so a search was made of the literature on fuel storage for information on cladding degradation. The authors of a report entitled "Control of Degradation of Spent LWR Fuel During Dry Storage in an Inert Atmosphere" (Cunningham et al., 1987) assessed numerous mechanisms for cladding failure during storage and concluded that creep rupture by diffusion-controlled cavity growth is the most important. The U.S. Nuclear Regulatory Commission (NRC) reached similar conclusions (NRC, 1985). In diffusion-controlled cavity growth, tensile stresses cause lenticular cavities to form along the grain boundaries and grow by grain boundary diffusion of vacancies. Analysis of constitutive equations and conditions indicates that diffusion-controlled cavity growth also dominates during disposal. Past applications of this model have predicted unrealistically short lifetimes. Part of the goal in this effort was to apply the model without excessive conservatism. To do so, a model of diffusion-controlled cavity growth that includes the effects of microstructure was developed.

Analysis of the model gives a temperature-dependent damage accumulation rate. The rule of thumb that maximum cladding temperatures should be kept below 350°C was examined. For one calculation, the rule was surprisingly accurate. But for fuels that cool slowly or that have been damaged by long dry storage at high temperatures, the rule may not be conservative, so the use of damage accumulation integrals is recommended.

### Cladding Failure by Diffusion-Controlled Cavity Growth

The method of damage accumulation was used: the amount of damage accumulated at time  $t$ ,  $D(t)$ , is given by

$$D(t) = \int_0^t \frac{d\tau}{L(\tau)} \quad (2.6.1.5-5)$$

where  $L$  is the lifetime of the material under the conditions at time  $\tau$ . When  $D(t) = 1$ , the material fails. The lower limit of integration is the time of fuel discharge, so the integral includes exposure during storage. In standard models of diffusion-controlled cavity growth (Raj and Ashby, 1975), failure occurs when cavities cover a certain area fraction of the grain boundaries. The lifetime  $L$  is

$$L = \frac{n\lambda^3 kT}{\delta D_{gb} \Omega \sigma m} \quad (2.6.1.5-6)$$

where  $n$  is a constant that depends on cavity shape and diffusion geometry,  $\lambda$  is the cavity spacing,  $k$  is Boltzmann's constant,  $T$  is temperature,  $\delta$  is the effective thickness of the grain boundary,  $D_{gb}$  is the grain boundary diffusivity,  $\Omega$  is the atomic volume,  $\sigma$  is the hoop stress

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in the cladding, and  $m$  is a constant that depends on microstructure. The values of each of these factors are discussed below.

Several factors are straightforward. The atomic volume  $\Omega$  is the volume of the crystallographic unit cell divided by the number of atoms per cell:  $\Omega = 2.327 \times 10^{-29} \text{ m}^3$ . If the gas inside the fuel rod is ideal and thermal expansion of solids is negligible,  $T/\sigma$  is a constant. The value of  $\sigma$  depends on the geometry of the fuel rod, the burnup of the fuel, and the amount of fission gas release. Einziger and Kohli (1984) state that  $\sigma = 90 \text{ MPa}$  at  $T = 623 \text{ K}$  ( $350^\circ\text{C}$ ) is conservative for most fuel, so these values were used. The cavity spacing  $\lambda = 10 \text{ }\mu\text{m}$  from Schwartz and Witte (1987) and NRC (1985) was taken.

Grain-boundary diffusivity is normally reported as  $\delta D_{gb}$ , but literature on diffusion-controlled cavity growth often separates the factors. Following Schwartz and Witte (1987) and NRC (1985),  $\delta = 9.69 \times 10^{-10}$  was used. For diffusivity,  $D_{gb} = 5.9 \times 10^{-6} \exp[(-131 \text{ kJ/mol})/RT] \text{ m}^2/\text{s}$ , where  $R$  is the gas constant was used. At temperatures of interest, this is the largest of the reviewed values.

From analysis of the diffusion geometry, the geometric constant  $n$ , for a lenticular cavity, is

$$n = \frac{3\sqrt{\pi}}{32} \frac{F_v(\theta)}{F_b(\theta)^{3/2}} \int_{A_i}^{A_f} \frac{dA}{f(A)} \quad (2.6.1.5-7)$$

where

$$F_v(\theta) = (2\pi/3) (2 - 3\cos\theta + \cos^3\theta) \quad , \quad (2.6.1.5-8)$$

$$F_b(\theta) = \pi \sin^2\theta \quad , \quad (2.6.1.5-9)$$

and

$$f(A) = \frac{(1 - \sqrt{A_c/A})(1 - A)}{\sqrt{A} [A(1 - A/4) - 3/4 - (\ln A)/2]} \quad (2.6.1.5-10)$$

Here  $F_v$  and  $F_b$  are defined so that  $F_v \rho^3$  is the volume of the cavity and  $F_b \rho^2$  is the area of the grain boundary that is cut out by the cavity. The function  $f$  takes account for the geometric effects of radial diffusion to the cavity. (NOTE: Raj and Ashby (1975) and NRC (1985) give slightly different equations for  $f(A)$ . Raj and Ashby's equation is clearly in error, since it is inconsistent with other equations in the paper. The form of the equation used by NRC (1985) suggests the derivation may be in error, but since some variables are not defined, that cannot be determined with certainty. Schwartz and Witte (1987) gives an equation with this form but it fails to mention, let alone treat, the singularity discussed below. Constants  $A_i$  and  $A_f$  are the initial and final values of the fractional areas that are decohered, that is, the values upon fuel discharge and at failure. Similar to NRC (1985) it was assumed that failure occurs at  $A_f = 0.15$ . This value is fairly conservative; some authors have used values as large as 0.5. Some authors have suggested that  $A_i$  should be  $A_c$ , the fractional area that is decohered by cavities of the critical size, where

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$$A_c = \left( \frac{4\gamma_s \sin\theta}{\sigma\lambda} \right)^2 \quad (2.6.1.5-11)$$

But such cavities have zero driving force for growth, so  $n$  is infinite. To avoid this singularity in  $n$ ,  $A_i$  was taken to be equal to  $2A_c$ . For reasonable choices of  $A_i$ , the exact value has only a small effect on  $n$ . For surface energies, Pescatore, et al. (1990) were followed by taking  $\gamma_s = 2\gamma_{gb} = 2 \text{ J/m}^2$ .

The constant  $m$  describes the effect of microstructure. Standard models of diffusion-controlled cavity growth assume a uniaxial tensile stress and grain boundaries that are normal to the stress axis. But this geometry is inappropriate for cold-formed cladding, so the model was modified. The cavity growth rate is proportional to the normal traction on the grain boundary. The principal stresses used are those for a pressurized, thin-walled tube:  $\sigma$  in the circumferential direction,  $\sigma/2$  in the axial direction, and 0 in the radial direction. The average normal traction over the surface of an ellipsoidal grain with semi-axis lengths of  $a$ ,  $b$ , and  $c$  in the circumferential, axial, and radial directions was then calculated. The constant  $m$  is the ratio of the average normal traction to the hoop stress  $\sigma$ ;  $m$  depends on  $a/c$  and  $b/c$ .

For cold forming, it can be assumed that the grains have a constant volume (the product  $abc$  is a constant) and that no grain-boundary sliding occurs. Under these conditions,  $b/c = (a/c)^2$ . From photomicrographs of cladding, it was estimated that  $a/c = 5$ . For conservatism,  $a/c = 3$  was used and resulted in  $m = 0.164521$ . The dependence of  $m$  on  $a/c$  is shown in Figure 2.6-2.

Using the data above, the lifetime  $L$  was calculated as a function of temperature; the results are plotted in Figure 2.6-3. Cladding in a repository was also simulated. The repository contained 21 pressurized-water reactor packages in 7.62-m (25-ft) drifts with a thermal loading of 282 kW/ha (114 kW/acre); equivalently, the mass loading was 247 MTU/ha (100 MTU/acre). The characteristics were 42.21 GWd/MTU burnup, 3.92 percent  $^{235}\text{U}$  initial enrichment, and emplacement 22.48 years after discharge. The temperature and damage function  $D$  are plotted in Figure 2.6-4. The damage occurs mostly during the first 100 years; as the temperature drops, damage accumulates slowly because grain boundary diffusion is slow.

For convenience, repository designs have often been evaluated by the rule that the cladding temperature must not exceed 350°C. The previous calculation was modified to test that rule, increasing the temperature by fixed increments until failure occurred at 10,000 years. This criterion was satisfied for a peak temperature of 354.9°C, which is in surprising agreement with the temperature-limit rule. For other fuels and repository designs the methods may not agree so well. The discrepancy may be especially large for fuel that has been damaged by dry storage at high temperatures.

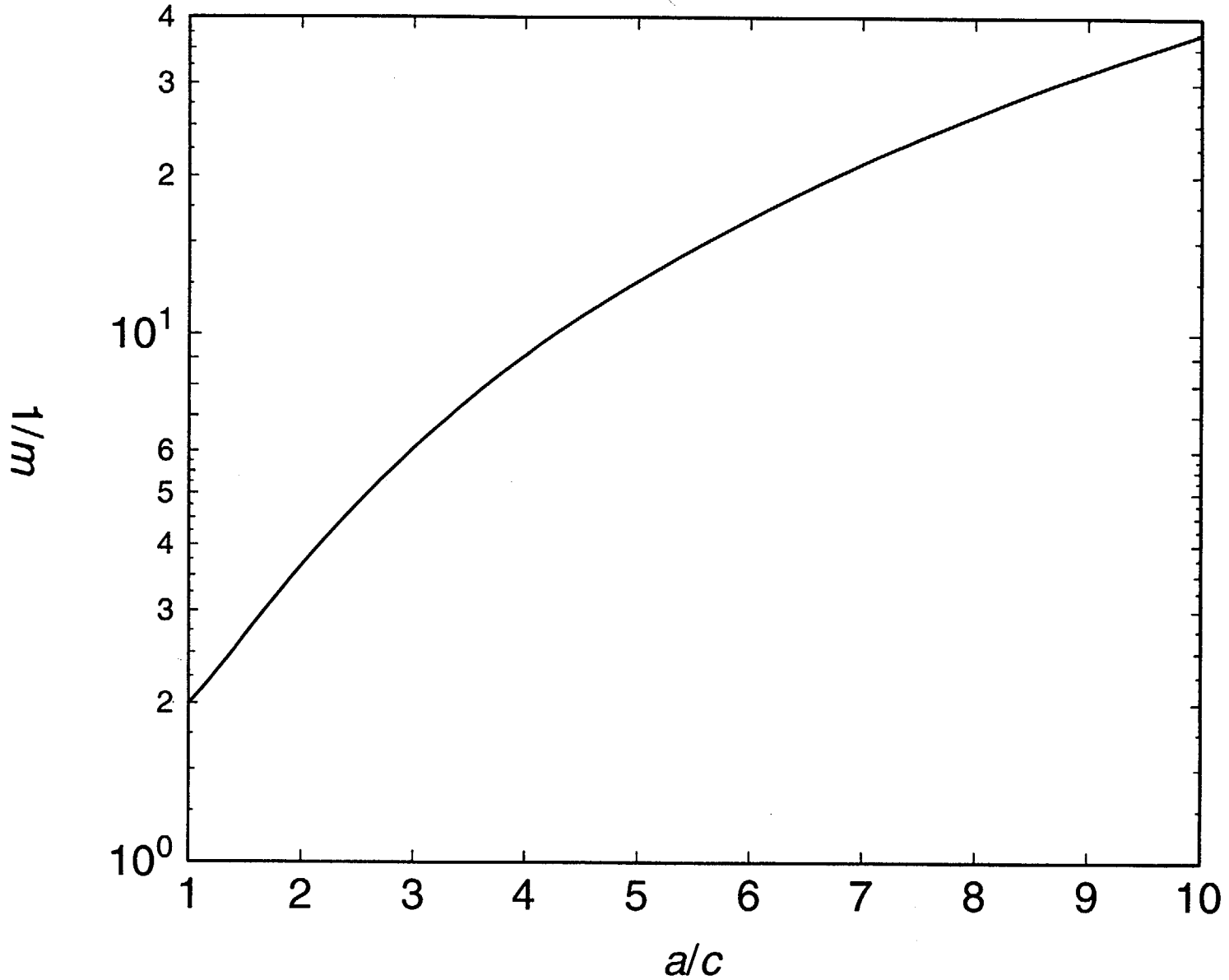


Figure 2.6-2. Microstructure constant  $m$  as a function of ratio  $a/c$   
 (where  $a$  and  $c$  are the grain semiaxis lengths in the circumferential and radial directions)

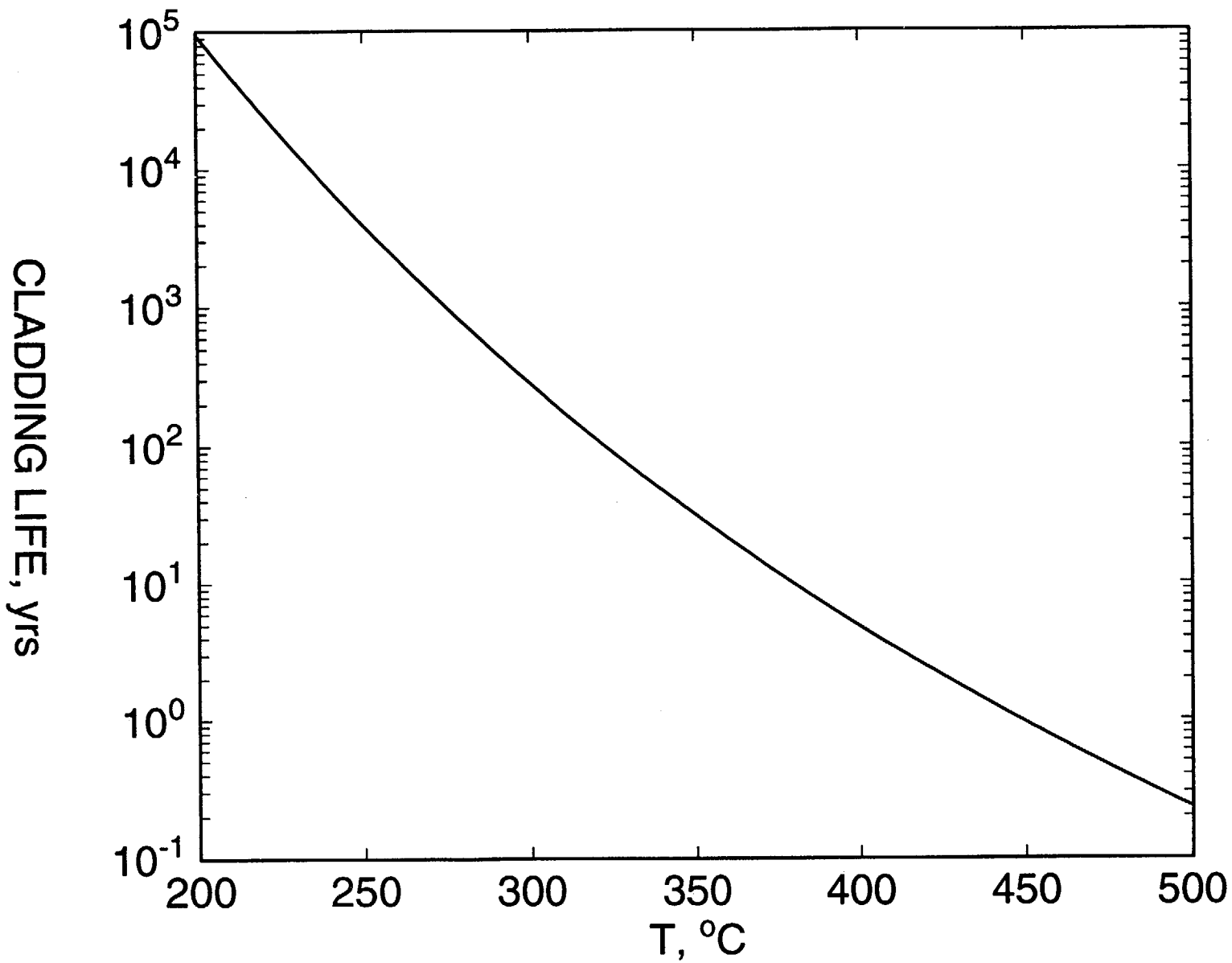


Figure 2.6-3. Predicted cladding life as a function of temperature for isothermal exposure



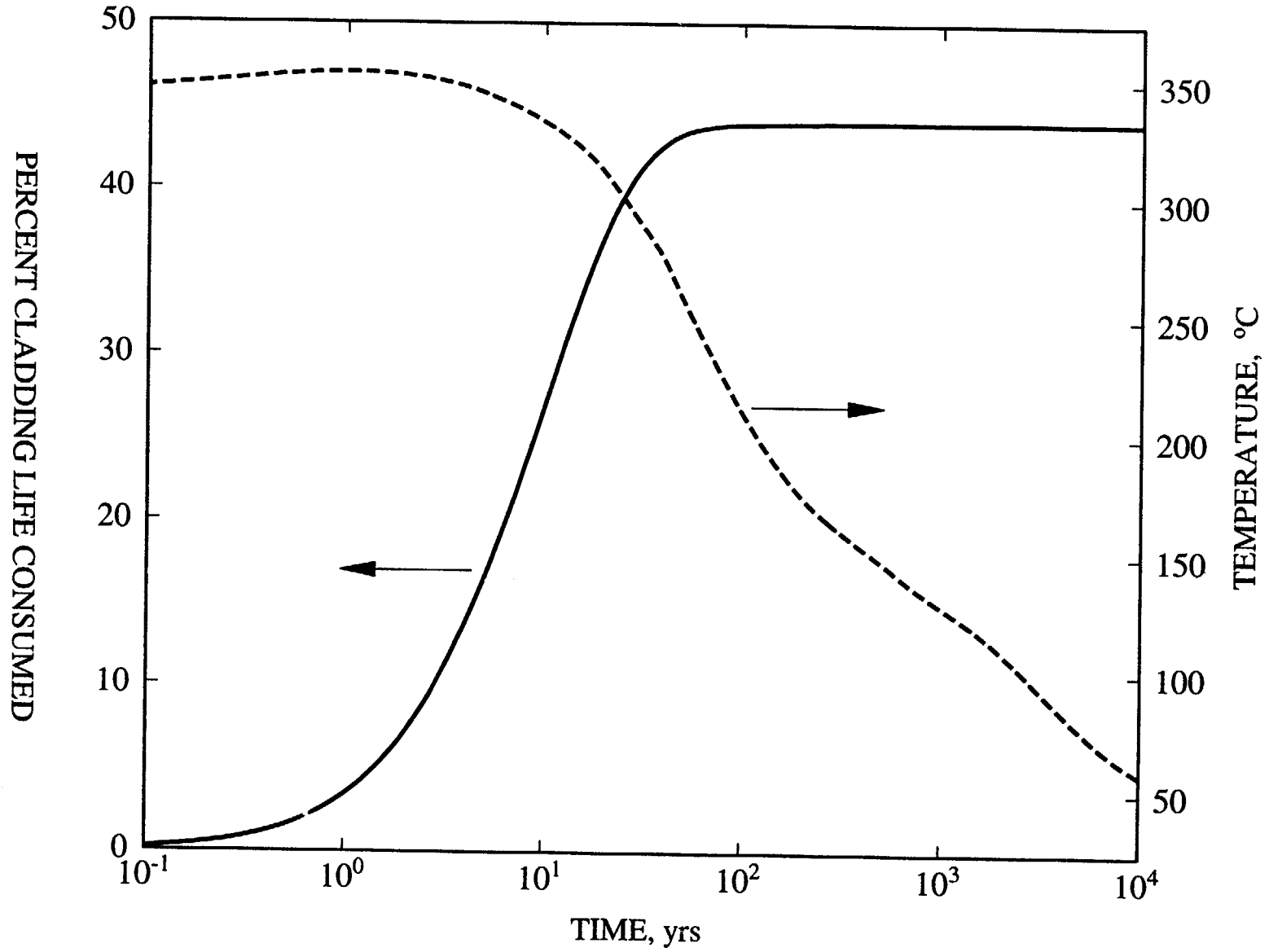


Figure 2.6-4. Temperature and fraction of cladding life consumed as functions of time for one repository design

## **2.6.2 Postemplacement Near-Field Environment (SCP Section 8.3.4.2)**

### **2.6.2.1 Design Activity 1.10.1.1 - Consideration of 10 CFR Part 60.135 (a) Factor**

A meeting was held in Las Vegas, Nevada, on April 16, 1993, to discuss possible revision of the Yucca Mountain Site Characterization Project (YMP) thermal goals originally detailed in the Site Characterization Plan (SCP). Some of the goals need to be changed to reflect the greater diversity of repository and waste package designs being considered in the Advanced Conceptual Design phase.

A Thermal Goals Workshop was held on May 12, 1993, in Las Vegas, Nevada. The goals were established in the SCP in 1988, but since then new considerations in the repository design, and improved knowledge of the site, necessitate review of the goals to determine: the original rationale for the goal; whether the individual goals are still relevant; and if the goals need to be changed and what the changes should be. The recommendations were incorporated into a report prepared for YMPO.

In support of the thermal loading systems study, Lawrence Livermore National Laboratory (LLNL) staff developed a new suite of repository-unsaturated zone-saturated zone-scale models for repository areas of 230, 301, 460, 709, and 1050 ha (570, 744, 1139, 1755, and 2598 acres). For 63,000 MTU of spent nuclear fuel, these repository areas correspond to areal mass loadings of 273, 206, 136.6, 88.7, and 60.3 MTU/ha (110.5, 83.4, 55.3, 35.9, and 24.4 MTU/acre). The models employ a relatively fine gridblock spacing at the outer perimeter of the repository in order to more accurately account for the effect of edge-cooling. A "youngest fuel first" receipt scenario with a ten year cut-off for the youngest fuel [referred to as YFF(10)] is being assumed. The calculations also account for the emplaced inventory of boiling water reactor waste packages containing 40 assemblies and pressurized-water reactor waste packages containing 21 assemblies.

Also, in support of the thermal loading systems study, LLNL staff developed a preprocessor "PBHEAT" that calculates the heat generation tables for the V-TOUGH code. This preprocessor incorporates the GETHT6 subroutine developed by the M&O which calculates kilowatts per metric ton uranium for a given fuel type (pressurized-water reactor or boiling water reactor), age, burnup, and enrichment. PBHEAT is capable of producing a blended heat generation curve (averaged over the entire repository area), based on the yearly increments of pressurized-water reactor and boiling water reactor waste packages and the yearly averaged spent nuclear fuel ages, burnups, and enrichments for each of these increments. Rather than assuming that all of the heat generation instantaneously begins at  $t = 0$  year, the heat generation curve produced by PBHEAT accounts for the "ramping up" of the heat output that occurs over the emplacement period. PBHEAT can also be used to calculate the heat generation curve for specific increments of the emplaced waste packages, thereby accounting for the spatial variability of heat generation within the repository. For 30-year-old pressurized-water reactors with a burnup of 33 GWd/MTU and an enrichment of 3.2 percent, PBHEAT produced nearly the identical heat generation curve produced by the pressurized-water reactor heat generation preprocessor, HEATCAL, which was developed several years ago at LLNL.

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A YMP Colloid Workshop was held May 3-5, 1993, in Santa Fe, New Mexico, where results of the analysis of inorganic colloids in Nevada Test Site ground waters were provided. A strategy for addressing issues related to colloid transport of radionuclides was developed. An initial draft of a strategy document is currently being edited.

### **2.6.2.2 Study 1.10.4.1 - Characterize Chemical and Mineralogical Changes in the Postemplacement Environment**

The revised Study Plan 8.3.4.2.4.1, "Characterization of the Chemical and Mineralogical Changes in the Post-Emplacement Environment," was returned by the LLNL editor, with several editorial suggestions. The comments were being addressed.

The April and June Geochemistry Integration Task meetings were participated in. They focused on the colloid workshop at Los Alamos National Laboratory (Los Alamos) and developing a Project strategy for addressing the issue of colloidal mediated transport of radionuclides.

Activity 1.10.4.1.1 - Rock-water interactions at elevated temperatures. The contract for the work on the New Zealand natural analog site was initiated. A visit by two LLNL scientists to evaluate several potential sites for conducting validation activities using EQ3/6 was completed. A prioritized list of site studies has been developed, and a draft memorandum describing the site work has been written. The screening process to select specific sites for study has been started, with initial work focusing on Champagne Pool, where fluid mixing is occurring. The first sampling of waters and solids has been done by the Crown Research Institute collaborators and analysis of the materials is under way. When the results are available, modeling of the mixing process and associated precipitation of metal phases will begin. Simultaneously, evaluation of the GEMBOCHS data base is being done at LLNL to determine what additional solid phases may be required to adequately simulate the mixing/precipitation process. Particular consideration is being placed on the sulfides, oxides, and hydroxides of antimony, iron, and other metals that may participate in the precipitation process. Staff again visited New Zealand in August 1993. The purpose of this visit was to finalize methods for transferring data from one organization to the other, and for establishing arrangements for collaborative activities with the companies involved with the day-to-day operation of the geothermal fields and drilling activities. Data are also being collected and processed to develop a three-dimensional model of the geothermal field. This model will form the basis for understanding the areal distribution of properties and for selecting additional sites for subsurface studies. Discussions are under way with the principal corporations controlling proprietary data to schedule a meeting to discuss how best to handle requests for such information. Discussions were also held concerning the first phase modeling activities. Samples collected are being analyzed and used in initial modeling exercises with the use of the EQ3/6 data base. Activity diagrams were compared with previous studies to ensure that consistency was maintained.

Models of mineral evolution in the vicinity of waste packages were further developed. A reference set of computations that will be used as a comparison for calculations involving

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flow and transport has been initiated, using UE-25 J#13 water chemistry and rock systems idealized from the known stratigraphy. The current calculations do not consider the role of moving water. Computations have also been initiated in which the dissolution and precipitation kinetics of various silicates are used to bound estimates of the rates at which mineralogical and chemical equilibrium may be achieved in the vicinity of waste packages, and also in the areas surrounding the repository in the altered zone. Initial calculations indicate that local equilibrium will be achieved in periods from a few months to a few years at the nominal SCP areal power density, and at higher thermal loads, for most regions. The exceptions are those areas nearest emplacement drifts where fluid velocities may be high, and those areas that never exceed approximately 60°C.

The samples obtained of the fracture system at the Large Block facility in late June were sectioned and have been submitted for analysis. These are being evaluated for mineralogical and petrological properties.

Activity 1.10.4.1.2 - Effect of grout, concrete, and other repository materials on water composition. This activity is now reported under 1.10.4.5.1 as a result of the Rev. 9 revision of the Site Characterization Program Baseline.

Activity 1.10.4.1.3 - Composition of vadose water from the waste package environment. No progress during the reporting period; this was an unfunded activity.

Activity 1.10.4.1.4 - Dissolution of phases in the waste package environment. No progress during the reporting period; this was an unfunded activity.

Activity 1.10.4.1.5 - Effects of radiation on water chemistry. No progress during the reporting period; this was an unfunded activity.

Activity 1.10.4.1.6 - Effects of container and borehole liner corrosion products on water chemistry. No progress during the reporting period; this was an unfunded activity.

Activity 1.10.4.1.7 - Numerical analysis and modeling of rock-water interaction. No progress during the reporting period; this was an unfunded activity. This activity is also reported under 1.10.4.5.1, because the activity was divided between geochemistry and man-made material activities (in Site Characterization Program Baseline, Rev. 8).

**Forecast:** The study plan is scheduled to be sent to YMPO. Work will continue on modeling the evolution of mineralogical properties and water chemistry. Emphasis is being placed on the effects of geochemical processes on hydrological properties. Testing modeling capabilities on field work will continue. Emphasis will be placed on developing guidelines for selecting modeling strategies where thermodynamic data or field information are not complete. Experimental studies of water-rock interaction will be conducted using vitric material in environment of low relative humidity. This information will allow completion of characterization of reaction processes likely to occur in the vicinity of the repository. Evaluation and development of codes capable of coupling hydrology and chemistry will continue, with the goal of designing experiments against which codes can be tested.

### 2.6.2.3 Study 1.10.4.2 - Hydrologic Properties of Waste Package Environment

Activity 1.10.4.2.1 - Single-phase fluid system properties. Study Plan 8.3.4.2.4.2, "Hydrological Properties of Waste Package Environment," is being prepared and will be submitted for approval in FY 1994.

Activity 1.10.4.2.2 - Two-phase fluid system properties. Work continues to measure electrical resistivity as a function of moisture content of Topopah Spring Tuff samples from USW GU-4 and USW GU-3 holes at room temperature, using UE-25 J#13 water as pore fluid. The purpose of following this experimental procedure is to determine the effect of the electrical conductivity of pore fluid on the relationship between the bulk electrical conductivity of a rock sample and the degree of saturation in it. The samples from USW GU-3 are being used for the high temperature measurements. For the USW GU-3 samples, the wetting phase measurements at 40°C have been completed, and the drying phase measurements at 40°C were started. The preparation of samples machined parallel to the core axis was also started. It was decided to use a humidity chamber to hold the moisture content in a sample when it is at high temperature. The measured bulk resistivity using UE-25 J#13 water as pore fluid at water saturation levels less than 80 percent is very similar to that when distilled water is used as pore fluid. When the saturation level is greater than 80 percent, the bulk electrical conductivity using UE-25 J#13 water as pore fluid did not decrease with respect to increase of water saturation, as was observed when distilled water was used as pore fluid. The electrical conductivity of UE-25 J#13 water at high temperatures has been determined to be near 100°C.

The determination of electrical resistivity as a function of water saturation using disc samples from USW G-4 core at room temperature was completed and the measurement at 40°C was started. These measurements included wetting and drying cycles, using UE-25 J#13 water and distilled water, on samples machined parallel and perpendicular to the axis of the original core section. Very little anisotropy in the measured electrical conductivity with respect to the core axis was found. The measurement of electrical conductivity as a function of frequency within the range of water saturation from 0 to 50 percent was completed for the USW G-4 sample. The data are being analyzed.

Work continued on the experiment to determine the moisture retention curve and one-dimensional imbibition using USW G-4 core. The data from this experiment will be used for calculating relative permeability as a function of water saturation. In the one-dimensional imbibition experiment, UE-25 J#13 water was introduced to the bottom of a sample that is 2.54 cm in diameter, and 10 cm long. The water was imbibed into the sample against gravity. Eight pairs of electrodes were mounted along the axis of the sample to determine the distribution of moisture content as a function of time. The imbibition rate of water was determined from the water level in a burette. The samples are at 90 percent relative humidity at 25°C. The wetting phase of the moisture retention curve at 25°C was completed. The sample was saturated with water, some of which will be extracted for chemical analysis. The Si concentration in the water is about five times that of virgin UE-25 J#13 water, indicating rock-water interaction during the six-week experiment at room temperature. To improve the accuracy of determining water saturation using electrical resistivity measurements during

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imbibition, a rectangular plate sample from USW G-4 core was prepared. A four electrode method will be used to determine electrical resistivity. The samples are in the drying phase. Data analysis is continuing.

Work continued on an experiment to determine the effect of fracture surface coatings on the imbibition of water into the matrix. Eight Topopah Spring Tuff samples machined from outcrops from Busted Butte, Nevada, were prepared for this purpose. Work progresses to determine the mineralogy of the coating material, the pore size distribution in the coating layers, and the porosity of the samples.

An intact Topopah Spring Tuff sample from the USW G-4 hole to be used to determine saturated water permeability has been put into a pressure vessel under a confining pressure of about 5 MPa. The sample is being resaturated with UE-25 J#13 water in the pressure vessel. The pore water pressure will be brought to equilibrium before measuring the water permeability.

Work continued on the analysis of thermohydrological behavior for a wide range of thermal loading conditions and hydrological properties. This analysis has been conducted at a variety of scales, including the mountain scale, subrepository scale, and drift-scale. Analyses have demonstrated that the only significant source of liquid water is from nonequilibrium fracture flow from three potential origins: meteoric sources, condensate generated under boiling conditions, and condensate generated under sub-boiling conditions.

The first source of liquid water arises from the ambient system; the second and third sources are generated by repository heat. Buoyant vapor flow, occurring either on a subrepository scale or on a mountain scale, may play an important role in the generation of the second and third sources of liquid water. Zones of sharply contrasting bulk permeability,  $k_b$ , are also found to influence condensate generation and drainage, both under boiling and subboiling conditions. Of particular concern are conditions that promote the focusing of vapor flow and condensate drainage, which could cause persistent two-phase conditions (often referred to as the heat-pipe effect) in the vicinity of waste packages. Repository heat can generate a mobile liquid phase in fractures even if temperatures are below the boiling point.

In addition to generating condensate flow, repository heat can redistribute the liquid saturation in the unsaturated zone, causing regions of net dryout below the repository and saturation buildup above the repository. These changes in the saturation distribution can impact ambient fracture flow, possibly amplifying the effects of natural infiltration in regions of saturation buildup and attenuating those effects in regions of net dryout. For high areal mass loadings, expressed in MTU/ha (or MTU/acre) that result in significant dryout, mountain-scale, buoyant, vapor flow can also increase the rate at which the dryout zone is rewetted. Repository-scale analyses have indicated that repository-heat-driven changes in the saturation distribution can persist for more than 100,000 years, even for low areal mass loadings that never drive temperatures close to the boiling point.

It is important to note that repository-scale analyses assume the repository thermal load to be uniformly distributed over a disk-shaped area with areally uniform thermohydrological

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properties. The vertical distribution of thermohydrological properties was included, assuming the major hydrostratigraphic units are horizontal. Effectively, the results of those calculations are representative of averaged, mountain-scale, thermohydrological behavior. How the spatial variability of heating conditions and hydrological properties may cause local thermohydrological behavior to deviate from averaged, mountain-scale behavior have been examined. The conditions under which buoyant, vapor flow begin to dominate hydrological and thermal behavior for both sub-boiling and above-boiling thermal loads have been examined.

### Thermal Loading Approach

The extent to which the three major sources of fracture flow may impact waste package performance and radionuclide migration depends on ambient site conditions as well as on the thermal-loading strategy that will eventually be adopted for the MGDS at Yucca Mountain. With respect to repository-heat-driven thermohydrological performance, there are three primary thermal loading approaches. These three approaches are best framed as three fundamental questions:

1. Can the thermal load be limited and distributed so that it has a negligible impact on hydrological performance of the MGDS?
2. For intermediate thermal loads, will the impact of thermohydrological processes and our understanding of those processes allow us to demonstrate that the MGDS meets regulatory compliance?
3. For higher thermal loads, that have the potential of generating extended-dry conditions, will the impact of thermohydrological processes and our understanding of those processes allow us to demonstrate that the MGDS meets regulatory compliance?

The first thermal loading strategy is to minimize the hydrological impact of repository heat so that the primary concern in assessing hydrological performance is the ambient hydrological system. The motivation for this approach is to avoid any potentially adverse effects of repository heat. The second approach is the baseline case that has been under consideration. The third approach would be to demonstrate that, for some period of time, repository heat is capable of dominating the ambient system with above-boiling conditions surrounding the repository. The primary motivations for this approach are to reduce the sensitivity of repository performance to hydrological variability; extend the period of radionuclide containment in the engineered barrier system; and reduce the probability of water contacting waste packages and the flow rates associated with transport.

Important uncertainties related to evaluating these options are the influence of buoyant, gas-phase convection and hydrogeological heterogeneity that may focus vapor flow and condensate drainage. The influence of these processes will largely determine what thermal loads are sufficiently "hot" (or whether any such thermal loads exist) to allow demonstration of that extended-dry condition that will prevail for some time in the vicinity of waste packages.

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### Use of Hypothesis Testing in Model Validation

A broad range of parameters and conditions are important in predicting thermohydrological performance. These include:

- (1) whether heat conduction dominates heat flow,
- (2) whether a region of above-boiling temperatures surrounding the repository corresponds to the absence of mobile liquid water at the waste package environment,
- (3) whether fracture density and connectivity are sufficient to promote rock dryout due to boiling and condensate shedding,
- (4) whether rewetting of the dryout zone back to ambient saturation lags significantly behind the end of the boiling period,
- (5) whether mountain-scale, buoyant, gas-phase convection may eventually dominate moisture movement in the unsaturated zone,
- (6) whether sub-repository-scale, buoyant, gas-phase convection dominates moisture movement at the repository, and
- (7) whether heterogeneity results in focusing enough vapor flow and condensate drainage to cause persistent local liquid flow at the waste package environment.

The first three hypotheses provide the basis for reliably predicting the spatial extent of the dryout zone surrounding the repository. The fourth hypothesis provides the basis for predicting how long the dryout zone persists. Demonstrating that hypotheses (5) through (7) are false is favorable for both above-boiling and sub-boiling performance. By showing that hypotheses (5) and (6) are false, a major potential source of fracture flow, particularly for sub-boiling conditions, as well as a potential mechanism for building up the saturation above the repository and re-wetting the dryout zone will be eliminated. By showing that hypothesis (7) is false, a major potential source of fracture flow for both sub-boiling and above-boiling conditions will be eliminated.

Resolution of hypotheses (1), (5), (6), and (7) is important even if temperatures never exceed the boiling point. Mountain-scale, buoyant, gas-phase convection will dominate heat flow only for a very large vapor flux that results in a large saturation buildup above the repository and/or a large condensate drainage flux in fractures. Therefore, hypotheses (1) and (5) are important for all areal mass loadings. Hypothesis (6) is particularly important for a thermal loading strategy that relies on a sub-boiling thermal load having a negligible impact on hydrological performance. Hypothesis (7) is important for all areal mass loadings, because focused vapor flow and condensate drainage can cause persistent liquid flow at the waste package environment for both sub-boiling and boiling conditions.



Mountain-Scale and Sub-Repository-Scale, Buoyant, Gas-Phase Flow

The repository-scale, unsaturated zone-saturated zone model has been used to study the thermohydrological impact of mountain-scale, buoyant, gas-phase flow over a wide range of  $k_b$  and areal mass loading, including 67, 121.5, and 382 MTU/ha (27.1, 49.2 [the reference SCP-CDR thermal load], and 154.7 MTU/acre). For a broad suite of cases, a homogeneous and isotropic  $k_b$  distribution was considered in the unsaturated zone and saturated zone. The impact of a layered, heterogeneous  $k_b$  distribution has also been considered. With the cross-sectional, drift-scale model, the thermohydrological impact of sub-repository-scale, buoyant, gas-phase flow over a wide range of  $k_b$  and areal mass loading, including 33.3, 67, 121.5, and 382 MTU/ha (13.5, 27.1, 49.2, and 154.7 MTU/acre) was investigated.

Mountain-scale, buoyant, gas-phase convection appears to occur within fracture networks having a connectivity with length-scale comparable to the unsaturated zone thickness and repository width. Sub-repository-scale, buoyant, gas-phase convection is predicted within fracture networks having a connectivity with length-scale comparable to the distance between the hot and cold regions of the repository. Buoyant, gas-phase, convection cells are predicted as the warmer, less dense column of gas within the footprint of the heated region is displaced by the cooler, denser column of gas outside of this region. As the initially cooler gas is heated, its relative humidity is lowered, causing it to evaporate water below the repository. The model results show that warm moist air is convected upward to where it cools above the repository, generating condensate that drains down fractures back toward the repository and/or is imbibed by the matrix, causing a saturation buildup above the repository. Because water removed below the repository may be replenished by water imbibed from the saturated zone, mountain-scale, buoyant, the modeling results suggest that vapor flow can result in a net saturation buildup in the unsaturated zone. Results support that mountain-scale, buoyant, vapor flow can dominate moisture movement on the order of 100,000 years.

Model results show that sub-repository-scale, buoyant, gas-phase convection will continue as long as significant temperature differences persist within the repository, dominating moisture movement for up to 1000 years for a center-to-center drift spacing of 38.4 m. These effects will persist longer for larger drift spacing. Sub-repository-scale, buoyant, vapor flow can move significant quantities of moisture, resulting in persistent dripping onto waste packages for temperatures that are well below the boiling point. For an areal mass loading of 33.3 MTU/ha (13.5 MTU/acre), which yields an areal power density of 24.7 kW/ha (10 kW/acre), for 30-year-old spent nuclear fuel, modeling results show that sub-repository-scale, buoyant vapor flow can drive significant moisture movement even though the peak drift wall temperature is only 42°C.

By considering a wide range in bulk permeability  $k_b$ , the threshold  $k_b$  (called  $k_b^{hyd}$ ) was identified at which buoyant, vapor convection begins to dominate hydrological behavior, and the threshold  $k_b$  (called  $k_b^{th}$ ) at which this convection begins to dominate thermal behavior. It was found that  $k_b^{hyd}$  is roughly the same for mountain-scale and sub-repository-scale, buoyant, gas-phase flow. It was also found that  $k_b^{th}$  is generally an order of magnitude larger than  $k_b^{hyd}$ . The development of a large above-boiling zone is found to suppress the effects of buoyant vapor flow, both on the mountain scale and sub-repository scale.

Focused Vapor Flow and Condensate Drainage Due to Heterogeneity

Two models were used to model focused vapor flow and condensate drainage which arise due to hydrogeological heterogeneity. These include the drift-scale model that accounts for the actual cross-sectional geometry of heat producing waste packages and the emplacement drifts, and the cross-sectional, uniform, heat flow model that smears the repository heat load, but is useful in investigating the effects of heterogeneity with a length-scale larger than the drift spacing. With the drift-scale model, it was assumed that a vertically oriented, high permeability zone intersects the emplacement drift directly over a waste package. With the cross-sectional, uniform, heat flow model, the sensitivity of focused vapor and condensate flow to the spacing between the highly permeable zones was investigated.

Zones of sharply contrasting  $k_b$  are found to influence vapor flow and the resulting condensate generation and drainage. It was found that if the contrast in  $k_b$  between the high- $k_b$  zone and the rest of the rock surrounding the drift (called the nominal- $k_b$  zone) is sufficiently large, then the  $p_g$  differential between these zones will drive water vapor back toward the drift and into the high- $k_b$  zone. In effect, the emplacement drift functions as a manifold that enhances the gas-phase communication between the high- $k_b$  and nominal- $k_b$  zones. If enough water vapor is focused into the high- $k_b$  zone, then the resulting condensate generation and drainage back down that zone may result in persistent two-phase conditions at the edge of the drift and water dripping onto the waste packages. These effects can occur under both sub-boiling and boiling conditions. Because the cross-sectional, uniform, heat flow model under represents the local heat flux in the vicinity of waste packages, it tends to overpredict the duration of two-phase conditions near the emplacement drifts.

The degree of vapor flow focusing into the high- $k_b$  zone, and the resulting duration of two-phase conditions at the repository horizon depend on three factors. First,  $k_b$  in the nominally fractured zone must be large enough not to significantly throttle the rate of vapor generation due to boiling (or due to evaporation under sub-boiling conditions). Second, a large contrast in  $k_b$  between the high- and nominal- $k_b$  zones results in a gas-phase pressure ( $p_g$ ), differential between these zones that preferentially drives vapor flow into the high- $k_b$  zone. If enough vapor enters and condenses in the high- $k_b$  zone, the return condensate flux will be large enough to maintain two-phase conditions at the repository horizon, possibly resulting in dripping onto waste packages. Third, there must be sufficient spacing between the high- $k_b$  zones to delay, or minimize, the interference between the high- $k_b$  zones with respect to the  $p_g$  distribution. Larger spacing between high- $k_b$  zones allows a greater  $p_g$  buildup within the nominal- $k_b$  zone, and increases the duration of this buildup. Moreover, larger spacing allows a greater volume of vapor generation to be focused into the high- $k_b$  zone.

Of course, the examples considered thus far are highly idealized relative to the complex geometry of real fracture networks, but they illustrates the principle that large contrasts in  $k_b$  between neighboring zones can result in focusing of vapor flow and condensate drainage, and, hence, persistent dripping onto waste packages. They also illustrate the principle that for a given contrast in  $k_b$ , the duration of two-phase conditions increases with spacing between the high- $k_b$  zones. Effectively, the high- $k_b$  zones are competing for a finite quantity of vapor

flow and condensate generation. Consequently, there is a trade-off between the duration of two-phase conditions and the number of locations where such conditions can occur in the repository. If there are too many such zones, there will be insufficient condensate focusing to cause persistent two-phase conditions at the repository horizon. The degree of focusing necessary to cause persistent two-phase conditions limits the number of locations where such conditions can occur.

In general, regardless of how it is generated, repository-heat-driven, condensate flow can drain away from the boiling zone, can drain back toward the boiling zone, can be imbibed by the matrix. Because the small matrix permeability,  $k_m$ , limits the rate of matrix imbibition, modeling results suggest that condensate drainage down fractures persists for considerable distances before being imbibed by the matrix. Note that the Equivalent Continuum Model used in these calculations does not explicitly represent this nonequilibrium drainage in fractures. Below the boiling zone, condensate drainage is away from the boiling zone, enhancing the dryout rate. Above the boiling zone, condensate tends to drain back toward the boiling zone, where it reboils, thereby retarding the net rate of dryout. Until boiling reduces the liquid saturation to zero, temperatures will be determined by two-phase thermodynamic equilibrium. The effect of vapor pressure lowering (which results from surface forces between the water and the matrix) can make it difficult to reduce the liquid saturation in the matrix to zero even though temperatures may be well above the nominal boiling point. Under such conditions, the fractures are likely to be completely free of mobile liquid water. Immobile water, tightly held by surface forces, may be present in the rock at temperatures above the boiling point.

It should be noted that very extreme examples of heterogeneity may have been considered. However, the same degree of heterogeneity was considered for a wide range of thermal loads, yielding very different outcomes. The two-phase effects of focused vapor flow and condensate drainage are seen to be more persistent in the vicinity of waste packages for marginal boiling cases, and continue long after temperatures have dropped below the boiling point. For increasing areal mass loading, the effects of focused vapor flow and condensate drainage were decreasingly persistent. For several extreme examples of heterogeneity, an areal mass loading of 121.5 MTU/ha (49.2 MTU/acre) (the reference SCP-CDR thermal load), resulted in two-phase conditions (with a mobile liquid phase in the fractures) for more than 1500 years at the emplacement drift, long after temperatures had dropped below boiling. For exactly the same degree of heterogeneity and an areal mass loading of 382 MTU/ha (154.7 MTU/acre), two-phase conditions at the emplacement drift ceased within nine years, and the effects of focused vapor and condensate drainage virtually vanished in the far-field long before temperatures dropped below the boiling point. Work continues to address condensate focusing that arises from preferential, gas-phase focusing. In future work, condensate focusing that arises from preferential, liquid-phase focusing of condensate, as well as from combinations of gas-phase and liquid-phase focusing that include the impact of climatological change will be addressed. The potential impact that climatological change may have on liquid-phase flow focusing will increase with time as the decaying heat load from the repository causes the mean condensate flux to decrease.

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**Forecast:** Modeling activities will continue. Study Plan 8.3.4.2.4.2 will be submitted to YMPO for approval.

Activity 1.10.4.2.3 - Numerical analysis of flow and transport in laboratory systems. At the Performance Assessment Model Validation Meeting held in Las Vegas, Nevada, on June 29, 1993, presentations were made on the following subjects: Repository-Heat-Driven Hydrothermal Flow: Modeling and Analysis (Buscheck); Analytical Expressions Quantifying the Influence of Convection on Fluid and Heat Flow (Nitao); and Modeling Statistical Variability in Condensate Drainage (Nitao).

**Forecast:** The work of building up a data base of electrical resistivity as a function of water saturation will continue. Laboratory model validation experiments will be started.

### **2.6.2.4 Study 1.10.4.3 - Characterization of the Geomechanical Attributes of the Waste Package Environment**

Study Plan 8.3.4.2.4.3 was approved by YMPO on December 11, 1992, and sent to NRC on December 31, 1992. The NRC accepted the study plan in a letter to the Office of Civilian Radioactive Waste Management (OCRWM) dated April 21, 1993, and posed four questions. The OCRWM responded to the NRC questions in a letter dated September 2, 1993. A response to NRC comments was prepared and forwarded to YMPO. This response included a description of proposed revisions to the study plan scheduled for FY 1995. In addition, a draft Activity Plan for Geomechanical Investigations has been prepared.

Set-up of laboratory facilities for geomechanics testing of rock samples has been started. Emphasis is on apparatus to support the Large Block Test to determine the effect of the cristobalite behavior at temperatures of 200° - 250°C on the mechanical properties of the rock.

Thin sections of several samples of Topopah Spring Tuff were prepared from core ends of samples to be tested on the geochemical and hydrologic tasks and a set of approximately 100 images of the microstructure of Topopah Spring Tuff were produced at a variety of magnifications in the range 50x to 1000x. The images are of samples taken from holes USW GU-3 and USW G-4. The purpose of this imaging of the microstructure is to gain quantitative information on the pore structure of the rock. The images were digitized and stored on computer disks, and two-point spatial correlation functions were computed for many of them. This function is a statistical way to measure the geometry of the pore space and provides the basis for estimating several parameters of interest such as local distribution of specific surface area and local estimates of pore size and connectivity. In addition, standard morphological measurements were made on several of the images. These results will aid in understanding the fundamental properties of the pore structure and in identifying any changes in pore structure that may occur during laboratory testing.

Activity 1.10.4.3.1 - Block stability analysis. No progress during the reporting period; this was an unfunded activity.

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Activity 1.10.4.3.2 - Borehole damage analysis. No progress during the reporting period; this was an unfunded activity.

Activity 1.10.4.3.3 - Geomechanical properties analysis. No progress during the reporting period; this was an unfunded activity.

**Forecast:** A major portion of the effort on this task for FY 1994 will be directed to geomechanics measurement and analysis of the Large Block Test. This includes development and testing of instrumentation for geomechanics measurements, laboratory characterization of geomechanical behavior of smaller blocks quarried from the site of the Large Block Test and modeling of the geomechanical behavior of the Large Block Test.

Work will continue on the interface of thermogeomechanics models with thermo-hydrologic models. This work will focus on developing the capability to use the temperature fields computed by the hydrologic models such as V-TOUGH and NUFT, as input to geomechanical models. In particular, temperature fields estimated for the Large Block Test will be interfaced to the FLAC geomechanics code. This will enable the geomechanics code to be used to develop estimates of stress field for various thermal-loading regimes, based on a temperature field that is consistent with that used by the hydrologists.

Work will start to obtain/develop a capability for discrete element analysis. The discrete element method is a technique for modeling rock behavior based on the movement along fractures of independent rock blocks. This method is well suited to analysis of the Large Block Test and the Exploratory Studies Facility (ESF). During FY 1994 the LDDA discrete element code will be evaluated for analysis of the Large Block Test.

### 2.6.2.5 Study 1.10.4.4 - Engineered Barrier System Field Tests

Study Plan 8.3.4.2.4.4 was submitted to YMPO for approval on July 9, 1993.

Activity 1.10.4.4.1 - Repository horizon near-field hydrologic properties. Comment resolution for the draft Scientific Investigation Plan for the Large Block Test has been completed and the plan is awaiting approval signatures by YMPO. Linkage of the Scientific Investigation Plan to (draft) Study Plan 8.3.4.2.4.4 also continues. The drafting of the Activity Plan was started.

The design of the loading frame has been finalized. The Mechanical Engineering Department (LLNL) personnel have prepared fabrication drawings of the frame. Preparation work for laboratory tests on smaller blocks and quarry of the large block has been started. Preliminary scoping model calculations indicate that it is possible to generate both a dryout zone and a condensate zone in the block. The procurement package for the load-retaining frame has been sent to potential vendors. Environmental management approval was received on May 25, 1993, to clear the potential test area. The LLNL staff assisted by Los Alamos, Sandia National Laboratories (SNL), Raytheon Services Nevada and Reynolds Electrical & Engineering Co., Inc. (REECO) personnel visited the Nevada Test Site June 1-2, 1993, to map

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fractures and select a test area. The REECo personnel then completed the clearing and rock surface cleaning activity. The LLNL staff continued mapping the fractures and sampled the fracture system. Emphasis was on identifying mineralogy of fractures, number of fracture generations, and characteristics of fracture alteration haloes and fracture surfaces.

A geomechanical numerical simulation of the Large Block Test was initiated. The purpose of this work is to aid in the experimental design of the test and to provide a point of reference for evaluation of various thermal and material models for predicting the block response. The initial focus is on evaluation of options for the placement of heaters and the rate and duration of heating/cooling cycles, and to assist in the design of the type and location of diagnostic instrumentation, especially for the geomechanical measurements. The numerical model used for this simulation is called FLAC which is a time-dependent, finite difference model capable of treating both mechanical and thermally induced stresses and deformations. It is a two-dimensional code in which materials are represented by arbitrarily shaped quadrilateral zones. FLAC is based on a Lagrangian scheme which is well suited for large material deformations, is capable of using several built-in material models including the ubiquitous joint model, and is installed on a Sun Sparc work station. Preliminary results for temperature, stress and displacement fields as a function of time from start of heating were prepared and compared to results from the V-TOUGH model.

The samples obtained of the fracture system at the Large Block Test facility in late June were examined by petrographic microscopy and x-ray diffraction. Preliminary examination of the thin sections indicates that dark alteration zones along the fracture margins are the result of fluid-rock interaction during vein formation in which oxidized iron phases are reduced, possibly from hematite to magnetite. Carbonate has invaded the rock along the vein margins, partially replacing the feldspar/cristobalite phases. The veins themselves consist of quartz margins, bladed calcite vein filling, and calcite-quartz polygonal mosaics in the vein center. Further work to more thoroughly characterize these materials will be undertaken in October.

Review of specifications was initiated for several geomechanical diagnostic systems for the Large Block Test. These include multiple point displacement extensometer systems, stress meters, acoustic velocity systems and a borehole scanner. This review led to the discovery that there may be two multiple point displacement extensometer systems on site and efforts to locate them were initiated.

The LLNL staff continued the hydrothermal modeling analysis of the Large Block Test. The 3 m x 3 m x 4.5-m-high block has an upper boundary with a constant temperature, pressure, and relative humidity (that allows gas to escape the block). Heat and fluid flow is represented between the block and the underlying rock. The model effectively extends infinitely downward below the ground surface. The block is being modeled with the use of a two-dimensional model, which represents the cross-section that is orthogonal to five parallel, uniformly-spaced, 300 W heaters. The two-dimensional, cross-sectional model assumes adiabatic boundaries on the sides of the block (i.e., perfect insulator) and is very useful in showing how long it takes for thermal interference between the heaters to occur.

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The block was modeled with an R-Z axisymmetric model which averages the heating from the individual heaters with a disk-shaped heat source. The 3 x 3 m cross-sectional area of the block is represented by a circular cross section with a 3.385-m diameter (giving it the same cross-sectional area).

The heater horizon is located 3 m below the top of the block. The R-Z axisymmetric model can represent the heat loss out of the sides of the block. The sides are modeled as having a layer of insulation with a specified thickness and thermal conductivity,  $k_{th}$ . Because of its large heat capacity and  $k_{th}$ , the loading frame (that confines the block) is assumed to be at a constant temperature. For the insulation layer, a  $k_{th}$  of 0.110 W/m°C was assumed which is a typical value for wood (Douglas Fir). A suite of calculations assuming the block to have adiabatic sides (which could be achieved through the use of guard heaters) was also run. Gas-phase and liquid-phase flow can occur across the upper boundary of the block. The upper boundary is either a constant temperature boundary or an adiabatic boundary which is capable of becoming a constant temperature boundary.

The model extends vertically downward to the water table (assumed to be at a depth of 568.1 m) and out to a radial distance of 205 m. For the time-scale of the Large Block Test, the model effectively extends infinitely in the radial and vertical (downward) direction. It was found that heat from the Large Block Test drives hydrothermal flow effects in the rock underlying the Large Block Test. These effects occur primarily within the first 10 m of rock underlying the Large Block Test. The initial vertical temperature, saturation, and pressure profiles correspond to the geothermal and pneumatostatic pressure gradients, and to a net recharge flux of 0 mm/year. Note that this yields an initial liquid saturation of 58 percent in the large block. In order to adequately represent gas-phase flow, it is necessary to start with a pneumatostatic pressure distribution.

In the parameter sensitivity study, three variables were considered: the insulation thickness (or whether adiabatic boundaries are maintained), the manner in which temperature is controlled at the upper boundary of the block, and bulk permeability,  $k_b$ .

The lateral insulation thicknesses of .3 and .6 m were considered. Even for a .6-m-thick insulation, the heat loss out of the sides of the block is substantial, causing sub-boiling conditions and condensate drainage to persist at the outer edges of the block. Condensate shedding around the perimeter of the block diminishes the magnitude of saturation buildup in the condensate zone overlying the boiling zone. Because of the intent to maximize the potential for refluxing, possibly resulting in the heat-pipe effect occurring above the heaters, condensate shedding along the cooler sides of the block is not desired. When the upper boundary is maintained at a constant (ambient) temperature, it takes about 0.5 year for a steady-state temperature profile to develop. The heat loss out of the top and sides of the block limits the spatial extent of dryout and condensate buildup.

When an adiabatic lateral boundary and constant temperature upper boundary are maintained, the boiling zone extends out to the lateral boundaries within 90 days, substantially limiting condensate drainage around the perimeter of the block. Consequently, the saturation buildup in the upper condensation zone is very pronounced, maximizing the potential for

refluxing above the heater horizon. A steady-state temperature profile is established within 0.5 year. Adiabatic sides also enable the development of a larger dryout zone; however, it was found that maintaining a constant (ambient) temperature upper boundary substantially limits the vertical extent of refluxing above the heater horizon. Consequently, sub-boiling conditions persist for much of the block overlying the heater horizon.

In order to maximize the vertical extent of refluxing (i.e., two-phase conditions) above the heater horizon, it is necessary to maintain an adiabatic upper boundary until the top of the block approaches the nominal boiling point. In a further suite of calculations, an adiabatic upper boundary was maintained until the temperature at the top of the block reached 83°C, and thereafter the upper boundary was maintained at 83°C. Controlling the upper boundary in this manner resulted in the upper two-phase zone being more than 1 m in vertical extent. The saturation buildup in this zone was substantially greater than the case where the upper boundary temperature was fixed at ambient temperature.

Also considered were the values of bulk permeability,  $k_b$ , of 10 and 100 microdarcy, 1, 10, and 280 millidarcy, and 5 and 40 darcy. For  $k_b$  of 1, 10, and 280 millidarcy, the vertical extent of the dryout zone is almost identical, and the effect of buoyant, gas-phase convection is negligible (i.e., does not cause the dryout zone to deviate from being vertically symmetrical about the heater horizon). For a  $k_b$  of 5 darcy, the effects of buoyant gas-phase convection begin to become noticeable, with more than 50 percent of the total steam flow being upward. For a  $k_b$  of 40 darcy, buoyant vapor flow dominates gas-phase flow, with all of the steam flowing upward, resulting in a much greater buildup of condensate above the heater horizon. The threshold  $k_b$  (where the effects of buoyant vapor convection begin to dominate gas-phase flow) is essentially the same in the Large Block Test as in the in situ heater tests and repository-heat-driven hydrothermal flow. For  $k_b$  values of 10 and 100 microdarcy, dryout due to boiling is effectively throttled, thereby reducing the volume of the dryout zone relative to the cases where  $k_b > 1$  millidarcy.

Activity 1.10.4.4.2 - Repository horizon rock-water interaction. No progress during the reporting period; this was an unfunded activity.

Activity 1.10.4.4.3 - Numerical analysis of fluid flow and transport in repository horizon near-field environment. No progress during the reporting period; this was an unfunded activity.

**Forecast:** The Activity Plan for the Engineered Barrier System Field Tests will be drafted. Work will continue on the preparations, procurement, etc. for the Large Block Test.

#### **2.6.2.6 Study 1.10.4.5 - Characterize the Effects of Man-Made Materials on Water Chemistry in the Postemplacement Environment**

Revision of Study Plan 8.3.4.2.4.5, "Characterization of the Effects of Man-Made Materials on the Chemical & Mineral Changes in the Post-Emplacement Environment" is currently being reviewed.



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Activity 1.10.4.5.1 - Effect of grout, concrete, and other repository materials on water composition. The revised Study Plan 8.3.4.2.4.1, "Characterization of the Chemical and Mineralogical Changes in the Post-Emplacement Environment," was completed in draft form.

As a result of contacts made at meetings, activities continued with emphasis on procurement of information on introduced materials. Emphasis has been placed on diesel fuel and other organic compounds, colloids, biodegradation of tracer fluids, and water. The sources and potential amounts of water under investigation are those that may result from human intrusion and construction of the repository.

Staff have initiated the first series of diesel fuel stability experiments. The preliminary results demonstrate that diesel fuel comprises a vast array of constituents of varying stabilities. There is good evidence of chemical reactions taking place at 200°C. Some of the products are carboxylic acids which may prove to be aggressive to waste canister materials.

Staff from LLNL met with M&O personnel to discuss concerns regarding organic materials in general. They also reviewed the present diesel fuel experiments and visited the organic materials experimental facilities. Interest was expressed in obtaining information regarding the stability of hydraulic fluids and the M&O agreed to supply information regarding the range of hydraulic fluids that may be used during the construction of the ESF.

An LLNL representative of the Man-Made Materials Task attended a meeting on Waste Isolation Analyses and Test Interference Evaluations, held July 2, 1993, in Las Vegas, Nevada. This interaction improves the coordination of results from the Man-Made Materials study with Waste Isolation Evaluations.

Geothermal power companies in Taupo, New Zealand, were visited in August 1993 by LLNL and YMPO staff. The purpose of these meetings was to discuss the development of a collaborative relationship that will provide long-term chemical information of interest to YMPO and to obtain access to chemical data, samples of degraded materials, boreholes for experimentation and sampling, and geothermal areas not accessible to the public. This study will benefit both the Geochemistry and the Man-made Materials Tasks at LLNL and will be conducted by both tasks. A contract is presently in place between the Institute of Geological and Nuclear Sciences, a Crown Research Institute of New Zealand, and the Geochemistry task at LLNL for the initiation of geochemical studies. Of particular interest to the power companies are many of the long-term materials degradation issues of the man-made materials task.

The potential for conducting studies on degradation of man-made materials in collaboration with New Zealand geothermal interests is being pursued as part of a geochemical analog project for the YMP. One area of mutual interest that will be addressed immediately is cement biodegradation. The rare opportunity to acquire cement samples from an usually inaccessible area that has been exposed to elevated temperatures over a period of five years and is showing extensive signs of biodegradation will present itself in mid-October 1993. A complete plant shutdown at this site, which only occurs once every two years for a period of two days, will take place at that time. During that window of opportunity, if

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foreign travel arrangements can be made in time, plans are to collect samples for culture and identification, as well as future experimentation. Another site, which contains some of the oldest (up to 40 years) synthesized materials, will be shut down for a similar period of time in February 1993. This shutdown will offer the opportunity to obtain other samples, primarily inorganic materials for analysis.

A paper entitled "Chemical and Mineralogical Concerns for the Use of Man-Made Materials in the Post-Emplacement Environment" (Meike) was submitted to YMPO for approval on August 9, 1993. This paper was originally prepared for M&O personnel and submitted in January 1993.

A paper entitled "Formation of Colloids from Introduced Materials in the Post-Emplacement Environment: A Report on the State of Understanding" (Meike and Wittwer, 1993) was presented at Focus '93. This literature review will provide the basis for determining the necessity of future experimental and analog studies.

Activity 1.10.4.5.2 - Effects of container and borehole liner corrosion products on water chemistry. No progress during the reporting period; this was an unfunded activity.

Activity 1.10.4.5.3 - Effects of man-made materials in presence of radiation field. No progress during the reporting period; this was an unfunded activity.

Activity 1.10.4.5.4 - Numerical analysis and modeling of man-made materials/water interaction. No progress during the reporting period; this was an unfunded activity.

**Forecast:** Work will continue on the diesel fuel stability experiments and the studies on degradation of man-made materials in collaboration with New Zealand geothermal interests.

### **2.6.3 Characteristics and Behavior of the Waste Form (SCP Section 8.3.5.10)**

#### **2.6.3.1 Activity 1.5.1.1 - Integrate Waste Form Data and Waste Package Design Data**

Subactivity 1.5.1.1.1 - Integrate spent fuel information. The responses to the review comments for the Preliminary Waste Form Characterization Report were completed and returned to YMPO.

Subactivity 1.5.1.1.2 - Integrate glass waste form information. No progress during the reporting period; this was an unfunded activity.

Subactivity 1.5.1.1.3 - Integrate waste package and repository design information. No progress during the reporting period; this was an unfunded activity.

**Forecast:** Integration of waste form data into the Waste Form Characterization Report will continue.

### 2.6.3.2 Activity 1.5.2.1 - Characterization of the Spent Fuel Waste Form

Subactivity 1.5.2.1.1 - Dissolution and leaching of spent fuel. The dissolution response of spent fuel is a part of the characterization and data input for performing waste package design activities and repository performance assessments. The dissolution response testing addresses spent fuel types, reactor burnups, oxidation phases, heterogeneous effects of radionuclides on and in pellet fragments, potential water temperatures, and water chemistries. Only the flow-through dissolution activities are currently supported. The activity plans for these tests contain test matrices that prescribe conditions and types of flow-through runs to be completed for dissolution model development.

The eight  $\text{UO}_2$  dissolution experiments begun in April 1993, as a part of the LLNL test matrix, were completed. These eight experiments are at temperatures of 50° and 75°C, and at subatmospheric oxygen levels of 0.2 and 2 percent. This group included three identical runs at midvalues of the variables to test for reproducibility of the runs. This completes the initial test matrix of nineteen experiments at alkaline conditions. These tests were continued at room temperature using the same buffers to obtain additional test replications and data. These results will provide additional data to test intrinsic  $\text{UO}_2$  dissolution models that are developed. These continuations, plus the original test matrix runs, gives 35 experimental runs under a wide variety of conditions to develop dissolution response models. Detailed analysis of the final results of the full test matrix is required before formal conclusions can be made.

Analysis has begun of the final results of the original test matrices at Pacific Northwest Laboratory (PNL) for spent fuel dissolution and at LLNL for  $\text{UO}_2$  dissolution. The trends in dissolution rates are similar in both matrices. There are a few experimental points in both matrices that do not seem consistent with the other data. These are being re-examined or repeated. Two experiments at LLNL are under way that are repeats of individual runs in the original test matrix. The two earlier runs had dissolution rates that varied considerably during the course of the experiments and were not consistent with other runs in the matrix.

Work is continuing at LLNL on the two long-term, room-temperature dissolution experiments ongoing since fall of 1992. These experiments use  $\text{UO}_2$  powder from a batch provided by PNL that had been used in similar experiments. Our Canadian colleagues at Pinawa, Manitoba, are performing similar experiments. The first buffer composition is 0.02 M sodium bicarbonate at a pH of 8. The second composition is a 'standard' saline solution with 0.01 M sodium bicarbonate and 0.1 M sodium chloride saturated with air; the pH is not controlled. Since February 1993, the uranium dissolution rate for the first nonsaline solution slowly increased to about 2 mg/m<sup>2</sup>·d in mid-April 1993. The experiments were stopped for about one month during a move of the equipment to another building. Upon resuming the experiment in mid-May 1993, the dissolution rate has increased to 2.5-4.0 mg/m<sup>2</sup>·d. The  $\text{UO}_2$  dissolution rate in the saline solution did not change during the one month stoppage. Its dissolution rate has also slowly increased over time, but is less variable at about 4-5 mg/m<sup>2</sup>·d.

Analysis and documentation are being completed for all the experimental data of the previous dissolution tests performed on  $\text{UO}_2$  and spent fuel. Following this report work, a

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sequence of experiments will be performed to examine the effects of oxidation state on uranium oxide dissolution. Two experiments with schoepite have begun at room temperature and 20 percent oxygen. One experiment includes hydrated schoepite ( $\text{UO}_3 \cdot 2\text{H}_2\text{O}$ ) as a sample; the other experimental sample is dehydrated schoepite ( $\text{UO}_3 \cdot \text{H}_2\text{O}$ ). The results of these two experiments will be compared with similar experiments previously conducted at very low oxygen concentrations. These prototypes will provide data to plan a test matrix of dissolution tests on the higher  $\text{UO}_2$  oxidation states. These experiments are similar to those experiments begun at PNL on spent fuel.

A test matrix for flow-through dissolution tests at PNL with three different spent fuels (Approved Testing Material [ATM]-104, ATM-105, and ATM-106), three oxidation states ( $\text{UO}_2$ ,  $\text{O}_4\text{O}_{9+x}$  and  $\text{O}_3\text{O}_8$ ), two temperatures (25° and 75°C), and three carbonate/bi-carbonate concentrations (0.2, 2, and 20 mmol) was completed and included in an addendum to the test plan. This addendum was included in the Activity Plan, "Flow-Through Dissolution Studies on Spent Fuel."

The flow-through dissolution tests at PNL on ATM-106 fuel (pressurized-water reactor fuel with a 50 GWd/MTIHM burnup and 18 percent fission gas release) in both oxidized (O/M ~2.4) and unoxidized forms are in progress. Preliminary results from the oxidized specimens do not indicate a high initial release of Tc such as was found in a previous test with oxidized ATM-105 fuel (boiling water reactor fuel with 31 GWd/MTIHM burnup and 0.6 percent fission gas release).

Another specimen of ATM-106 fuel was oxidized to  $\text{U}_3\text{O}_8$  by heating in air overnight at 425°C. The surface area (measured by Brunauer-Emmett-Teller surface area measurements) increased by a factor of about 40 compared with unoxidized particles of about 1 mm in size. The large increase in surface area is the result of substantial intra- and inter-granular cracking during oxidation. Flow-through tests on the  $\text{U}_3\text{O}_8$  material have been completed. Preliminary analytical results indicate that 15 percent of the total Cs inventory in the fuel was dissolved in the first 29 hours compared with only 4 percent of the total uranium. Thereafter, the U and Cs dissolution rates were equal. A possible explanation for the 11 percent excess of Cs over U dissolution is that some of the Cs may be associated with gas bubbles in the spent fuel matrix. Cracks caused by the oxidation probably intercepted many of these bubbles thereby exposing the associated Cs for immediate dissolution. It was anticipated that oxidizing the fuel to  $\text{U}_3\text{O}_8$  might also give rise to an increase in the initial dissolution of Tc; however, this was not observed.

Subactivity 1.5.2.1.2 - Oxidation of spent fuel. The oxidation drybath testing (D-20-45) activity on spent fuel at low temperatures (<200°C) continued at PNL. The drybath apparatus was initially designed to run two to three years; testing has continued for about eight years. The temperature control system in one drybath has failed; samples were transferred from the failed drybath to another and testing restarted. At the existing temperatures (<200°C), the spent fuel oxidation changes crystalline phase from a  $\text{UO}_2$  lattice to a  $\text{U}_4\text{O}_9$  lattice structure; however, the oxygen content is that of a  $\text{UO}_{2.4}$ . The excess oxygen atoms means that the  $\text{U}_4\text{O}_9$  phase is nonstoichiometric. Also, the  $\text{U}_4\text{O}_9$  with an O to U of (<2.4) is metastable, because the  $\text{U}_3\text{O}_7$  ( $\text{UO}_{2.33}$ ) lattice structure is also stoichiometrically accessible. Some

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previous spent fuel oxidation experiments indicate that the metastable  $U_4O_9$  phase ( $UO_{2.4}$  oxygen excess) transitions upon further oxidation directly to a  $U_3O_8$  phase. However, little was known of the phase transition kinetics nor the rate of oxidation and its associated mechanism.

Because of this spent fuel degradation by oxidation and the potential for higher dissolution rates of the higher oxidation phases, the oven drybath test plan and activity plan were updated to run a drybath at a higher temperature ( $\sim 250^\circ\text{C}$ ). In this temperature range, the transition testing of some existing  $U_4O_9$  (at  $UO_{2.4}$ ) and some "fresh"  $UO_2$  spent fuel multifragment samples were initiated. The phase transition kinetics of the two types of samples will be quantified through weight gain measurements and by selecting fragments at various time intervals of the weight gain measurements in order to systematically perform microscopic observations on them.

The first interim examination of the  $255^\circ\text{C}$  drybath test was completed at 195 hours of test time. Those samples that were initially unoxidized had oxidized to an O/M between 2.35 and 2.42 (i.e., essentially all the way to the 2.4 weight gain plateau). Those samples that had been oxidized to O/M  $\sim 2.4$  at  $175^\circ\text{C}$  had very little change in O/M which would be expected for samples already on the plateau. In the next interim examination of the drybath samples, the weight gain was as expected in the  $110^\circ$ ,  $130^\circ$ ,  $175^\circ$ , or  $195^\circ\text{C}$  drybath tests. However, the  $255^\circ\text{C}$  drybath test continued to provide new information:

1. The Turkey Point fuel samples oxidized to a higher plateau than the other fuels (in the lower temperature tests, it was the lowest O/M plateau).
2. A weight gain plateau appeared to be occurring, the samples continued to gain weight and O/M ratios of 2.5 have been reached by some samples.
3. While sample preparation for microscopic analysis indicated the spent fuel was friable, x-ray diffraction analysis detected only  $U_4O_9$  and no  $U_3O_8$ .

A third interim examination was conducted at 1667 hours. The samples continued to gain weight, but at a significantly reduced rate. No samples were removed for additional microscopic analysis. It appears that after the initial transient weight gain, the samples are all now gaining weight at the same reduced rate; this includes the samples with a higher initial O/M that were taken from earlier tests at  $175^\circ\text{C}$ . Future sample examinations as oxidation progresses will continue to be performed to obtain a time history of the phase change kinetics and the oxidation rate response.

In addition to the oven drybath testing at higher temperatures, thermogravimetric apparatus testing for phase change kinetics are being initiated. Thermogravimetric apparatuses were brought out of storage and one is now fully operational. The thermocouples in the other thermogravimetric apparatus is being calibrated, and should also be operational shortly. An  $^{18}\text{O}_2$  run indicated that the equipment was leak tight. During some calibration testing, fluctuations in the thermogravimetric apparatus balance were observed but were well within tolerable limits. These fluctuations are apparently caused by thermal convections and

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were also present in previous thermogravimetric apparatus runs. To restart the thermogravimetric apparatus testing activity, an update of the existing test and activity plans are required. Therefore, some preliminary tests are being performed in support of a thermogravimetric apparatus oxidation test plan, to calibrate the equipment, and to obtain baseline information to be used to determine a suitable test matrix.

For one of the preliminary thermogravimetric apparatus tests, a piece of unirradiated  $\text{UO}_2$  doped with eight percent  $\text{Gd}_2\text{O}_3$  was held at  $283^\circ\text{C}$  for 454 hours. This sample exhibited behavior similar to that of drybath tested spent fuel (an oxygen-to-metal ratio of 2.35 plateau was reached). This sample broke into powder while being removed. Subsamples for x-ray diffraction and scanning electron microscopy analysis were taken. An adequate subsample for transmission electron microscopy analysis was not obtained due to sample friability. Both x-ray diffraction and scanning electron microscopy confirmed the presence of  $\text{U}_4\text{O}_9$  and approximately three percent  $\text{U}_3\text{O}_8$ . The initial results from scanning electron microscopy analysis indicate the  $\text{U}_3\text{O}_8$  is dispersed throughout and not located on the grain boundaries.

In another preliminary thermogravimetric apparatus test, a fragment of BWR-ATM 105 fuel has run for over 300 hr at  $283^\circ\text{C}$ . An O/M ratio of 2.647 has been reached. The sample rapidly gained weight to an O/M of 2.35. However, a true plateau around an O/M of 2.4 was never attained since the sample continuously gained weight. But the weight gain rate,  $[d(\text{O/M})/dt]$ , decreased significantly after obtaining a 2.35 O/M at around 125 hours. It now appears that the rate of weight gain is slowing down and possibly may be approaching a second "plateau." The test is continuing.

Subactivity 1.5.2.1.3 - Corrosion of zircaloy. No progress during the reporting period; this was an unfunded activity.

Subactivity 1.5.2.1.4 - Corrosion of and radionuclide release from other materials in the spent fuel waste form. No progress during the reporting period; this was an unfunded activity.

Subactivity 1.5.2.1.5 - Evaluation of the inventory and release of carbon-14 from zircaloy cladding. No progress during the reporting period; this was an unfunded activity.

Subactivity 1.5.2.1.6 - Other experiments on the spent fuel waste form. No progress during the reporting period; this was an unfunded activity.

**Forecast:** A new sequence of experiments will be performed this coming year to examine the effects of oxidation state on uranium dissolution. Studies of spent fuel with matrix oxidation states of  $\text{U}_4\text{O}_9$  and  $\text{U}_3\text{O}_8$  will continue at PNL, with some variation in burnup, according to the ATM fuels available. The higher uranium oxide forms,  $\text{U}_3\text{O}_8$  and  $\text{UO}_3$ , will be studied at LLNL. These results will provide data to evaluate the effect of burnup on the spent fuel dissolution rates. In addition to the ongoing flow through dissolution testing activities at PNL and LLNL, dissolution testing on spent fuel under unsaturated conditions will be initiated at Argonne National Laboratory. The unsaturated

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testing conditions use relatively small amounts of water and will provide release rate data for dripping water flow (thin film flow) and partial surface wetting conditions.

The higher temperature oven dry bath oxidation testing will be continued to obtain phase change kinetics data for the transformations of  $\text{UO}_2$  to  $\text{U}_4\text{O}_9$  to  $\text{U}_3\text{O}_8$  to  $\text{UO}_3$ . In addition, the test plan and activity plan to restart the thermogravimetric analysis oxidation testing will be completed and thermogravimetric testing at the Quality Affecting level will be initiated. The two oxidation testing methods provide flexibility and breadth in atmospheric and temperature controls to provide the spent fuel oxidation rate and oxidation phase change data in the temperature range of  $200^\circ$  to  $300^\circ\text{C}$  that is required to assess spent fuel repository response issues.

### 2.6.3.3 Activity 1.5.2.2 - Characterization of the Glass Waste Form

Subactivity 1.5.2.2.1 - Leach testing of glass. The N2 tests (SRL actinide-doped glass) have been in progress for 92 months. The N3 tests (ATM-10, a West Valley actinide-doped glass) continue and have been in progress for 73 months.

Subactivity 1.5.2.2.2 - Materials interactions affecting glass leaching. No progress during the reporting period; this was an unfunded activity.

Subactivity 1.5.2.2.3 - Cooperative testing with waste producers. No progress during the reporting period; this was an unfunded activity.

**Forecast:** The N2 and N3 unsaturated tests will continue. A low level of geochemical modeling work will continue using input from experimental work not performed as part of the YMP.

### 2.6.3.4 Activity 1.5.3.1 - Integrate Scenarios for Release From Waste Packages

Subactivity 1.5.3.1.1 - Develop scenario identifications. The Yucca Mountain Integrating Model submodels are being incorporated into the Total System Performance Assessment (TSPA) 1993 source term.

Subactivity 1.5.3.1.2 - Separate scenarios into anticipated and unanticipated categories. No progress during the reporting period; this was an unfunded activity.

Subactivity 1.5.3.1.3 - Development of parameters describing the scenarios. Near-field environment/engineered barrier system model parameters were elicited and abstracted for use in TSPA 1993 source term. No scenario analysis was funded.

Subactivity 1.5.3.1.4 - Determine adequacy of design envelope of waste package. Information pertaining to this subactivity is provided under Subactivity 1.5.3.1.1.

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**Forecast:** Work will continue to incorporate the Yucca Mountain Integrating Model submodels into the TSPA 1993 source term.

### 2.6.3.5 Activity 1.5.3.2 - Develop Geochemical Speciation and Reaction Model

Subactivity 1.5.3.2.1 - Develop data base for geochemical modeling. GEMBOCHS Change Requests 2-5 and 7-15 using the CNGBOCHS system were resolved and submitted during this reporting period.

Programs FACET and JEWEL (formerly DBAPP and DOOUT) were used to generate five revised suites of thermodynamic data files (DATA0 suites R19-R23) that support the EQ3/6 geochemical modeling package. These new data files reflect various revisions associated with resolution of the change requests submitted this reporting period. These DATA0 suites together with their DATA1 analogs, were transferred to a dedicated directory on s60 where they can be accessed by local EQ3/6 users.

The development of a WINDOWS/4GL Graphical User Interface version of JEWEL was completed and beta testing of this new software has begun. This user-friendly, mouse-driven code facilitates point-and-click generation of thermodynamic data files for use with EQ3/6, GT, and other geochemical modeling packages. The development of a WINDOWS/4GL version of FACET has begun. This code will permit point-and-click review of GEMBOCHS data by onsite and offsite GEMBOCHS users; password-restricted to GEMBOCHS staff members.

GEMBOCHS was updated to include equilibrium-constant and reaction-enthalpy data from the CHEMVAL-II data base. A modified version of JEWEL which facilitates generation of CHEMVAL-II data files for use with EQ3/6 was created. Work has started on establishing a GEMBOCHS "patron" account. This login account will provide offsite GEMBOCHS users with direct access to GEMBOCHS software (which facilitates review and application of GEMBOCHS data) and the current DATA0 suite (for use with EQ3/6). These online services will provide convenient and timely access to GEMBOCHS for offsite YMP Participants.

Subactivity 1.5.3.2.2 - Develop geochemical modeling code. This activity maintains and develops the EQ3/6 software package for use in near-field environment characterization and site characterization. Version 7 is being maintained. Version 8, which involves a significant rewrite to support new capabilities, is being developed.

Testing and final preparation of Version 7.2 was completed in the reporting period. Update packages were distributed to YMP Participants and other YMP-related recipients. This new version is available in a 486 personal computer form, in addition to a UNIX work station form. It is the first version of EQ3/6 produced by LLNL for the personal computer. It contains special personal computer interface software to complement the existing UNIX interface software. It also contains two new input file reformatters, XCON3 and XCON6. These allow input files for the EQ3NR and EQ6, respectively, to be changed from a compact



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format to a menu-style format and vice versa, and from one supported version level to another. The input file formats for Version 7.2 are slightly different from those employed in Versions 7.0 and 7.1. These reformatter codes can be used by current users to update their old input files to Version level 7.2;

A new suite of data files (R22) is included in Version 7.2. It contains corrections to the thermodynamic data for two magnesium hydroxysulfate minerals. It also reflects a reorganization of the reactions involving aqueous organic species. The EQ3/6 test library was rebaselined using these new data files

Internal use of this version has uncovered a few minor bugs, which are being addressed for a Version 7.2a update. Version 5.11 of the Lahey FORTRAN compiler has been received and is being tested to see if it will eliminate a memory manager fault when running the personal computer version other than in a DOS window under Microsoft Windows 3.1. The Version 7.2a update will be distributed in late-October 1993.

Work is continuing on Version 8.0. As specified in the Software Design Description, this version is a major rewrite incorporating major changes in the data structure in order to accommodate improvements in numerical methods and the addition of new functional capabilities. The new capabilities planned for Version 8.0 include:

1. Allowing for redox disequilibrium in reaction-path calculations (important to treating the metastable persistence of dissolved components such as sulfate, nitrate, and organics;
2. A generic ion-exchange model; and
3. Correction of supporting data, mostly thermodynamic, to pressures off the 1.013 bar steam saturation curve.

The data restructuring has been completed. The new structure, which is common to both EQ3NR and EQ6, is significantly different from that previously employed in either code. Both codes formerly had different data structures, which was why EQ3NR had a redox disequilibrium capability, but EQ6 did not. The new structure is more like the old one in EQ3NR, although it incorporates some important new features. All chemical species are now defined by a common set of arrays. The set of basis species is defined by a point array, instead of being equated to a particular subset of aqueous species. Thus, basis switching no longer requires switching species indices. The new structure allows a species of any type (e.g., aqueous, gas, mineral, solid solution component, exchange species) to be defined as a basis species. This is important to maximizing numerical stability.

The new structure also incorporates a dual basis concept. All mass balances are defined in terms of a convenient, familiar set of basis species (e.g.,  $\text{Na}^+$ ,  $\text{Ca}^{2+}$ ,  $\text{Cl}^-$ ) as defined in the supporting data file. A second set of basis species is used to define the reduced set of unknowns used to solve the set of governing equations. Defining mass balances in terms of a familiar set of species is important because it helps prevent misinterpretations of mass balance

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quantities in code input and output. Mass balances computed using a basis set selected to maximize code numerics may appear to have physical significance (e.g., correspondence with chemical analyses), when instead they may have only mathematical significance.

Version 7 was heavily dependent on COMMON blocks to define the data structure. It was also heavily dependent on INCLUDE files (mostly to contain these COMMON blocks). Among EQLIB, EQ3NR, and EQ6, there were about 134 COMMON blocks, 147 INCLUDE files, and 2052 references to INCLUDE files. This has been reduced to 16 COMMON blocks, 11 INCLUDE files, and 52 references to INCLUDE files. This was accomplished by making greater use of calling sequences to handle data flow. The resulting code is much more modular and hence much easier to maintain and develop.

The general rewrite has been largely completed. The redox disequilibrium capability in EQ6 is now in the code. The software (EQ3NR as well as EQ6, as this code has been extensively changed even though no new capabilities have yet been added) is now in a testing phase. The test case library from Version 7 is being converted to Version level 8 format, using extended versions of the XCON3 and XCON6 input file reformatter codes that were created for Version 7.2. New problems are being added to test the redox disequilibrium capability in EQ6.

Software validation activities leading to the certification of Version 7 of EQ3/6 for use in quality affecting work continued through the reporting period, and have now covered all of the software with the exception of EQ6.

At the request of the Quality Assurance Manager, Quality Procedure 3.2 and associated Technical Implementing Procedures (TIP-YM-10 through TIP-YM-20) are being reviewed.

**Forecast:** The current testing phase for Version 8 of EQ6 will be completed in early FY 1994. The new capabilities for handling the generic ion exchange model and thermodynamic pressure corrections will then be added. After final testing and preparation, including preparation of the relevant code documentation, Version 8.0 will be released. This is currently planned to take place at the end of July 1994. Activities will then begin for Version 9.0, focusing on the addition of sorption models.

Software validation activities for Version 7 will continue through the first few months of FY 1994, focusing on the EQ6 code. This version should then be ready for certification for use in quality affecting work. Software validation activities for Version 8 will commence when Version 8.0 completes the final testing phase.

The beta testing of the WINDOWS/4GL JEWEL and a user's manual for this software will be completed.

The prototype development of a WINDOWS/4GL FACET will be completed.

Work will continue to establish a GEMBOCHS "patron" account.

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As dictated by availability and/or user requirements, additional or revised thermodynamic data will be incorporated into GEMBOCHS and new or improved extrapolation algorithms will be incorporated into JEWEL. As required by GEMBOCHS and/or EQ3/6 modifications, FACET and JEWEL will be used to generate revised suites of thermodynamic data files (DATA0 suites) that support EQ3/6.

### **2.6.3.6 Activity 1.5.3.3 - Generate Models for Release From Spent Fuel**

Subactivity 1.5.3.3.1 - Generate release for spent fuel models. No progress during the reporting period; this was an unfunded activity.

**Forecast:** No activity is planned for FY 1994.

### **2.6.3.7 Activity 1.5.3.4 - Generate Models for Release From Glass Waste Forms**

Subactivity 1.5.3.4.1 - Generate release models for glass waste forms. No progress during the reporting period; this was an unfunded activity.

**Forecast:** Activity plan for glass release models will be developed in FY 1994.

### **2.6.3.8 Activity 1.5.3.5 - Waste Package Performance Assessment Model Development**

Subactivity 1.5.3.5.1 - Development of system model. This activity has focused on development of an engineered barrier system/near-field environment source term model for use in TSPA 1993 which has improved mechanistic submodels and incorporates thermal effects. This source term will allow TSPA 1993 to examine alternative designs and thermal loading strategies.

Work continues on the scoping study of cladding temperature history for various drift emplacement heat loadings, and of cladding creep endurance. Drift backfill 75 years after waste emplacement is assumed. Based on recent literature, the temperatures are somewhat higher than in the earlier parameterization of thermal results, but feasible repository loadings can meet both dryout and cladding goals. The cladding creep model was extended to incorporate reduced pressure load due to the progress of creep. This effect had been included in some previous papers, but just examined and not included in others; noninclusion is somewhat conservative.

The main contributors to elevated temperatures in the fuel cladding are the heating of the rock mass (dependent on the areal power density) and the temperature difference across the backfill (dependent on the heat generation rate of the package at any given time and on the thermal conductivity of the backfill). The container wall-to-center difference contributes only on the order of 10 percent of the total heat rise, assuming a 21-pressurized-water reactor-assembly container. The current analysis based on recent papers gives somewhat higher

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temperatures than reported previously. There are still some feasible loading plans that will provide an areal power density of 223-247 kW/ha (90-100 kW/acre) using 30-year-old spent fuel (areal mass loading of 301 to 336 MTU/ha [122 to 136 MTU/acre]) and still meet the cladding strain limit as calculated by a conservative approach. These loadings have 10 to 12 pressurized-water reactor assemblies per waste package, rather than 21 assemblies as in the preliminary analysis. Increasing the loading per package would require some other design choices affecting the heat transfer.

The cladding creep rate is dependent on temperature and stress. Creep reduces the stress. In the initial analysis used above, this source of reduction was not included. Further analysis showed that including it makes an appreciable difference, with improved performance. The stress is generated by internal gas pressure in the fuel rod. The internal gas is a fill gas plus a small amount of fission gas released to the fuel rod's void space. During reactor operation, the fuel pellets swell, reducing the void volume by 30 to 50 percent. Gas pressure depends on temperature and volume. The cladding creep increases the volume progressively. The creep model was extended to include the strain-dependent effects and it was found that it makes an appreciable difference in extending creep lifetime and a modest difference in increasing the allowable temperature. Analysis is continuing. Note that creep of cladding can occur mainly in two time periods: the first decade of temporary dry storage, if utilized, and the first few decades after backfill is emplaced in repository disposal. It is urged that there be coordination of creep allowables in these two design periods before changing any allowables to take the benefit of the finite-strain effect on creep.

The LLNL staff is developing a summary model of the near-field environment of the waste package. This will consider the thermal transient and dryout based on papers by LLNL personnel and others in the field. The product will be time histories, in table or algorithm form, of temperature, fractional saturation, fraction of waste packages wetted, and liquid water flux. A calculational procedure was implemented to evaluate the distance of fracture flow penetration due to refluxing of condensate water above the repository. This procedure includes a spatial variability in water flux and in fracture sizes, and hence a spatial variability in distance of refluxing.

Information on the source term was presented to SNL for use in TSPA 1993. As part of this effort, Near Field and Performance Assessment staff modeled an important near-field hydrological process, localized water penetration beyond a boiling front, through a dried-out zone, down to the level of a repository. At random locations, this flux could wet some waste packages. In order for penetration to happen at some location, it is necessary that the localized water flux be greater than the amount of water that can be evaporated by the heat flux from the repository. This heat flux is assumed to be essentially uniform, whereas water fluxes are known to exhibit spatial heterogeneity. Using a lognormal distribution to characterize this heterogeneity (as is suggested in the literature), numerical results have been derived for the fraction of waste packages that get wet under the assumptions of 141 and 282 kW/ha (57 and 114 kW/acre) initial areal power density, both at the center and edge of the repository. For representative assumed input values, the fraction of waste packages in the repository center zone that get wet is on the order of a few per thousand for the first 50 to 100 years. The fraction then drops by about an order of magnitude in the 141 kW/ha

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(57 kW/acre) case. The fraction drops by about three orders of magnitude in the 282 kW/ha (114 kW/acre) case, to an expected value well below one waste package in the whole repository center zone after a few hundred years.

Staff continued providing both SNL and the M&O with detailed temperature, saturation, and liquid flux histories throughout the repository and unsaturated zone for repository-unsaturated zone-saturated zone-scale model calculations using V-TOUGH. This is being done in support of TSPA 1993. We applied a blended repository thermal loading history provided by the M&O that is based on the oldest fuel first waste receipt scenario, yielding an average spent fuel age of 26 years. Calculations for areal power densities of 70.5, 141, and 282 kW/ha (28.5, 57, and 114 kW/acre) (yielding areal mass loadings of 71.7, 143.5, and 287 MTU/ha [29, 58, and 116 MTU/acre]) were conducted. The 141 kW/ha (57 kW/acre) case (which falls within the thermal loadings described in the SCP-CDR) has a boiling period duration,  $t_{bp}$ , of 2600 years at the repository center.

At the request of the M&O, the liquid-phase velocity field at various times and the liquid-phase velocity history at various points from the repository horizon down to the water table have been provided based on the repository-unsaturated zone-saturated zone-scale hydrothermal calculations using V-TOUGH. These results can be used to calculate radionuclide transport in the unsaturated zone on the basis of averaged liquid-phase fluxes. Because of the spatial variability of liquid-phase flux, basing transport calculations on average fluxes may not accurately reflect the flow field calculated by V-TOUGH. In order to more accurately reflect the V-TOUGH-calculated flow field, it is preferred to track packets of particles released from waste package locations, as they are driven by the flow field in the underlying natural barrier system. Staff developed a family of "particle tracking" post-processors for V-TOUGH, called P-TRACK, PT-PLOT, and PT-MOVIE. P-TRACK calculates the x-y location versus time for each of the particles. PT-PLOT calculates the pressure, temperature, and saturation history for each of the particles. PT-MOVIE is a graphics program that produces a video animation of the moving particles. Colors can be used in PT-MOVIE to "tag" when or where the particles were released, or can be used to indicate the value of either pressure, temperature, or saturation of the moving particles. P-TRACK and PT-PLOT can be the basis for conducting radionuclide transport calculations where retardation may be treated as a function of pressure, temperature, and saturation. PT-MOVIE is an extremely valuable aid to visualize the spatial and time dependence of transport, as well as the relationship between transport and temperature and saturation.

Staff began work on documenting the stochastic model for condensate drainage. This model is being used for performance assessment modeling and predicts the spatial variability of condensate drainage onto waste packages. The condensate flux is modeled as a lognormal random field in space. The waste packages can become wet in those regions where fluxes are sufficiently focused that they overcome the vaporizing effect of the above-boiling thermal field. The mean condensate flux is the conditional expectation of the flux given that the flux exceeds a critical flux proportional to the mean condensate flux calculated by the V-TOUGH calculations. The proportionality factor is a function of the thickness of the dryout zone. In general, the thicker the dryout zone, the higher the threshold flux required for breakthrough to the waste packages.

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The following two workshops were hosted at LLNL to develop models and data for TSPA 1993. LLNL is responsible for a near-field environment/engineered barrier system source term which incorporates thermal processes:

1. June 11, Thermal History Workshop (participants from LLNL, U.S. Department of Energy, SNL and M&O).
2. June 23, Hydrothermal Water Flux Workshop (participants from LLNL, SNL and M&O).

A paper entitled "Post-Closure Performance Assessment of Waste Packages for the Yucca Mountain Project" (O'Connell et al., 1993) was approved by YMPO on August 25, 1993, and was published.

The PANDORA-1.1 user's manual is in technical editing for reviewers' stylistic comments and for ease of use.

The performance assessment function is continuing its development of a new-generation waste package/engineered barrier system performance assessment code. This work is being carried out on behalf of the M&O by the staff of PNL. Two working documents were written that describe progress in this effort. The first is "Mathematical Document for the AREST Code Development" and the second is "Software Requirements Specification for the AREST code Development." These documents are currently in M&O technical review. The focus of the AREST code upgrade effort is to ensure that the detailed waste package model accounts for the principal processes affecting container degradation, waste form alteration, and radionuclide release to the host rock.

The M&O performance assessment staff developed a model to perform thermal calculations in the vicinity of waste packages placed horizontally in drifts. The main features of this finite difference model include radiative heat transfer from the waste package to the drift wall and conduction heat transfer in the host rock. The effects of heat convection and moisture content in the host rock are neglected in this model. This model is presently being used to perform bounding calculations to determine the ranges of drift diameters and waste package spacings for various emplacement configurations, such that the allowable temperature limits of waste package and the host rock are not exceeded.

The M&O and University of California, Berkeley, staff completed documents entitled "Mass Transfer Induced by Thermal Effects in Unsaturated Porous Media" and "Evaporation of Water on a Heated Surface in a Cavity in Unsaturated Porous Media." The first report is an analysis of the evaporation of water from a liquid film on a heated surface into a surrounding unsaturated porous medium. The second report is a study of the steady-state heat and mass transfer near a heat source in an unsaturated porous medium to evaluate potential heat pipe effects. These reports are undergoing internal review.

A Performance Assessment Thermal Modeling Meeting was held in Las Vegas, Nevada, on June 29, 1993. The meeting presented a range of modeling results, from coupled

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multiphase thermal flow analyses through thermal-conductance-only evaluations. The M&O performance assessment staff presented talks discussing results of hydrothermal calculations performed with VTOUGH entitled "Subrepository Scale Hydrothermal Analysis in Support of TSPA," results of near field calculations for in-drift emplacement of robust canisters entitled "Bounding Thermal Calculations for Individual Waste Package Placement," and a summary of thermomechanical calculations for predicting spall from the drift walls entitled "Very Near Field Thermomechanical Analysis Using Discontinuous Deformation Method."

Subactivity 1.5.3.5.2 - Development of uncertainty methodology. A paper entitled "The Role of Multiple Barriers in Assuring Waste Package Reliability" (Bradford) has been submitted to YMPO for approval.

Subactivity 1.5.3.5.3 - Water flow into and out of a breached container. No progress during the reporting period; this was an unfunded activity.

**Forecast:** Work will continue to complete LLNL contributions to TSPA 1993 including the temperature dependent processes in the engineered barrier system and near-field environment.

Work will begin on the engineered barrier system sensitivity studies based on TSPA 1993.

Work will continue on trade studies for waste package-Advanced Conceptual Design.

### **2.6.3.9 Activity 1.5.4.1 - Deterministic Calculation of Releases From the Waste Package**

While not funded in FY 1993, improved waste package models were developed and release calculations were performed in support of the TSPA 1993 source term as described above.

**Forecast:** No activity is planned for FY 1994.

### **2.6.3.10 Activity 1.5.4.2 - Probabilistic Calculation of Releases from the Waste Package**

This activity is currently in the prototype and planning stage. The revised Scientific Investigation Plan for waste package performance assessment has been approved for interim use and has been submitted to the Project. Improved waste package models were developed and release calculations were performed in support of TSPA 1993 as described above.

**Forecast:** No activity is planned for FY 1994.

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### **2.6.3.11 Activity 1.5.5.1 - Determine Radionuclide Transport Parameters**

Subactivity 1.5.5.1.1 - Radionuclide distribution in tuff wafers. Work in this area that is also pertinent to determining the radionuclide distribution in tuff cores is reported under Subactivity 1.5.5.1.2. No significant activity occurred pertaining exclusively to distributions of radionuclides in tuff wafers due to reduced funding levels in FY 1993.

Subactivity 1.5.5.1.2 - Radionuclide distribution in tuff cores. Samples of single crystals of clinoptilolite to be used for diffusion experiments were added to #1N Na, K and Ca chloride salts, heated to 85°C, and are currently maintained at that temperature. These crystals were removed from the reaction flasks and embedded in epoxy in preparation for analysis by scanning electron microscopy and electron and ion probes. The single crystals were oriented so that (010), (100), and (001) crystal planes would be exposed for subsequent diffusion experiments. Additional single crystals were added to #1N Na, K, and Ca chloride salts at 85°C for future analysis. The preparation of a status report on diffusion in clinoptilolite was initiated.

Flow testing of the saw-cut fracture at ambient temperature showed that the automatic flow monitoring system is working. Small oscillations in the differential pressure and consequent flow are readily detected using this system. Flow-rate stability was difficult to maintain, apparently due to microbial fouling of the saw-cut fracture. At low differential pressures, the bacterial growth effectively shut down fracture flow. A sample injection loop was added to the flow-through apparatus and will be used for testing the behavior of a conservative tracer (Br<sup>-</sup>). Preparation of a report on the test phase for the flow-through apparatus was initiated. Transmission electron microscopy analysis of effluent showed the presence of iron (hematite) and silicon oxides (quartz) that may be related to the sawing process.

A sample of Well UE-25 J#13 water was analyzed for colloids using light scattering. Samples of this water were prepared for transmission electron microscopy analysis.

**Forecast:** Work will continue on the flow testing experiment and the diffusion experiments using samples of single crystals of clinoptilolite.

### **2.6.4 Characteristics and Configurations of the Waste Packages (SCP Section 8.3.4.3)**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

### **2.6.5 Waste Package Production Technologies (SCP Section 8.3.4.4)**

During the reporting period, a report entitled "Waste Package Engineering Development Task Plan" (CRWMS M&O, 1993n) was issued. This plan satisfies the requirement specified



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in the Waste Package Implementation Plan for a description of planned activities associated with Work Breakdown Structure 1.2.2.4.2.

The Waste Package Engineering Development Task Plan is to cover the entire engineering development period. Thus, the waste package engineering development tasks will be subject to periodic review by the M&O Waste Package Development Department, to verify that they still meet the waste package development needs. The plan will be revised as necessary to accommodate changes in the Waste Package Development Program; it is a controlled document and changes to it shall be controlled in accordance with applicable procedures.

The principal goal of the Advanced Conceptual Design phase of the Waste Package Program is to evaluate and develop a set of waste package design concepts that will satisfy NRC requirements. As part of this development process, evaluation of each waste package concept will be based on both technical feasibility and cost effectiveness of the manufacturing processes (for containment barrier fabrication, closure, and inspection). Designs that will be evaluated for fabrication will include spent nuclear fuel and defense high-level waste. Spent nuclear fuel waste package concepts will also include the multipurpose canister disposal container.

The specific engineering development tasks described herein involve test and evaluation of full or reduced-scale sections of various waste package design concepts during the Advanced Conceptual Design phase. The tasks will focus on key manufacturing uncertainties specific to each design concept. As the manufacturing processes are developed, and as the results of the prototype testing become available, proposed process specifications will be developed and preliminary fabrication drawings generated for each of the selected Advanced Conceptual Design and License Application Design design concepts.

Early in the License Application Design phase of the program, the evaluation of concepts developed during Advanced Conceptual Design will be completed and the final two (primary and alternative) waste package designs for spent nuclear fuel and defense high-level waste will be selected. The required manufacturing processes will influence the selection of the designs selected for further evaluation and refinement. Manufacturing studies during License Application Design will include full-scale prototypes that will be subjected to realistic system-imposed conditions.

The five basic areas of the plan are described in the following sections.

### **2.6.5.1 Design Activity 4.3.1.1- Waste Package Fabrication Process Development**

The objective of the interrelated tasks of fabrication, closure, and inspection is to identify and demonstrate the optimum manufacturing process for container manufacturing consistent with the functional and performance requirements of the application. The solution is complex because the manufacturing method affects the characteristics and properties of the product being produced. The effects must be understood and integrated into the overall

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program to achieve a selection of both materials and manufacturing methods that meet the design requirements, and perform satisfactorily for 1000 years and more. Processes selected should be technically conservative to ensure safety and long-term performance. In this regard, manufacturing costs should not impose sacrifices in construction methodology (i.e., cost is a concern, but not a top priority).

The objective of this development task is to select and develop fabrication techniques for several waste package container design configurations, with the exception of the lid closures (that subject is addressed separately in the next section), that are technically and economically acceptable and also may be conditioned during fabrication to minimize stresses. The multibarrier container configuration is a right cylinder made of two layers of material, probably configured with some integral lifting feature. The two layers may be a cylinder within a cylinder, or a single cylinder made of two-layer clad material. The waste material, whether multipurpose canister, spent nuclear fuel, or defense high-level waste, is then placed into the container at the repository site and the lids are installed. The development concerns are the fabricability of the design configurations and their relative cost, plus the need to minimize tensile stresses within the fabricated container.

### **2.6.5.2 Design Activity 4.3.1.2 - Waste Package Closure Process Development**

The objective of this development task is to select and develop waste package remote closure welding processes that are technically and economically acceptable, and will also minimize stresses. Viable methods of repairing defective closure welds must also be developed. This remote closure task, as well as the waste package remote nondestructive examination task that follows, must be performed in concert with the waste package container fabrication task, because of the strong technical interrelationships between these tasks.

Installation of the waste package closure lids will take place at the MGDS repository surface facility, following placement of the waste within the waste package container. Each of the two closure lids must be separately remotely welded into place and remotely inspected to complete the envelope for each corrosion barrier. The primary development concerns are the combined choice of weld joint configurations and welding techniques to result in lowest possible post-weld tensile stress conditions, and of joint configurations that can be inspected. Various standard industrial remote closure welding processes will be investigated for each of the selected waste package container design configurations (evolved from the previous task). Other areas that must be considered include: quality of the closure welds (weld integrity, and good mechanical properties of the welds and heat affected zones), economy and time involved in making the closure welds (high deposition rate and minimizing amount of weld filler material), fully automatic remote closure welding equipment, the ability to use the same equipment for both the thin inner weld and thick outer weld, the capability of hardening the welding equipment to the anticipated levels of radiation exposure, and viable methods for repair of defective welds or for container replacement if weld repair should be unfeasible.

The fabrication industry is making continual advances in development of fully automatic remote welding equipment and process control to meet the combined challenges of:

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stricter quality standards, consistent quality and reduced rejection rate; adaptation to computer numerical control; computer monitoring of weld process parameters for quality assurance; cost control and labor cost reduction; improved health and safety standards; increased productivity through improved operating factors; and the expansion of worldwide competition.

This Program shares most of the aforementioned challenges. This development task is expected to benefit greatly from recent and near-future automatic remote welding advances, with the expectation that the needed level of technology already exists, or will be available. The implementation and adaptation of that technology to the circumstances of the waste package closure welds is what remains, which is the major endeavor of this development task. The waste package closure circumstances that require complete isolation of the welding activity within a hot cell, plus effects of the radioactive environment upon the welding equipment, are circumstances which tend to be outside those of the more stringent industrial welding conditions.

### **2.6.5.3 Design Activity 4.3.1.3 - Waste Package Closure Inspection Development**

The objective of this development task is to select and develop nondestructive examination technique(s) that are technically and economically acceptable, and can accommodate the selected waste package materials, thicknesses, and geometries. As previously indicated, certain closure configurations may be incompatible with available nondestructive examination techniques, thus this task must be performed in concert with waste package closure configuration design activities. The nondestructive examination technique(s) finally chosen will have to prove the quality of both inner and outer closure welds for the chosen configuration for each waste package closure joint, both for the License Application Design prototype welds and for each and every closure weld made during production.

The types and sizes of flaws that might be encountered in the remotely welded joints must be well understood. Ongoing evaluations of weld test samples produced by the recommended weld methods will provide the data base necessary to characterize the weld defects and for subsequent nondestructive examination tests. Weld inspection methods must be selected which are capable of detecting the types of defects or flaws potentially produced by the weld method.

The condition of the completed weld (contour, surface finish) must be compatible with the inspection techniques. Post weld cleaning and metal removal may be necessary to provide a surface free of undercutting, splatter, ripple, etc.

Joint geometry will be a major concern in the development of the closure weld nondestructive examination. The ideal case would be one in which there are no reflective surfaces on or near the inner portion of the weld which might interfere with interpretation of the test results. Likewise, it is desirable that the exterior surface in the vicinity of the weld be a simple shape and that there is a clear straight line access to the weld in two orthogonal directions.

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### **2.6.5.4 Design Activity 4.3.1.4 - Remote In-Service-Inspection Development**

The performance of the waste package, as specified by 10 CFR 60, requires a performance confirmation period. The objective of this development task is to select and develop remote in-service-inspection equipment and techniques that are technically and economically acceptable, and which can withstand the radiation dose and temperatures of the waste package environment. The needed equipment will consist of sensors, transmitters, and cabling to be installed in a selected area within the repository for the purpose of monitoring conditions therein. The sensors may be mounted on or around waste packages and/or sample material coupons, mounted on and within the drift rock walls both near and far from emplaced waste packages, and would also be located within any environmental monitoring stations as might be placed in the drifts. Parameters which may be expected to be of interest in order to monitor conditions within the repository will include: temperature, pressure, humidity, pH level, air velocity, strain gages, radioactivity level, and seismic accelerometers.

### **2.6.5.5 Design Activity 4.3.1.5 - Internal Filler Material Process Development**

The use of waste package internal filler material versus filling the void space with an inert gas is an issue to be resolved. The choice will be determined by the benefits or penalties related to use of filler materials, as derived from future engineering studies and performance assessment analyses. Filler materials may be solids placed while in a liquid state such as low melting temperature metals, graded coarse granular solids such as iron shot, or fine materials such as dry cementitious mixes (e.g., sand and cement). Cementitious materials would be placed in the dry unreacted state. The material would remain unreacted until such time as the barriers might breach and water would enter the waste package interior, causing the material to react with the water and to solidify.

The purpose of this development task is to perform engineering development activities as may be defined by, and in support of, future engineering trade studies in regard to use of filler material within the waste package. The engineering study must first compare use of filler materials versus an inert gas in the void spaces within the waste package, followed by the comparison of various candidate filler materials. Specific activities will include the following areas: material placement including infiltration and uniformity of distribution in the presence of the internal basket and spent nuclear fuel assemblies, effective thermal conductivity measurements, and additional material properties at elevated temperatures as may be required.

This development task will support both the waste package and multipurpose canister engineering development activities. Filler material, if used, would be added remotely to a spent nuclear fuel container/canister following placement of the spent nuclear fuel assemblies into the basket, prior to closure of the container/canister. A manner of measuring the quantity of filler material would be required to establish that placement of the proper total quantity was accomplished, to confirm absence of voids within the space. In the case of the multipurpose canister, addition of filler material would take place at the MGDS.

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Use of waste package filler materials would assist in achieving several technical objectives. Among these are:

- Minimization of waste package internal void space to minimize the amount of water that could enter the waste package in the event of repository flooding and a breach of the waste package containment barriers
- Aid in transferring heat from the fuel rods
- Criticality control
- Chemical buffering for radionuclides

The use of fillers would increase waste package or multipurpose canister weight and cost.

**Forecast:** The Waste Package Engineering Development Task is scheduled to begin in FY 1994 and will continue through conclusion of the License Application Design phase.

### **2.6.6 Waste Package Performance (SCP Section 8.3.5.9)**

#### **2.6.6.1 Activity 1.4.1.1 - Integrate Design and Materials Information (Metal Container)**

Revision of the Scientific Investigation Plan for the Metal Barrier Task (SIP-CM-01) has begun.

Staff from LLNL met with M&O staff on August 17, 1993, to discuss interfaces between the work scopes for the two organizations. The discussions principally involved evaluations and selections of waste package materials for the different configurations being considered in the Advanced Conceptual Design phase. A follow-up meeting on this subject was scheduled for September 2, 1993.

**Subactivity 1.4.1.1.1 - Mechanical properties.** No progress during the reporting period; this was an unfunded activity.

**Subactivity 1.4.1.1.2 - Microstructural properties.** No progress during the reporting period; this was an unfunded activity.

**Subactivity 1.4.1.1.3 - Physical properties.** No progress during the reporting period; this was an unfunded activity.

**Subactivity 1.4.1.1.4 - State of stress in the container.** No progress during the reporting period; this was an unfunded activity.

**Subactivity 1.4.1.1.5 - Characterization and inspection of weld integrity.** No progress during the reporting period; this was an unfunded activity.

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Subactivity 1.4.1.1.6 - Characterization of the container surface. No progress during the reporting period; this was an unfunded activity.

**Forecast:** Work will continue on the assessment of degradation modes affecting bimetallic metal systems in preparation for the Advanced Conceptual Design of robust packages. Work will continue on the crack growth studies at Argonne National Laboratory.

### **2.6.6.2 Activity 1.4.1.2 - Integrate Design and Materials Information (Alternate Barriers Investigation)**

No progress during the reporting period; this was an unfunded activity.

**Forecast:** No activity is planned for FY 1994.

### **2.6.6.3 Activity 1.4.2.1 - Selection of the Container Material for the License Application Design**

Subactivity 1.4.2.1.1 - Establishment of selection criteria and their weighting factors. No progress during the reporting period; this was an unfunded activity.

Subactivity 1.4.2.1.2 - Material selection. No progress during the reporting period; this was an unfunded activity.

**Forecast:** No activity is planned for FY 1994.

### **2.6.6.4 Activity 1.4.2.2 - Degradation Modes Affecting Candidate Copper-Based Container Materials**

No progress during the reporting period; this was an unfunded activity.

**Forecast:** No activity is planned for FY 1994.

### **2.6.6.5 Activity 1.4.2.3 - Degradation Modes Affecting Candidate Austenitic Materials**

Subactivity 1.4.2.3.1 - Assessment of degradation modes in austenitic container. The statement of work from Principal Investigators at Argonne National Laboratory was received and the interlaboratory agreement for continuation of the slow crack growth rate studies on Alloy 825 and other austenitic alloys was finalized. The studies involve application of a tensile load to precracked compact tension specimens exposed to laboratory-simulated J-13 well water at 95°C. The studies measure crack propagation by the very small changes in electrical resistance manifested as the crack grows, and the technique is sensitive to crack rates less than 10-12 m/s. The crack growth studies have been maintained since 1991.

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During that period, the crack propagation on Alloy 825 has been imperceptible. A progress report will be drafted at the end of FY 1993 on results to date.

The mechanical components of the crack growth measurement system have been completed for the new corrosion testing laboratory at LLNL. The initial system operation was checked out for the pump, heater assemblies, system leak check, and the efficiency of the heat exchangers. The heaters and heat exchanger operated as designed, and the pump appears to operate at a maximum of 26.5 L/h (7 gal/hr), a flow rate better than expected. A missing switch that controls the interlocks for pump and heater shutdown was ordered. The G.E. data acquisition and reversing DC system was turned on. A Project work plan was prepared for the crack growth testing and other experimental work. This work at LLNL will complement the work being performed at Argonne National Laboratory.

Subactivities 1.4.2.3.2 through 1.4.2.3.9. No progress during the reporting period; these were unfunded activities.

**Forecast:** Subactivity 1.4.2.3.1 - Work is proceeding on running shake-down tests to evaluate the software performance. Work is planned for conducting slow crack growth studies on carbon steels and other ferrous materials under repository-relevant environment conditions. Degradation mode studies of candidate austenitic materials will continue.

Subactivities 1.4.2.3.2 through 1.4.2.3.9 - No activity is planned for FY 1994.

### **2.6.6.6 Activity 1.4.2.4 - Degradation Modes Affecting Ceramic-Metal, Bimetallic/Single Metal, or Coatings and Filler Systems**

Subactivity 1.4.2.4.1 - Assessment of degradation modes affecting ceramic-metal systems. No progress during the reporting period; this was an unfunded activity.

Subactivity 1.4.2.4.2 - Laboratory test plan for ceramic-metal systems of the alternate barriers investigations. No progress during the reporting period; this was an unfunded activity.

Subactivity 1.4.2.4.3 - Assessment of degradation modes affecting bimetallic metal systems. A high sensitivity thermogravimetric analysis unit will be procured. This unit will be used in an experimental study to discern at what point there is a transition between "dry" oxidation and "wet" corrosion. It is expected that the study will be conducted on a corrosion allowance material (such as carbon steel) with temperature, humidity, and surface condition as the principal variables. The transition between dry and wet conditions is very important with respect to performance of the container material and the design strategy for keeping the waste package in a "dry" condition for an extended period of time.

An experimental arrangement is being designed for use in conjunction with the thermal gravimetric analysis system for monitoring the low corrosion and oxidation rates in low and high humidity environments. Experiments are planned over a temperature range from

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ambient to above the normal boiling point of water and humidities ranging from very dry to saturation. Staff has been in contact with Cahn Microbalances, Inc. on the status of the thermogravimetric analysis unit.

Following discussions with U.S. Geological Survey (USGS) Principal Investigators, staff visited the REECo Subdock in Area 25 on May 11, 1993, to examine a carbon steel tubing string that had been removed from Well USW H-5 on the north side of Yucca Mountain. The string had been used as a conduit for an instrument package placed in the well and had been exposed in the well for more than ten years. The string was about 1100 m in length and traversed both the unsaturated and saturated zones. The water level was 705 m from the surface, the well was cased to a depth of around 750 m. It was very evident which part of the string was immersed in water and which part was exposed to the atmosphere. There was little corrosion of the part that was exposed to the atmosphere. In fact, most of the original stenciling on the tubing was still intact. The part immersed in the water showed abundant corrosion products, apparently ferric oxide.

Samples from different parts of the string were shipped to LLNL for characterization. The steel used for the string is American Petroleum Institute Grade J-55, a common carbon-manganese steel used in petroleum wells. Samples of a string recently pulled from the WT-2 well were received at LLNL for evaluation. Samples exposed in the saturated zone from this well appear to be much less corroded than those obtained from the H-5 well, even though the time of exposure was the same (ten years). Information received from USGS Principal Investigators involved in these wells, and others, suggests that the depth of the well, the particular tuff layer, the fracture pattern in the rock, and the flow rate are important in determining the corrosion rate, since these factors govern the transport of oxygen that can reach the corroding steel surface. A report on the observations of steel exposed in these wells is being prepared. This information will be incorporated in the evaluation of steel as an overpack material in different waste package designs being considered by the Project.

Work continues on compiling information on the corrosion and oxidation behavior of carbon steels, cast irons, and low-to-intermediate-alloy steels. An experimental plan for studying the degradation (oxidation and corrosion) of materials in humid environments is also being prepared. The emphasis of this work will be on carbon steel and other iron-base materials and will focus on the effect of humidity and temperature in the transition from oxidation under "dry" conditions to corrosion under "wet" conditions. A system was designed for generating different humidity levels. This system will be used in conjunction with the thermal gravimetric analysis unit that was recently ordered as part of the YMP capital acquisition and will be used for the degradation mode survey on this family of materials.

Staff has completed a draft of the degradation mode survey on carbon steels, cast irons, and low-alloy steels. These materials are corrosion allowance materials that could be used in multiple-barrier waste package designs. The survey is undergoing internal technical review.

Subactivity 1.4.2.4.4 - Laboratory test plan for bimetallic/single metal material systems.  
No progress during the reporting period; this was an unfunded activity.



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### Subactivity 1.4.2.4.5 - Assessment of degradation modes in coatings and filler systems.

No progress during the reporting period; this was an unfunded activity.

Subactivity 1.4.2.4.6 - Laboratory test plan for coatings and filler systems of the alternate barriers investigations. No progress during the reporting period; this was an unfunded activity.

**Forecast:** Subactivity 1.4.2.4.3 - The expected delivery date of the thermogravimetric analysis unit is October 15, 1993. Assessment of degradation mode studies affecting bimetallic metal systems will continue in FY 1994.

Subactivities 1.4.2.4.1, 1.4.2.4.2, 1.4.2.4.4 through 1.4.2.4.6 - No activity is planned for FY 1994.

### **2.6.6.7 Activity 1.4.3.1 - Models for Copper and Copper Alloy Degradation**

No progress during the reporting period; this was an unfunded activity.

**Forecast:** No activity is planned for FY 1994.

### **2.6.6.8 Activity 1.4.3.2 - Models for Austenitic Material Degradation**

Subactivities 1.4.3.2.1 through 1.4.3.2.5. No progress during the reporting period; these were unfunded activities.

Subactivity 1.4.3.2.6 - Pitting, crevice, and other localized attack. Staff met with personnel from the Performance Assessment Technical Area to discuss previous work with pitting survivability models and how this work might be applicable to the performance of a corrosion resistant material under repository environmental conditions.

Subactivities 1.4.3.2.7 and 1.4.3.2.8. No progress during the reporting period; this was an unfunded activity.

**Forecast:** The studies in Subactivity 1.4.3.2.6 will continue. No activity is planned for the other subactivities for FY 1994.

### **2.6.6.9 Activity 1.4.3.3 - Models for Degradation of Ceramic-Metal, Bimetallic/Single Metal, and Coatings and Filler Alternative Systems**

No progress during the reporting period; this was an unfunded activity.

**Forecast:** Work on this activity will begin during FY 1994.

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**2.6.6.10 Activity 1.4.4.1 - Estimates of the Rates and Mechanisms of Container Degradation in the Repository Environment for Anticipated and Unanticipated Processes and Events, and Calculation of Container Failure Rate as a Function of Time**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

**2.6.6.11 Activity 1.4.5.1 - Determination of Whether the Substantially Complete Containment Requirement is Satisfied**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

**2.6.6.12 Activity 1.5.5.2 - Radionuclide Transport Modeling in the Near-Field Waste Package Environment**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

## SECTION 2.7 PERFORMANCE ASSESSMENT

The Performance Assessment Program was assigned two high-level priorities for fiscal year (FY) 1993: (1) to support Exploratory Studies Facility (ESF) construction and surface-based testing support through Waste Isolation Evaluations, and (2) to carry out the Total System Performance Assessment (TSPA) 1993 exercise. In addition, the performance assessment function is providing input to one of the top Regulatory & Licensing Department's initiatives, which is the evaluation of possible alternative regulatory requirements.

### Waste Isolation Evaluations

In terms of the first initiative, the M&O Performance Assessment Department provided the following 46 ESF construction and surface-based testing support Waste Isolation Evaluations:

- Waste Isolation Evaluation for YMP Temporary 69-kV Power Distribution System
- Waste Isolation Evaluation, Road Oyl and EMC<sup>2</sup>, Dust Suppression and Soil Stabilization Products
- Waste Isolation Evaluation, Need for Separate Rock Storage Areas for Topopah Spring and Calico Hills Muck
- Waste Isolation Evaluation, TFM (Tracers, Fluids, and Materials) for C-Well Pump Tests
- Waste Isolation Evaluation, TFM for UE-25 NRG#4, Electrical Grounding Grid
- Waste Isolation Evaluation, Drilling of USW SRG-5
- Waste Isolation Evaluation, Drilling of UE-25 NRG#2 and UE-25 NRG#2A, Supplement #1
- Waste Isolation Evaluation, Drilling of UE-25 NRG#5, Supplement #1
- Waste Isolation Evaluation, Package 1A Water Supply System for the Exploratory Studies Facility
- Waste Isolation Evaluation, Package 1B Surface Buildings, Parking, and Compressed Air Facility
- Waste Isolation Evaluation, Fran Ridge Large Block Experiment
- Waste Isolation Evaluation, Concrete Batch Plant
- Waste Isolation Evaluation, Drilling of UE-25 NRG#2B

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- Waste Isolation Evaluation, Package 1A Water Distribution System for the Exploratory Studies Facility
- Performance Assessment Concerns Regarding a Diesel Transportation System to Service Tunnel Boring Machine (TBM) Operations
- Waste Isolation Evaluation, Package 2A Extension of the North Ramp Starter Tunnel
- Waste Isolation Evaluation, Tracers, Fluids, and Materials for North Ramp Starter Tunnel Testing and Construction, Supplement #1
- Waste Isolation Evaluation - Different ESF Ramp/Drift Sizes - Thermo-Mechanical and Flow and Transport
- Waste Isolation Evaluation TFM for North Portal Pad Substation & 69-kV Power and Feeder System
- Waste Isolation Evaluation, ESF Subsurface Wastewater Pond, Pkg 1B
- Waste Isolation Evaluation, Shop, Pkg 1B (Package 1B Surface Buildings Supplement #1)
- Waste Isolation Evaluation, H-Road Widening and Paving, Pkg 1B (Pkg 1A Water Supply System Supplement #1)
- Waste Isolation Evaluation, Package 1B Sewer System
- Waste Isolation Evaluation, ESF Explosives Storage Area, Pkg 1B
- Waste Isolation Evaluation, Excavation Trenches along Solitario Canyon Fault
- Waste Isolation Evaluation, Drilling and Testing of USW SD-12
- Waste Isolation Evaluation, ESF Package 1A North Ramp Alcove #1
- Waste Isolation Evaluation, TFMs for North Ramp Starter Tunnel Testing and Construction, Supplement #2
- Waste Isolation Evaluation, ESF Package 1A North Ramp Alcove #1: Rev. 01
- Waste Isolation Evaluation, TFMs for FY-1993 ESF Phase 1A Construction, Rev. 02
- Waste Isolation Evaluation, Package 1A Water Supply System for the ESF, Rev. 01

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- Waste Isolation Evaluation, USW UZ-14 Perched Water Grouting Plan
- Waste Isolation Evaluation, USW NRG-7 Drill Pad and Access Road
- Waste Isolation Evaluation, Midway Valley Alice Ridge Trenching
- Waste Isolation Evaluation, Package 1A Water Distribution System for the ESF, Rev. 01
- Waste Isolation Evaluation, TFM's for North Ramp Starter Tunnel Testing and Construction, Supplement #2, Rev. 01
- Waste Isolation Evaluation, Seismic Reflection Line, ESF Support
- Waste Isolation Evaluation, TFM's for the UE-25 C-Well Complex, Rev. 01
- Waste Isolation Evaluation, ESF Package 1B Explosives Storage Area, Rev. 01
- Waste Isolation Evaluation, ESF Package 1B Surface Buildings, Parking, and Compressed Air Facility, Supplement #1, Rev. 01
- Waste Isolation Evaluation, TFM, for the ESF North Portal Pad 69-12.47 kV Electrical Power, Site Grounding and Lightning Systems, Rev. 01
- Waste Isolation Evaluation, H-Road Widening and Paving, Rev. 01
- Waste Isolation Evaluation, ESF Package 1A North Ramp Alcove #1, Rev. 02
- Waste Isolation Evaluation, TFM's for North Ramp Starter Tunnel Testing and Construction, Supplement #2, Rev. 02
- Waste Isolation Evaluation, Additional Grouting of Perched Water Zones in USW UZ-14
- Waste Isolation Evaluation, Drilling of USW NRG-7

Preparing Waste Isolation Evaluations involves the inspection of design analyses, drawings, and specifications from a performance assessment viewpoint to ensure that the facilities will not impact waste isolation and to recommend design changes if necessary. In support of surface-based testing, this includes the review of designs of facilities such as access roads, drill pads, and water lines. For the ESF, it includes reviews of the ESF design packages being prepared during FY 1993: the North Ramp Starter Tunnel redesign, the North Portal surface facilities, the North Ramp, the South Portal, and the Topopah Spring Level main drift.

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The M&O performance assessment staff conducted the following three generic evaluations in support of ESF design and surface-based testing (all currently undergoing internal review): (1) an evaluation of ESF and surface-based testing tracers, fluids and materials, to determine their potential impacts on waste isolation and to recommend any constraints on their use; (2) an evaluation of ranges of ESF ramp and drift sizes being considered, to determine differences in impacts, if any, on potential repository preclosure radiological safety and postclosure waste isolation; and (3) a comparison of drill-and-blast ESF excavation with mechanical excavation techniques (including tunnel boring machines) with respect to potential repository preclosure radiological safety and postclosure waste isolation impacts.

In addition, Sandia National Laboratories (SNL) completed two performance assessments in support of establishing water use controls and requirements for the ESF.

### Total System Performance Assessment

The second performance assessment initiative was the effort called TSPA 1993, which included work in many areas of data analysis and model development supporting the top-level analyses. This is discussed in more detail in Section 2.7.6. A brief summary of these activities follows.

#### TSPA Calculations

- SNL completed and published sensitivity studies on TSPA 1991 (April 15, 1993).
- The M&O and SNL constructed the TSPA 1993 problem set and developed source-term and site system data with Los Alamos National Laboratory (Los Alamos), Lawrence Livermore National Laboratory (LLNL), M&O, and U.S. Geological Survey (USGS) participation.
- The M&O and SNL completed the bulk of the TSPA 1993 calculations, and are drafting reports to be completed by end of calendar year 1993.
- The M&O, through Golder Associates Inc., issued three documents describing the Repository Integration Program total system code, one giving the structure, another providing user guidance, and the third describing the Yucca Mountain data set (February 22, 1993, April 20, 1993, and September 30, 1993).

#### Source-Term Modeling and Model Development

- The M&O, through Pacific Northwest Laboratory (PNL), prepared two documents providing the mathematical description and software requirements for the next generation source-term model currently being developed (June 15, 1993, and September 30, 1993).

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- The LLNL staff prepared the source term for the TSPA 1993 exercise participants, and provided a preliminary version of the Yucca Mountain Integrating Model to SNL (August 1993).

### Development of Scenarios for use in TSPAs

- The SNL staff continued to make progress in describing volcanism scenarios, and is ready to publish the first report on this topic entitled "Scenarios Constructed for Basaltic Igneous Activity at Yucca Mountain and Vicinity."
- The SNL staff continued work to define nominal flow scenarios.

### Unsaturated and Saturated Zone Flow Modeling and Model Development

- The M&O submitted a draft report on the Review and Selection of Unsaturated Flow Models (September 30, 1993).
- The SNL staff completed development of a transient gas flow model for use in TSPA 1993 (September 30, 1993).
- The SNL staff developed an updated three-dimensional saturated zone flow model for their use in TSPA 1993.
- Work on understanding unsaturated flow was described by Lawrence Berkeley Laboratory (LBL) in a number of presentations to various audiences, and two documents were produced describing a TOUGH-2 code enhancement and application.

### Calculations and Experimental Work Supporting TSPA

- The M&O, through the University of California at Berkeley, produced two draft papers on thermal effects in the near field environment (September 15, 1993).
- The USGS staff reported progress in experimental and modeling work addressing infiltration rates and the potential for lateral flow in Yucca Mountain was reported in four conference papers and two draft reports.
- Joint experimental work on validating radionuclide transport modeling and on understanding fracture flow continued between SNL and Los Alamos.

### Alternative Regulatory Requirements

The M&O performed calculations in support of U.S. Department of Energy (DOE) positions on potential new environmental standards for Yucca Mountain. The calculations were begun using the model UCBNE-41, which was the basis for the National Academy of Sciences Waste Isolation System Panel report (Pigford et al., 1983). Initial results were

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compared to results, and sensitivity analyses were conducted over ranges of parameters that include values similar to those at Yucca Mountain. More detailed assessments were conducted using the Repository Integration Program. This model is the basis for the M&O contribution to TSPA 1993. In addition, the effects of natural uranium ore bodies are being compared to the effects of a potential repository. These calculations consist of a series of simple performance assessments of a repository at Yucca Mountain, and have been used to begin to formulate DOE positions on issues related to environmental standards for Yucca Mountain. The DOE positions as well as the calculations that support them will be ready for presentation to the National Academy of Sciences' Committee on Technical Bases for Yucca Mountain Standards when that body requests DOE input. The preliminary results of the calculations were presented to the Nuclear Waste Technical Review Board in July 1993, and the detailed results will be presented to that technical oversight group early in 1994.

Detailed descriptions of performance assessment accomplishments for the second half of FY 1993 are presented in the appropriate subsections of Sections 2.6 (2.6.3.8) and 2.7 (all).

### **2.7.1 Waste Retrievability (SCP Section 8.3.5.2)**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

### **2.7.2 Public Radiological Exposure - Normal Conditions (SCP Section 8.3.5.3)**

A report entitled "Preclosure Radiological Safety Evaluation" (Schelling and Smith, 1993) closed out SNL participation in this activity. This report describes the use of standard probabilistic risk assessment methods to evaluate the impact of ESF design changes (from the original vertical shaft configuration to the current dual ramp configuration) on previous public radiological risk evaluations and to estimate the level of uncertainty in the assessment results. This activity has now been transitioned to the M&O.

**Forecast:** No direct activity in FY 1994; see Section 2.7.3 for related work.

### **2.7.3 Worker Radiological Safety - Normal Conditions (SCP Section 8.3.5.4)**

The M&O conducted an initial preclosure probabilistic risk assessment on items important to safety for the ESF components that could be incorporated into the Mined Geologic Disposal System (MGDS). This initial study was conducted using proprietary spreadsheet software to provide a timely response. Individual areas of work included collection and analysis of mining rock-fall data and transportation accident data; quantifying radioactive waste container releases arising from energetic events; radionuclide transport in the MGDS ventilation system; atmospheric dispersion; and potential exposure levels to the



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general public outside the restricted area. Statistical methods were used to incorporate, in the overall assessment, the uncertainties present in the accident and rock-fall data.

The preliminary findings of the probabilistic risk assessment showed that if the MGDS is to have a high reliability two-stage high-efficiency particulate air filter then the ESF components to be incorporated into the MGDS do not have to be on the Q-List. If only a single stage high-efficiency particulate air were to be deployed in the MGDS and a thin (10 cm) walled container is used, then ESF (and the waste transporter) are marginal in meeting the statutory requirement and thus would have to be included on the Q-List. An analysis of the ESF/MGDS system indicated that the greatest uncertainty in the predictions arise from the simple (1½ dimension) model used to predict the response of, and subsequent release from, the nuclear waste container following a rock-fall or transporter accident.

Rock-fall likelihoods and consequences were estimated from an analysis of mining rock-fall data and underground transportation accident data. Using the Bureau of Mines Accident Data Analysis program, such data was obtained from the collection of mining accidents managed by the Health and Safety Analysis center of the Mine Safety and Health Administration. The analysis was performed using mining accident statistics over the period of the last ten years and the configuration of the ESF main drift shown in ESF Title II Design.

The M&O performed numerical calculations using the Discontinuous Deformation Analysis method to assess tunnel stability under the expected range of thermal loads. Specifically, the model enables the representation of a discontinuous system of rock blocks separated by joints, allowing relative movement of individual rock blocks that may be undergoing block deformation, rigid rotation, and translation. Friction/cohesive discontinuous joint surfaces are considered. Elastic blocks and elastic contact between blocks were addressed; however, energy dissipation occurs during sliding. Quasi-static mechanical effects of the tunnel excavation, thermal effects of a ten-year temperature field (added instantaneously to the rock mass around the tunnel), and thermal effects of instantaneous removal of the temperature field around the tunnel were modelled to provide qualitative descriptions of thermal loading effects on the stability of a repository drift.

**Forecast:** This work will be documented for review by the M&O and subsequently by DOE. The report will contain recommendations for future work. At present two areas can be identified for improvement: (1) container modeling, and (2) incorporation of actual Yucca Mountain meteorological conditions into the atmospheric dispersion calculations.

### **2.7.4 Accidental Radiological Release (SCP Section 8.3.5.5)**

Potential effects of accidental rock falls were addressed in Section 2.7.3.

**Forecast:** See Section 2.7.3.

### **2.7.5 Ground-Water Travel Time (SCP Section 8.3.5.12)**

The Ground-Water Travel Time Issue Resolution Working Group met in Las Vegas in September 1993, and is currently examining the technical aspects of ground-water flow at Yucca Mountain. The primary objective is to develop a methodology for demonstrating compliance with regulations related to natural barrier performance that is technically prudent and acceptable to the NRC.

#### **2.7.5.1 Activity 1.6.2.1 - Model Development**

The M&O performance assessment staff finished its previously reported review of unsaturated flow models in use in the Yucca Mountain Site Characterization Project (YMP), and recommended a limited subset of those in use for continued development. Review results were summarized in a paper entitled "Review and Selection of Unsaturated Flow Models" (Reeves et al., 1993) presented at the 1993 High-Level Waste Conference. A draft report was submitted to YMPO for review.

**Forecast:** The completed report will be published after YMPO review. Its recommendations are already being implemented, and are reflected in the discussions of cooperative code development work in Section 2.7.5.3.

**Subactivity 1.6.2.1.1 - Development of a theoretical framework for calculational models.** M. Harr from Purdue University visited SNL August 9-11, 1993. While at SNL, he reviewed the methods for generated random, auto-correlated fields (covered in the memo discussed above) that were developed at Purdue as a software package in support of YMP.

The performance assessment staff from DOE and the M&O were briefed by SNL in Las Vegas, Nevada, on August 23, 1993, on advanced geostatistical simulation and economic decision modeling that has been done in support of the DOE/Headquarters Office of Environmental Restoration and Waste Management, Environmental Restoration Demonstration Testing and Evaluation Division. Possible applications to the YMP were discussed. A copy of the Purdue software was also demonstrated and a copy of the package was left with DOE for review.

**Subactivity 1.6.2.1.2 - Development of calculational models.** No progress during the reporting period; this activity was not funded in FY 1993. See related work in Section 2.7.5.3.

**Forecast:** No activity is planned for FY 1994. See related work in Section 2.7.5.3.

### 2.7.5.2 Activity 1.6.2.2 - Verification and Validation

#### Subactivity 1.6.2.2.1 - Verification of codes.

##### Appropriateness of One-Dimensional Calculations:

A report entitled "The Appropriateness of One-Dimensional Yucca Mountain Hydrologic Calculations" (Eaton) was written to help in defining the calculational regimes for which one-dimensional calculations are valid for approximating aqueous flow for TSPA-type calculations. The report is in policy review at YMPO, and a summary of the report will be included in the TSPA 1993 report.

##### Fracture Permeability Effects on Dryout:

The effect of fracture permeability on the dryout of a nuclear waste repository was investigated in a series of calculations using the multiphase code TOUGH2. The material properties used in this study were based on values from Buscheck and Nitao (1993). The calculated saturation results based on these material characteristics for a highly fractured media predicted considerable dryout in the vicinity of buried waste and a large perched water region above the potential repository horizon for times exceeding 10,000 years. However, when the permeability of the fractures were reduced by a factor of  $10^4$ , the size of the dryout and perched regions were significantly reduced. Furthermore, when the values for fracture permeability were reduced by more than a factor of  $10^4$ , these regions were essentially nonexistent. The latter reduction represents a decrease in fracture aperture from 100 to  $5.1 \mu\text{m}$ . It should be noted that the algebraic model used to define the material properties can also significantly affect calculated values of water perching and dryout in the vicinity of the repository. These results indicate the importance of accurately modeling fractures when calculating the presence of multiphase flow in the vicinity of a potential repository.

##### Barometric Pumping Simulations:

The SNL staff have been modeling the amount of water vapor extracted from Yucca Mountain via fluctuations in barometric pressure. A method-of-lines code for two-phase flow in porous media and for modeling barometric pumping of water vapor in a discrete fracture/matrix system has been undergoing testing and application to estimate respired moisture from Yucca Mountain. The code compared well with results obtained by recomputing a heat pipe problem done at LBL using TOUGH. The coupling between fracture and matrix models was tested by simulation of an analytical solution to periodically driven diffusion in a fracture/matrix system. This comparison was also excellent.

Two barometric cycles are being studied: the diurnal cycle and a five-day cycle typically caused by storm fronts. The latter cycle appears to be most effective in transporting moisture out of the upper layers of Yucca Mountain.

**Forecast:** The results of the fracture permeability study are based on material properties provided by LLNL investigators. Since the time that those property values were

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developed, new information has required some modification of the data set by SNL. The new data set will be used for ancillary calculations to be reported as part of TSPA 1993. In addition, a subset of the calculations reported here will be rerun to determine the degree to which the new data set causes changes in the predicted effects.

Documentation of the results of all of these studies is under way and will be included as ancillary calculations in the SNL report on TSPA 1993.

### Subactivity 1.6.2.2.2 - Validation of models.

#### Flow and Transport Through Single Fractures:

The purpose of this task is to challenge existing conceptual models of fracture flow and explore possible rapid transport mechanisms that may be relevant to performance assessment at Yucca Mountain. The SNL staff made three presentations on the results of this work at the Spring '93 American Geophysical Union Meeting in Baltimore, Maryland, May 24-28, 1993: "Influence of Fracture Saturation and Wetted Structure on Fracture Permeability" (Nicholl and Glass, 1993a), "Infiltration Flow Instability in Unsaturated Fractures" (Nicholl and Glass, 1993b), and "Gravity-Driven Fingering in Rough-Walled Fractures: Analysis Using Modified Percolation Theory" (Glass, 1993).

A paper entitled "Gravity-Driven Infiltration Flow Instability in Initially Dry Non-Horizontal Unsaturated Fractures" (Nicholl et al., 1993) was submitted to the journal Water Resources Research. A copy of the paper was sent to YMPO; and a paper entitled "Behavior of Individual Gravity-Driven Fingers in an Initially Dry Fracture" (Nicholl and Glass) is in SNL internal technical review.

A collaborative effort was established as part of the international cooperative research project work at LBL to consider the effects of gaseous exsolution/dissolution on fracture flow. Questions regarding the potential significance of such effects in the vicinity of excavations have arisen during field testing. A second collaborative effort was also established with LLNL to participate in the nonisothermal large block heater test at the Fran Ridge test site. Fracture connectivity will be examined under natural gradient conditions within the Topopah Spring welded tuff. A third collaborative effort was initiated with staff of the University of Nevada, Reno, to analyze fracture flow data obtained from laboratory experiments in individual analog fractures under both saturated and unsaturated conditions.

Development of a methodology to manufacture analog fractures continued. Numerically controlled milling techniques may be used to directly manufacture analog fracture surfaces to predetermined specifications. Two such surfaces may then be used to create a controlled analog aperture field. The ability to replicate a specific aperture field is limited by the physical dimensions of the cutter and the increment between cutting centers. Methods of moving the cutter head may also impart structural features to the surface. Such physical limitations were explored in preparation for subsequent fracture manufacture.

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Casts of both manufactured fractures and natural fractures will be used for actual experimentation. Methodologies for making transparent casts were further refined. Various casting materials were considered as a means of varying mechanical properties and surface wettability of the analog fracture. A significant effort was directed towards obtaining better control of boundary conditions in the analog fracture. As a result, a technique allowing inflow and outflow manifolds to be machined directly into the fracture surfaces was developed.

Development of experimental techniques to explore the effects of air entrapment on fracture permeability and tracer migration continued. The cooling system for the high-resolution camera was reworked to include filtration of the water supply and a relay to shut off the camera, should the supply of cooling fluid be interrupted during a long term test. The computer actuated solenoids controlling flow through the fracture were restructured to minimize mixing of tracer fluids prior to entry and to also minimize air entrapment around the valves themselves. Aperture field of the analog fracture to be used was characterized using simple light absorption theory. Saturated permeability was measured for a baseline and a sequence of unsaturated experiments were initiated. Results of this sequence will be submitted to the 1994 High-Level Waste Conference.

### Fracture/Matrix Interaction:

The purpose of this task is to challenge existing conceptual models describing the transfer of fluids and solutes between fractures and the host matrix (fracture-matrix interaction), and to explore the impact of fracture-matrix interaction on rapid transport mechanisms.

Experimental apparatus allowing observation of fracture wetted structure as a function of matrix pressures was updated and refined. A high resolution digital camera was installed; this system yields 1024 x 1024 pixels of spatial resolution at 4096 gray levels intensity resolution. A relay to shut off the camera if flow of cooling fluid ceases was also fabricated and installed. Low resolution cameras (256 x 256 pixels, 256 gray levels) to provide backup data and monitor manometers were also installed. Software controlling data acquisition and pressure variation was refined and tested. The experiment was slightly reconfigured to allow for a greater range of pressure variation. Additional light shielding was added to attenuate spurious data resulting from internal reflections and light leaks. After collecting a series of test images, the utility of the IP-Lab software package by Signal Analytics for image analysis was explored. First drafts of the experimental procedure and data sheets for the scientific notebook were written.

A large format test chamber for investigating the effect of matrix imbibition on saturated fracture flow has been constructed. Experiments make use of naturally and synthetically fractured slabs of volcanic tuff. The new test chamber is capable of securing multiple fractured rock slabs measuring 60 by 60 cm. Refinement of the experimental technique has also been made to achieve desired boundary conditions (upper flux boundary and lower prescribed tension boundary). A suite of rock slabs have also been cut (from Topopah Spring Tuff) for use in these experiments.

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The enlarged test system has recently been tested using two slabs of Topopah Spring Tuff. X-ray absorption was used to image the transient saturation fields as fluid imbibed into the tuff slabs from a 100  $\mu\text{m}$  slot fracture. Following full saturation of the matrix by a KI solution, deionized water was introduced into the fracture and the transient diffusion of the deionized water into the KI saturated matrix was imaged by x-ray absorption. Tuff slab heterogeneity was noted to have significant influence on the imaged imbibition and diffusion fields.

A Philip's industrial x-ray machine, which was purchased for imaging of flow experiments in the YMP Unsaturated Flow and Transport Laboratory, was temporarily set up at the Non-Destructive Testing Laboratory at SNL. The x-ray unit is currently being utilized in experiments, such as the tuff-slab test. Design of a facility for permanent operation of the x-ray is in progress.

**Forecast:** Unsaturated flow experiments conducted on a block of fractured welded tuff, performed approximately one year ago by USGS, yielded some unexpected and currently unexplainable results. In an attempt to understand what happened in this experiment, a joint laboratory program involving USGS and SNL was initiated. A suite of experiments are being designed to take advantage of the special capabilities developed by each of the participants in the experiment. In particular, SNL will contribute x-ray imaging capabilities as well as expertise in unsaturated flow experimentation. Current plans call for the USGS tuff block to be shipped to SNL early in FY 1994.

Experiments continue in efforts to develop real-time x-ray analysis capabilities. Currently, investigations are conducted in two systems, a simple x-ray detector/image intensifier system, and the more sophisticated Siemen's Polytron. The goal is to achieve a high image contrast for unsaturated flow systems with short time constants.

### Field, Lab, and Numerical Experimentation to Determine Scaling Laws for Effective-Media Properties in Heterogeneous Media:

The purpose of this task is to challenge existing conceptual models for the scaling of effective media properties which are critical to performance assessment at Yucca Mountain. Experiments and analyses are designed to investigate fracture-matrix interaction in the plane of the fracture and in the plane normal to the fracture. These activities provide critical understanding necessary for the formulation of effective media properties that integrate over fracture-matrix interaction subscale processes. Both basic understanding and the effective property formulations are required by other model validation activities, including collaborative initiatives with USGS to examine fracture matrix interactions using x-ray imaging technology developed at SNL in support of this activity.

Several of the activities are aimed at acquiring the understanding necessary to develop models for scaling data collected at one scale and applied to another. This effort will be coordinated with complementary work on geostatistical characterization of heterogeneity (see Section 2.2.3.7).

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To improve measurement precision and facilitate data collection, an automated gas permeameter test system has been constructed. The permeameter consists of four mass flow meters (0-50, 0-500, 0-2000, and 0-20,000 sccm), two pressure transducers (0-100, and 0-350 kPa gauge), a barometer, and temperature sensor that are connected to a regulated source of compressed nitrogen. Operation of the electronic permeameter instruments and solenoids (electronic valves) are controlled by specially adapted personal computer-based software. An x-y positioning system coupled with a pneumatic piston was also automated for positioning and compressing the permeameter tip seal against the rock surface. This system allows over 400 measurements to be made in an eight-hour period, unattended. Data collection routines have also been automated and are used on a periodic basis to assess instrument stability and precision.

Tests have been completed aimed at evaluating permeameter sensitivity, measurement repeatability, and temporal stability. Data collected to date indicate that measurement sensitivity and repeatability are within the specifications of the electronic permeameter equipment (0.5 percent full scale). Calibration of the mass flow meters, and pressure transducers has also been accomplished. An improved seal material has been identified and tested (room temperature vulcanizing silicone rubber) that will facilitate measurements made on rough rock surfaces. Additional permeameter tip seals were designed and constructed. At present a suite of tip seals exist that represent measurement scales spanning five orders of magnitude on a per volume basis.

**Forecast:** A task order has been established and a statement of work developed for acquiring tuff boulders from the Yucca Mountain site. Four tuff blocks have been identified for experimentation, each exhibiting varying degrees of welding and bedding as well as extent and size of lithic/pumice/lithophysae inclusions. Once the boulders are collected they will be sawed into blocks measuring 1.0 to 1.3 m<sup>3</sup>. Until the large tuff blocks are received (expected by early October 1993), measurement of gas permeability at multiple scales is being conducted on tuff slabs to be used in the fracture-matrix interaction studies described above.

### Fast Pathway Analysis in Unsaturated Fractured Tuff: Analog Field Site Investigation

This study addresses issues concerning the occurrence of localized zones of saturation in otherwise unsaturated media which may act as fast pathways through the unsaturated zone at Yucca Mountain.

Through detailed literature review, a data base was formed that details characteristics of sites in which localized flowing water (seeps or weeps) are present. Efforts were made to correlate various boundary conditions and system parameters with the occurrence of such features. This search has investigated numerous sites across the southwest including the Apache Leap Tuff site in Arizona and the Nevada Test Site.

### Caisson Test:

An intermediate-scale experiment is being carried out jointly between SNL and Los Alamos to evaluate instrumentation and models that might be used for transport-model

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validation for the YMP. The experiment involves the detection and prediction of the migration of fluid and tracers (Ni, Li, and Br) through 6-m-high x 3-m-diameter caisson filled with quartz sand.

Caisson design. The final design of the caisson, including locations of time domain reflectometry probes and ceramic and hollow fiber solution samplers, was completed and submitted to Los Alamos prior to filling of the caisson.

Ni sorption and solubility. Systematic studies of sorption of Ni by Wedron 510 sand under atmospheric conditions at two different Ni concentrations (100 ppb and 200 ppb) in the presence and absence of LiBr (17 ppm Li and 200 ppm Br) showed no dependence of Ni sorption on Ni concentration over the range studied, and suggest that Ni sorption under atmospheric CO<sub>2</sub> conditions is equivalent or slightly higher than under CO<sub>2</sub>-free conditions. The studies of Ni and Li sorption suggested that Li at high concentration can compete with Ni for sorption sites. Studies aimed at refining the sorption curve for Ni of Wedron 510 sand under nominally CO<sub>2</sub>-free conditions yielded data that are being used to calculate surface complexation constants.

A kinetic batch sorption study was run to determine the time dependency of Ni sorption by Wedron 510 sand. After one-half hour, 94 percent of the Ni had been sorbed, suggesting that equilibrium was reached during previous batch experiments, which were mixed for two to three days.

Satisfactory solubility data for Ni has been obtained over the pH range 7-10. The measured solubility exceeds that for crystalline Ni(OH)<sub>2</sub> by an order of magnitude or more, and suggests that there is no danger of precipitation occurring in the batch sorption studies using 100 ng/mL initial Ni for pH <8.5. The precipitate formed in the Ni solubility experiment was identified as predominantly Ni(OH)<sub>2</sub> by x-ray diffraction.

LiBr Sorption. A second systematic study of sorption of Br by Wedron 510 sand under CO<sub>2</sub>-free conditions was completed and reduced the uncertainty of the K<sub>d</sub> value for the conservative tracer for the caisson experiment. Studies of Li sorption under atmospheric conditions were performed. Measured sorption was close to 0 at pH = 7, and dropped to -5 percent at pH >8. In contrast, experiments run under CO<sub>2</sub>-free conditions show sorption of 20-25 percent at pH = 7, dropping to about 5 percent at pH = 10. It is probable that Na added at pH >7 as NaOH, almost certainly acts as an ionization suppressant during AA analysis, increasing the signal for Li in the electrolyte, and causing a spurious drop in the K<sub>d</sub> values measured for Li in samples above pH = 8. The offset between the atmospheric and CO<sub>2</sub>-free data sets may be due to a similar effect.

LiBr column experiments. Two LiBr pulses were eluted from saturated Wedron 510 sand columns (5-cm diameter by 30-cm tall). Analysis of Br by ion-selective electrode and Li by flame atomic absorption and fitting of the breakthrough curve by CXTFIT determined retardation factors of 1.06 and 0.96 for Li and Br, respectively. Dispersion coefficients were 0.017 and 0.0023, respectively, for Li and Br. The two runs differed in the way the sand columns were packed, the first with micro-layering and the second homogeneously. The



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results indicated that these differences in the packing method did not significantly affect the breakthrough curve. The retardation factor of less than one for Br is consistent with anion exclusion, causing the Br to flow in the center of the pores where the velocity is higher than average. Kinetic batch sorption experiments were conducted for Li with Wedron 510 sand. Preliminary results show that there is a finite sorption rate that would affect breakthrough curves. The column breakthrough data were analyzed with a kinetic sorption expression with the CXTFIT code to compare the extracted reaction rate constant with the rate constant measured in the batch experiments.

Several unsaturated hanging column experiments with Wedron 510 sand and a LiBr tracer were performed. Both a pulse and a continuous feed of LiBr solution were used, and retardation factors and dispersivities for Li and Br were calculated. Similar experiments with different flow conditions are under way, and experiments with Ni transport were designed.

Interlaboratory calibration studies. The atomic absorption results for Ni and Li analyses were independently checked on a number of samples by inductively-coupled plasma mass spectrometry, with good agreement between the two methods. Ni sorption experiments were performed using the batch sorption techniques described in Los Alamos Detailed Technical Procedures TWS-INC-DP-05-R2 and LANL-INC-DP-86-R0. The data from these experiments were compared with those collected in previous studies at SNL. A solution produced by leaching the Wedron 510 sand and adding a Ni spike was prepared for an interlaboratory calibration with the University of Nevada, Las Vegas. Techniques for analysis of Ni, Br, Li, Ca, and Mg used at SNL and the University of Nevada, Las Vegas for the caisson test were compared. In addition, several Li samples were prepared to be run by inductively-coupled plasma spectrometry as an accuracy check on our atomic absorption method.

Forecast: SNL and Los Alamos will complete an intermediate-scale experiment at the Experimental Engineered Test Facility at Los Alamos. The experiment involves the detection and prediction of the migration of fluid, colloids, and tracers (Li, Br, Ni) through unsaturated quartz sand in a 6-m-high x 3-m-diameter caisson. The purpose of the test is to demonstrate a framework for the validation of reactive transport models in saturated and unsaturated porous and fractured media at Yucca Mountain. The experiments will be designed to provide well-controlled conditions and a well-characterized geomeedia to allow separation of uncertainties due to chemical and physical processes. Criteria for acceptable agreement between predicted and observed tracer migration will be formulated as part of model validation tests and will reflect various sources of uncertainty in the experimental and model design.

Documentation of procedures is nearly completed. A draft Technical Procedure, "Batch Sorption Experiments Under Atmospheric and CO<sub>2</sub>-free Conditions," was prepared and describes the procedures used to perform batch sorption experiments at SNL in support of the caisson experiment. Draft Technical Procedures for Br analysis by ion-specific electrode and the Li analysis technique by flame atomic absorption were prepared.

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### Reactive Transport Model Experimentation

Experimental studies to test key assumptions used by performance assessment models to represent geochemical interactions are being designed. Current performance assessment models assume that sorption of radionuclides by heterogeneous mixtures of minerals under unsaturated flow conditions can be estimated or bound by  $K_d$  values measured on bulk rock samples obtained under saturated conditions. During the report period, efforts were focused on designing experiments to relate the sorption behavior of bulk rocks to trace minerals by developing a model for sorption by mineral mixtures, and on obtaining sorption data under unsaturated conditions.

Development of methods to carry out in situ batch sorption studies in unsaturated media continued at the Massachusetts Institute of Technology. Several alternate methods to extract pore solutions from unsaturated sand for pH and uranium analyses were compared. Kinetic studies of uranium sorption/desorption were carried out. A dedicated Nd:YAG laser for uranium fluorescence imaging studies was installed and is operational at Massachusetts Institute of Technology. Studies of in situ pH measurements and fracture-matrix interaction using analog materials are being designed in collaboration with SNL.

Efforts directed towards obtaining surface complexation constants for Li and Ni sorption by pure quartz and goethite and Ni sorption onto a Min-U-Sil, a quartz standard, under  $\text{CO}_2$ -free conditions continued. In an effort to minimize diffusion of  $\text{CO}_2$  through the sample vessels, a glove cabinet (plastic sheeting on a wire frame) was set up with  $\text{N}_2$  atmosphere for storage of the samples during equilibration. A measurement protocol was developed for making reproducible pH measurements in batch-sorption systems. Additional modifications to the Ar scrubber for the autotitration system have improved overall system stability by an order of magnitude.

An initial titration curve was measured for raw Wedron 510 sand and showed that the stirrer can effectively suspend a 1:1 solid:solution mixture of electrolyte and sand. The sand settles quite rapidly; therefore, a high stirrer setting is required, possibly leading to grain-to-grain collisions and consequent production of clay-size particles. Shielding the electrode from the direct flow eliminated this problem.

A new 250-mL reactor vessel was built and prepared for the autotitrator. This permitted titrations to be performed on smaller load sizes, typically 100 mL electrolyte + 100 g sand. This factor-of-four decrease conserves specially treated (e.g., carbonate-stripped or acid-washed) sand required for the experiments. A series of alkalimetric titration curves were obtained at ionic strengths of 0.0006, 0.0032, 0.011, and 0.094 M for an aliquot of Min-U-Sil that had been cleaned by boiling in 6 N HCl. Double-extrapolation plots were prepared for Min-U-Sil data obtained from the British Geologic Survey for the CHEMVAL2 modeling exercise. The data support an intrinsic acidity constant in the range  $10^{-6.9}$  to  $10^{-8.1}$ , and an association constant for  $\text{Na}^+$  of  $10^{-7.4}$  to  $10^{-7.7}$ , and will be used to verify our technique. Three alkalimetric titrations of acid-washed Wedron 510 sand were performed at ionic strengths of 0.0018, 0.0030 and 0.012. It was determined that leakage of filling solution through the ceramic frit of the pH electrode is significant when titrating systems of low ionic

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strength. At high ionic strength ( $<0.01$ ) such a change is negligible, but at lower ionic strength this effect must be explicitly accounted for to obtain precise surface acidity constants. The titration protocol has been modified so that the acid burette tip is removed from contact with the solution during alkalimetric titration.

Synthetic goethite was prepared for sorption experiments and analyzed by x-ray diffraction to confirm purity and crystallinity. A batch Ni sorption experiment was run under atmospheric conditions, using the surface area of goethite that is believed to be equivalent to 20 g of Wedron sand, the weight used in previous sorption experiments. A batch Ni sorption experiment was also run using acid-cleaned Min-U-Sil with a grain surface area equivalent to that of 20 g of Wedron sand.

**Forecast:** Documentation is in preparation. An abstract entitled "Unraveling Multi-Solute Sorption by Mineral Mixtures through Surface-Complexation Studies of Simple Systems: Sorption of Ni and Li by a Natural Sand" (Ward et al., 1993) was accepted for oral presentation at the Geological Society of America Annual Meeting.

### Reactive Transport Model Development

The LEHGC code is a coupled reaction/transport simulator which solves systems of transport and geochemical equilibrium equations. The chemical processes, assumed to occur under conditions of local equilibrium, include aqueous complexation, adsorption (surface complexation), ion exchange, and precipitation/dissolution. The LEHGC code is currently being modified to improve computational efficiency, add additional sorption and ion exchange sites, and is being ported to a massively parallel computer.

During the past six months, linkage of the new version of EQMOD with the flow module was completed; the new version of the chemical speciation module contains multiple sorption and ion-exchange sites. Four alternative PCG solvers were incorporated into LEHGC1.1. Testing of both the incorporated new EQMOD and the PCG solvers was completed. Preliminary work on adapting the LEHGC code for simulations of colloidal transport in fractured media began. Post-processing software was adapted to produce contours for two-dimensional simulations. Formal technical review of "User's Manual for LEHGC: A Lagrangian-Eulerian Model of HydroGeological Transport in Saturated-Unsaturated Media - Version 1.0" was completed.

A strategy was devised for implementing the LEHGC code on a massively parallel machine. The code was ported to the 1024-node nCUBE, compiled and executed on a single node; results compared well with previous calculations on a SUN work station and CRAY supercomputer. The subroutines and associated data to be distributed to multiple nodes were identified and specific locations were identified for "scatter-gather" operations. Once the code is successfully executing on multiple nodes, timing studies will be carried out to determine the benefits of this massively parallel implementation.

**Forecast:** SNL will continue development of a coupled reaction/transport simulator which solves a system of both transport and geochemical equations for radionuclide transport.

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The code (LEHGC) will simulate equilibrium chemical processes and will include aqueous complexation, adsorption (surface complexation), ion exchange, oxidation-reduction and precipitation/dissolution. Transport in fractures and transport of contaminants by colloids will be simulated. The code will be adapted to a massively parallel computing architecture enabling simulations of transport that include complex chemical behavior on the time and spatial scales required for regulatory compliance assessments.

Transport predicted by performance assessment codes using retardation factors measured on bulk mixtures will be compared to the tracer behavior predicted by the LEHGC code using surface complexation models. This information will be used to develop probability density functions for  $K_d$  determinations for future TSPAs, and will provide input to geostatistical models for  $K_d$  determinations at Yucca Mountain.

### 2.7.5.3 Activity 1.6.3.1 - Analysis of Unsaturated Flow System

Subactivity 1.6.3.1.1 - Unsaturated zone flow analysis. A report entitled "Processes, Mechanisms, Parameters, and Modeling Approaches for Partially Saturated Flow in Soil and Rock Media" (Wang and Narasimhan, 1993) was completed, printed, and distributed.

The M&O and SNL provided an outline for bounding modeling studies for fractured porous materials. Discrete fracture realizations from the Golder Associates Inc. FracMan code obtained by USGS will be combined with SNL measurement of fracture characteristic and relative fluid conductivity to enable doing the subsequent bounding modeling investigations.

A subrepository scale hydrothermal model was developed to provide hydrologic inputs for TSPA 1993. This model uses a two-dimensional axi-symmetric mesh to represent a generic waste-emplacement "panel" and its surrounding drift. Model objectives are to compute temperature histories at the center and the edge of the panel and the associated saturation/flux values. Presently the VTOUGH runs have been completed for one repository panel with areal power densities of 141, 189, and 282 kW/ha (57, 76, and 114 kW/acre).

A member of the M&O performance assessment staff presented a paper entitled "Effective Hydraulic Conductivity in Bounded, Strongly Heterogeneous Porous Media" (Paleologos and Neuman, 1993) at the Spring Meeting of the American Geophysical Union. It is the first time that solutions for bounded domains appear in the stochastic literature and the results generated significant interest.

Dripping fractures are known to occur in underground openings in unsaturated rock. Presumably they are caused by nonequilibrium fracture flow from perched water zones. Using TOUGH2, the M&O investigated the extent to which the condensate front surrounding the repository could feed a perched water zone, thus leading to a relatively early return of liquid water to the cooler regions of the repository. Results indicate the water vapor barrier accompanying perched water partially blocks the upward diffusion of water vapor. This

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effect reduces condensate formation above the perched zone and enhances the downward directed release of vapor and liquid to the saturated zone.

The M&O and USGS staff involved in Study Plan 8.3.1.2.2.8, "Characterization of Fluid Flow in Unsaturated, Fractured Rock," have facilitated scheduling efforts of Golder Associates Inc., who are assisting in application of FracMan/MAFIC analysis capability to obtain discrete fracture realizations using the USGS field fracture mapping data. The Golder software provides the capability for the transfer of discrete fracture realization data for use in either the TOUGH and FEHM coupled multiphase thermal flow codes which will be used in support of the USGS fracture flow study plan.

A Hydrologic Data/Thermal Modeling Interchange at USGS-Denver in May 1993 was jointly chaired by the M&O and YMPO. The meeting provided thermal modeler feedback on the new USGS data set provided in February 1993 for the thermal studies, discussion of long term needs for measurements of the air phase relative permeabilities, and consideration of the potential measurement implications of some initial thermal modeling sensitivity results involving particular ranges of bulk matrix-fracture permeability.

The M&O, LBL, and USGS have coordinated the planned hypotheses testing and sensitivity evaluations concerned with Study Plan 8.3.1.2.2.9, "Site Unsaturated-Zone Modeling and Synthesis." Specific efforts are to better satisfy the following performance assessment needs: demonstrate the rationale for selecting between alternative conceptual models, and provide a basis for testing the abstraction or roll-up methodology for system simulators used in TSPAs.

### Geohydrologic Data Development

The M&O performance assessment staff is coordinating the implementation of Study Plan 8.3.1.2.2.3, "Characterization of the Percolation in the Unsaturated Zone - Surface-Based Study," with assistance from the Principal Investigators involved, to enable YMPO to retrieve better data for the spatial infiltration distributions to represent Yucca Mountain. The spatially varying infiltration is needed as basic input to both the USGS/LBL Site Scale Three-Dimensional Flow Model and the Los Alamos Site Scale Three-Dimensional Transport/Retardation Model. Both modeling efforts are to become vital parts of the process level performance assessment evaluations.

### Probability Distributions

The SNL staff performing modeling and analysis for TSPA 1993 required probability distributions for both bulk and matrix hydrologic data. In response to the concern that the relatively abundant matrix hydrologic values do not provide the true characterization of Yucca Mountain, information on fracture properties was also developed.

Basic data acquisition, reduction and analysis necessary to provide probability distributions to TSPA analysts were completed. The SNL staff performing TSPA modeling

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were provided with initial basic statistics, beta distribution parameters, and upscaled beta distribution parameters for the matrix material properties.

Data for TSPA analyses were extracted from site and analog data for statistical reduction and depicted as probability distributions. The basic statistics report the number of data, expected value (mean), coefficient of variation, and maximum and minimum of the data. From the basic statistics, beta probability distribution parameters were derived by the RS/1 statistical package. If a normal distribution could not be generated because of the lack of sufficient data, Shannon's maximum entropy routine was employed reporting the mean, the maximum and minimum, and the alpha and beta curve parameters of the distribution. Then the curve parameters were upscaled for the beta probability distribution parameters that account for the vertical correlation length and mean thickness of the hydrogeologic units. Data reported include the mean thickness of the unit, upscaled coefficient of variation, upscaled alpha and beta distribution parameters, and model specific input parameters (p and q). The same approach was used for porosity, conductivity, and bulk density. For the desaturation parameters, Van Genuchten fits were generated for desaturation tests reported in "Fracture and Matrix Hydrologic Characteristics of Tuffaceous Materials from Yucca Mountain" (Peters et al., 1984), "Statistical Analysis of Hydrologic Data for Yucca Mountain" (Rutherford et al., 1992), and the data generated by USGS-OFR-90-569 (Flint and Flint, 1990), currently being used for the INTRAVAL exercise. To support and visually complement the numerical analyses, graphical representations of the basic statistics and beta probability distributions were developed (histograms and beta probability distribution plots, both normal and log normal) for inclusion in the TSPA 1993 report.

The fracture parameters, including fracture frequency, fracture spacing, fracture porosity, fracture hydraulic conductivity, fracture air-entry parameter, fracture orientation and fracture aperture were also completed. Fracture data from downhole measurements were analyzed for fracture distributions from USW G-4 as a test case to evaluate utility to the performance assessment problem. An attempt was initiated to derive the applicable information to correlate fracture aperture size as a function of the second moment of log saturated permeability versus log pore-size, according to an approach developed by LBL staff. The success of the approach would allow the availability of a more realistic range of aperture for the TSPA models.

A program was written to sample fracture frequency and bulk conductivity distributions to create a distribution of fracture apertures using the cubic law. Distributions for the fracture air entry parameter were also generated. A root-finding subroutine was added to help generate varieties from a beta probability distribution and code was added to allow comment input files to be used.

### INTRAVAL

The M&O, through Golder Associates Inc. staff, supported YMP participation in the international model validation program, INTRAVAL, through meeting participation and incorporation of data into the modeling process. The YMP INTRAVAL modeling results were presented at a meeting in Seattle, Washington, August 3-4, 1993. The meeting

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participants, USGS, SNL, LBL, the Commission, and State of Nevada, presented the model predictions for the moisture content in the UE-25 UZ#16 well drilled at Yucca Mountain. The predictions were compared, for the first time, with the UE-25 UZ#16 core moisture measured results made available at the meeting. The fracture data are being used on the extension of the FracMan/MAFIC codes for the interpretation of in situ air injection tests as part of YMP in a cooperative effort among the M&O, Golder Associates Inc., and USGS. Specifically, the saturated discrete fracture generation and solution capability of these codes is being extended to evaluate compressible air flow in fractured systems.

At SNL, development has continued on the east-west INTRAVAL cross section. Most of the indicator simulations have been converted to porosities. The north-south cross section was rerun with the third INTRAVAL data set incorporated and other corrections. Graphics were produced for the north-south cross section. Work has continued on the east-west INTRAVAL cross section with the gradational change in porosity in the shardy base added. The adaptive grid algorithm GAG was tried on the cross section, but produced poor results. Changes are being made to GAG to improve the results. A report on the SNL modeling effort for INTRAVAL was completed and submitted for review by the INTRAVAL participants. A presentation of SNL results was prepared for the INTRAVAL wrap-up meeting in Stockholm, Sweden, in late-August 1993. The presentation was given by a representative of the DOE staff who attended the meeting.

### Performance Assessment Data Base

Configuration of the INGRES system continues for the Performance Assessment Data Base to facilitate ease of data retrieval and presentation of the data in the format required by the analysis. Assistance has been provided to the analysts for the retrieval and reconfiguration of data. Work is continuing on the configuration of information in ARC/INFO to make use of Yucca Mountain data more flexible. A number of programs were written to link various routines in the geostatistical software from the Stanford (University) Center for Reservoir Forecasting. The Performance Assessment Data Base staff has initiated a review of the data base design and the requirements for the integration of the test results from construction monitoring, thermomechanical testing, and properties testing at Yucca Mountain.

### Probability Modeling

Modifications to the entropy fit program were made in response to problems discovered during early generation of the probability distributions for TSPA 1993. The changes included:

- A change in the computation of normalizing constant from adaptive integration to an analytical formula has been made. A more complicated change for bimodal and trimodal beta distributions was also completed.
- Display of the cubic line search iteration was added.

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- The maximum number of nonlinear iterations has been added to the input file so it can be adjusted by the user.
- Error tolerances were adjusted to increase robustness. Step size used in computing derivatives was made more robust.

Staff completed modifications of probability software originally installed on a VAX. Specifications for the user interfaces are being developed for experience gained during the elicitations. A user interface in an RS/1 shell has been written and installed on a personal computer.

**Forecast:** Documentation is progressing on the parameter generation for TSPA 1993 and for a stand alone document, which will contain more detail on the specifics of the data development. Subjects to be covered in both documents are stratigraphy development, data sources, and probability distribution function development for matrix, bulk, and fracture parameters. The hydrologic data availability has highlighted a critical need for bulk hydrologic conductivity data from the units above the Calico Hills horizon. The available bulk data for the Topopah Spring units are minimal to nonexistent. The relative sensitivity of these parameters will be investigated as part of the TSPA follow up analyses run in FY 1994. This information may then be used to help guide site investigations.

Subactivity 1.6.3.1.2 - Saturated zone flow analysis. An SNL staff member attended the Hydrology Integration Task Force meeting held in Denver, Colorado, May 17-18, 1993. The topic of focus was the C-Well testing, the current results, and future test plans.

A memo on the details of the modeling that will form the basis for flow and transport in the saturated zone for TSPA 1993 was completed and is currently in review by SNL and USGS staff. Information on the SNL saturated zone model was also made available to the M&O at their request.

**Forecast:** No activity is planned in FY 1994.

### **2.7.5.4 Activity 1.6.4.1 - Calculation of Pre-Waste-Emplacement Ground-Water Travel Time (GWTT)**

Subactivity 1.6.4.1.1 - Performance allocation for Issue 1.6. No progress during the reporting period; this was an out-year activity.

Subactivity 1.6.4.1.2 - Sensitivity and uncertainty analyses of ground-water travel time. See work reported under Subactivity 1.6.4.1.3.

Subactivity 1.6.4.1.3 - Determination of the pre-waste-emplacment ground-water travel time. The SNL participation in the INTRAVAL project centered on verification of numerical approaches for two-dimensional ground-water travel time calculations that were already under development. An extension of the INTRAVAL work, using the insights obtained during that



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exercise, was begun. The calculations were revised to incorporate zeolitic materials that are not included in the shallow calibration cross-section and to deal with some problems identified with the boundary conditions. Documentation of this work has also been started.

**Forecast:** This work will lead to calculations to predict ground-water travel time, as defined in 10 CFR Part 60. Activities planned for FY 1994 include performing sensitivity studies on parameter fields generated using theoretical and measured scaling models and geostatistical models developed for Yucca Mountain. These results will also be provided to guide future work in constructing experiments on scaling and geostatistics and to continue to support any validation initiative that may be a follow-on to the INTRAVAL studies completed in 1993. The objective of this work is to better conduct uncertainty and sensitivity studies to determine the hydrologic parameters of most importance in estimates on ground-water travel time; to continue the definition and development of an appropriate method for performing two-dimensional ground-water travel time calculations; and to continue work on upscaling of lab scale properties to a scale appropriate for simulating Yucca Mountain.

### **2.7.5.5 Activity 1.6.5.1 - Ground-Water Travel Time After Repository Construction and Waste Emplacement**

No progress during the reporting period; this was an out-year activity. See, however, the description of the thermohydrological calculations being made for the TSPA 1993 exercise in Section 2.7.6, which is related work.

**Forecast:** No activity is planned for FY 1994.

### **2.7.5.6 Activity 1.6.5.2 - Definition of the Disturbed Zone**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

### **2.7.6 Total System Performance (SCP Section 8.3.5.13)**

The TSPA combines the effects of the waste package and other engineered barriers and the site to determine the release of radionuclides to the accessible environment due to all significant processes and events. Several evaluations of total system performance have been conducted by a number of organizations. These earlier assessments have included SNL preliminary evaluations reported in the Environmental Assessment (DOE, 1986), which reported the results of performance evaluations by Thompson et al. (1984) and Sinnock et al. (1984). The PNL staff performed a preliminary total system risk assessment in 1988 (Doctor et al., 1992). Independent of the DOE program, NRC completed Phase 1 of their Iterative Performance Assessment in 1990 (NRC, 1990), and the Electric Power Research Institute completed a Phase 1 performance assessment in 1990 (McGuire et. al., 1990), and a Phase 2

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evaluation in 1992 (McGuire et al., 1992). Recent assessments have been performed on behalf of the YMP and reported in TSPA 1991 (Eslinger et al., 1993; Barnard et al., 1992).

The bulk of the work on the recent SNL performance assessment was done in FY 1991, therefore it was named "TSPA 1991." In FY 1992, SNL staff performed a number of sensitivity studies on the TSPA 1991 results (Wilson, 1993a). The results of TSPA 1991 were incorporated in the iterative TSPA process through the planning of the second iteration, TSPA 1993, that was in progress at the end of FY 1993. The participants in the TSPA 1993 calculations are SNL and the M&O. The LLNL staff is providing the source term data and model, and USGS and Los Alamos are providing updated site and experimental data.

The M&O was tasked in FY 1993 to evaluate the probabilistic total-system code Repository Integration Program. The M&O tested the code by benchmarking it against the TSPA 1991 problem. The conclusions (INTERA, 1993) were that the Repository Integration Program approach is a viable method for performing total system assessments. The M&O is applying the Repository Integration Program in TSPA 1993.

The differences between TSPA 1993 and TSPA 1991 include: (1) factoring in nonisothermal conditions to capture the effects of the thermal pulse associated with the disposal of spent fuel in the unsaturated zone, (2) improvements in the conceptualizations of unsaturated and saturated hydrologic flow, (3) enhancement of the radiological source term and the treatment of near-field processes, and (4) inclusion of geostatistical correlations for relevant parameters. The larger of these differences, in terms of affecting system performance, is expected to be the inclusion of thermal effects. The motivation for including these effects is to help answer the question of what the optimal areal mass loading or areal power density may be for a repository in the unsaturated zone.

Beyond TSPA 1993, there are TSPAs planned to support all of the major decision points in the Yucca Mountain Site Characterization Program. In the 1995-1996 timeframe, an interim site suitability evaluation will be done that will be supported by a total system assessment. In the 1997-1999 timeframe, the Environmental Impact Statement scoping process will be under way, and the draft Site Recommendation Report and the draft Safety Analysis Report will be in progress. Each of these major decision-making documents will be supported by TSPAs.

SNL is involved in producing a series of calculations that will form the basis for their contribution to the second iteration of total system performance assessments, TSPA 1993. The SNL document will consist of enhancements and expansions upon simulations reported in TSPA 1991. These will include calculation of radionuclide release and transport by aqueous and gaseous flow, as well as by conditions caused by human intrusion and basaltic volcanism. Of particular interest in this new suite of calculations is: inclusion of a more sophisticated source term and near field models (based on work by LLNL), coupling of thermal effects, enhanced treatments of retardation and solubility, incorporation of more site data and use of geostatistical correlations, and better treatment of disturbed conditions (including climate change). Although SNL will be reporting these results in a SAND document, a separate DOE

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document will be generated to compare and contrast both the SNL and M&O TSPA 1993 results.

Preliminary complementary cumulative distribution functions generated for the aqueous flow and transport portion of TSPA 1993 show a particularly interesting result. When compared to those generated for TSPA 1991, complementary cumulative distribution functions for releases from the engineered barrier system are only slightly different, even though a significantly more sophisticated source term model was used. However, the TSPA 1993 complementary cumulative distribution functions for releases to the accessible environment are quite different from TSPA 1991. The changed infiltration rate distribution appears to be the dominant parameter influencing this change. Specific calculations are discussed in Activities 1.1.3.1 and 1.1.5.1, below.

SNL hosted a meeting in Albuquerque, New Mexico, on September 20, 1993, to discuss preliminary results of the TSPA calculations done by SNL and the M&O. Representatives from LLNL and USGS were also present. A number of areas were identified for refinement and for sensitivity studies that will be incorporated into the final simulations.

The M&O completed the preliminary calculations for its TSPA 1993 contribution. The waste package/engineered barrier system file use in the Repository Integration Program code includes temperature-dependent corrosion rates; spent fuel and high-level defense waste dissolution rates; radionuclide solubilities; saturation- and flux-dependent corrosion rates; radionuclide diffusion from the waste package; and correlation of solubilities. Abstracted results from two-dimensional repository panel scale hydrotherm calculations were provided as input to Repository Integration Program calculations of waste package and far-field performance assessment. The  $^{14}\text{C}$  travel time distributions provided by SNL were transformed into Repository Integration Program-usable gas velocity distributions as a function of time of release from the waste package. A set of radionuclide release calculations were completed for waste packages placed in vertical boreholes and in-drift emplacement mode for three areal power densities: namely 28, 57, and 114 kw/acre. The results are to be presented to YMPO October 21-22, 1993.

The M&O supported the Nuclear Waste Technical Review Board meeting in Denver, Colorado, July 13-15, 1993. The meeting agenda was, in part, to present to the full board the progress on TSPA 1993, and support to the National Academy of Sciences study on technical bases for Yucca Mountain standards. The M&O made presentations on "Performance Assessment Efforts in Support of National Academy of Sciences Study" and "Total System Performance Assessment (TSPA) II: Repository Integration Program (RIP) Abstractions Analyzing Nominal Conditions."

The M&O and Golder Associates Inc. submitted a draft document entitled "Application of RIP (Repository Integration Program) to the Proposed Repository at Yucca Mountain: Conceptual Model and Input Data Set" to YMPO for review. The report documents a description of the preliminary data set constructed as a conceptual model for applying the Repository Integration Program to the proposed Yucca Mountain site.

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The M&O completed the first draft of the "YMP Performance Assessment Strategy." The principal objective of the document is to provide a common understanding of the general strategy and methodology for performance assessments, and to outline the need for TSPAs in support of future programmatic needs. The final draft of the Performance Assessment Strategy will be issued as a YMP document with input from all performance assessment participants and YMPO. It is currently being reviewed by the Participants.

### **2.7.6.1 Performance Assessment Activity 1.1.2.1 - Preliminary Identification of Potentially Significant Release Scenario Classes**

Subactivity 1.1.2.1.1 - Preliminary identification of potentially significant sequences of events and processes at the Yucca Mountain repository site. Work related to this activity is reported under Subactivity 1.1.2.1.2.

Subactivity 1.1.2.1.2 - Preliminary identification of potentially significant release scenario classes. A report entitled "Scenarios Constructed for Basaltic Igneous Activity at Yucca Mountain and Vicinity" (Barr et al.) has completed review comment resolution and has been submitted to the printer for publication.

The definition of nominal case scenarios is in progress at SNL. The M&O worked with SNL to clarify the importance of the "Nominal Flow System Cases," and helped explore ways of simplifying presentation of these scenario classes. The documentation of "Nominal Cases" now in review is the basis for a proposed definition of YMP site and repository hydrologic baseline cases. Such baseline cases are necessary to conduct the combined process hypothesis testing and sensitivity evaluations which establish the detail level conceptual modeling required, provide a testing basis for abstracted TSPA models, and allow prioritization of hydrologic site characterization data.

The SNL staff attended a Nuclear Energy Agency/Organization for Economic Cooperation and Development meeting in Paris, France, June 17-18, 1993. The meeting addressed the possibility of forming an international data base on features, events, and processes related to radioactive waste isolation. The meeting was also attended by representatives from Sweden, Switzerland, Canada, NRC, and the Waste Isolation Pilot Plant project. The consensus of the group was that such a data base could be very useful to the international community. The group agreed to work on several methods of incorporating the information already available in the various programs. A second meeting in November will review the results of these efforts. In conjunction with this trip, visits were made to the radioactive waste isolation programs at Bureau de Recherches Geologiques et Minières in Orleans, France, and Swiss National Cooperative Society for the Storage of Radioactive Wastes in Switzerland. Presentations were made on TSPA 1991 results and the status of TSPA 1993 at both locations.

**Forecast:** Scenarios developed under this element form the basis for numerical and analytical modeling of features, events and processes that might contribute to release and transport of radionuclides.

Activities in FY 1994 will include completing the final draft of the Nominal Flow scenario selection document, "Scenarios Constructed for Nominal Flow in the Presence of a Repository at Yucca Mountain and Vicinity" (Barr et al.), incorporating comments from YMPO review; completing the tectonic and human intrusion scenario selection documents, investigating the need for construction of event trees describing disturbances due to repository construction and operation; and participating in the Nuclear Energy Agency/Organization for Economic Cooperation and Development working group to form a data base for features, events and processes. These activities are linked with efforts being conducted by SNL, USGS, Los Alamos, LLNL, and LBL.

**2.7.6.2 Performance Assessment Activity 1.1.2.2 - Final Selection of Significant Release Scenario Classes to be Used in Licensing Assessments**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

**2.7.6.3 Performance Assessment Activity 1.1.3.1 - Development of Mathematical Models of the Scenario Classes**

**Subactivity 1.1.3.1.1 - Development of models for releases along the water pathways.**

For the TSPA 1993 (see Section 2.7.6.6) composite-porosity flow model, SNL constructed a new set of stratigraphic columns for the three potential repository footprints. The footprints were based on variations in power densities. Reconfiguration of each footprint has required construction of different stratigraphic cross-sections from which to draw the columns used for the one-dimensional calculations. Distributions for the hydrogeologic parameters of the stratigraphic units were incorporated into the total system performance assessment computer code, TOSPAC, input files. The parameter distribution generation is reported in Activity 1.6.3.1.1.

A short "graphic" about TOSPAC was written for inclusion in the SNL Software Catalog. Other modifications to the SNL codes, necessary to complete the TSPA 1993 calculations, were also completed. A new automatic mesh generator for TOSPAC was completed. The mesh generator will allow TSPA 1993 to efficiently calculate flow and transport for problems with different water-table heights and a wide range of percolation rates. This should help minimize mass-balance problems during transport calculations.

The TSPA 1993 "weeps" model was modified to incorporate LLNL's source-term model, Yucca Mountain Integration Model, and to incorporate thermal-effects data provided by SNL. Specifics of the modification include incorporating the number of containers outside the boiling isotherm as a function of time, the volume of rock encompassed by the boiling isotherm, and the temperature histories of representative containers.

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Subactivity 1.1.3.1.2 - Development of a model for gas-phase releases. Disposal Safety, Inc. developed new gas-flow and  $^{14}\text{C}$ -travel-time calculations that will be used to modify the gaseous flow model for TSPA 1993. Two-dimensional stratigraphies were generated by SNL for the gas-flow calculations and used by Disposal Safety, Inc. for their simulations. Information on the TSPA problem setups (including repository area and heat output, stratigraphy, and material properties) was also transmitted to Disposal Safety, Inc. Using this input, they completed the gas-flow calculations for TSPA 1993. Upon receipt of this information, SNL distributed the information to the M&O for inclusion in their TSPA 1993 calculations. The calculations are similar to the ones used in TSPA 1991, with two major improvements: gas flow and heat flow are now coupled and the calculations are time-varying rather than steady-state. Extremely short transport times were calculated by Disposal Safety, Inc. for  $^{14}\text{C}$ , given the hydrologic parameter values for the model. Subsequent studies are being run that will vary the relevant parameters to determine their relative sensitivities.

Subactivity 1.1.3.1.3 - Development of a model of releases through basaltic volcanism. The thermal pulse calculation to model an igneous dike near a waste package is completed. The calculation involves evaluating transcendental functions, which require the application of numerical analysis techniques. Now the range of temperatures can be approximated that may be expected in rock surrounding a basaltic intrusion. This calculation will be combined with a modified version of the TSPA 1991 VOLCAN program to calculate conditions for waste package failures.

Subactivity 1.1.3.1.4 - Development of a model of releases through human intrusion. A report entitled "Analyses of Releases Due to Drilling at the Potential Yucca Mountain Repository" (Barnard, 1993) was submitted as an invited paper for the 1993 American Nuclear Society winter meeting.

The human intrusion direct release model developed for TSPA 1993 calculates releases due to drilling into a repository where the waste package configuration is based on four variations of the thermal loads and emplacement schemes (defined in Activity 1.5.1.1). The human intrusion analyses also reflect the probabilities of drilling into both glass and spent-fuel waste. Preliminary results of calculations for the in-drift emplacement model indicates that interception of the much larger waste package may lead to releases of very high amounts of radionuclides in any one drilling event. Final analyses and sensitivity studies have been completed.

**Forecast:** See Section 2.7.6.6, Performance Assessment Activity 1.1.5.1.

### **2.7.6.4 Performance Assessment Activity 1.1.4.1 - The Screening of Potentially Significant Scenario Classes Against the Criterion of Relative Consequences**

Work related to this activity is reported under Section 2.7.6.1, Activity 1.1.2.1.

**Forecast:** See Section 2.7.6.1, Performance Assessment Activity 1.1.2.1.

**2.7.6.5 Performance Assessment Activity 1.1.4.2 - The Provision of Simplified, Computationally Efficient Models of the Final Scenario Classes Representing the Significant Processes and Events Mentioned in Proposed 10 CFR 60.112 and 60.115**

Work related to this activity is reported under Section, 2.7.6.6, Activity 1.1.5.1.

**Forecast:** See Section 2.7.6.6, Performance Assessment Activity 1.1.5.1.

**2.7.6.6 Performance Assessment Activity 1.1.5.1 - Calculation of an Empirical Complementary Cumulative Distribution Function**

Input Parameters for TSPA 1993

Geochemistry. SNL hosted a meeting on April 13, 1993, to elicit distributions for solubility to be used for TSPA 1993 from Los Alamos personnel. Probability density models of the distribution of solubility were generated for 15 radionuclides through elicitation of a panel of experts from Los Alamos. As a result of this interaction, a number of changes to the software used to generate the distributions will be made to facilitate the elicitation process.

The SNL staff coordinated and hosted an elicitation of sorption data for TSPA 1993 in Albuquerque, New Mexico, on June 1, 1993. The geochemistry experts elicited were from Los Alamos, Jacobs Engineering, and SNL with observers from the M&O also present. The  $K_d$  distributions were elicited for 15 radionuclides. The solubility and sorption distributions resulting from these elicitations are being used in both SNL and the M&O contributions to TSPA 1993.

Members of SNL staff attended the YMP Colloid Workshop. Results of an SNL analysis were included in a presentation entitled "Colloids: A Performance-Assessment Perspective" (Wilson, 1993b). The purpose of the analysis was to examine the question of whether transport of radionuclides by colloids will be significant for repository performance at Yucca Mountain.

Infiltration and climate change. A meeting was coordinated and hosted by SNL personnel on May 26, 1993, with participants from USGS, Raytheon Services of Nevada, and the M&O. The purpose of this meeting was to discuss the best approach for representing infiltration and water flow at Yucca Mountain resulting from both current and future climatic conditions. The results of this discussion are being used as the basis for the percolation flux used in TSPA 1993.

On June 25, 1993, staff of both SNL and Tech Reps Inc. met to discuss the climate-change information being gathered by the DOE Waste Isolation Pilot Plant project in New Mexico. The Waste Isolation Pilot Plant is using a doubling of precipitation as the upper bound of a climate change in the next 10,000 years. On the basis of information obtained from the Waste Isolation Pilot Plant and USGS, climate change will be represented

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in TSPA 1993 as dry, interpluvial periods (like the present) where ground-water flux is characterized by an exponential distribution with a mean value of 0.5 mm/year; and wet, pluvial periods characterized by an exponential distribution with a mean value of 10 mm/year. The time period under consideration has been extended from 10,000 years (TSPA 1991) to 1,000,000 years (TSPA 1993).

### Source Term and Near-field Development

A report entitled "Review of Radionuclide Source Terms Used for Performance Assessment Analyses" (Barnard, 1993b) completed SNL management review and was transmitted to YMPO for policy review.

A meeting was held on May 26, 1993, at LLNL, to formulate a source term for use by the M&O in their contribution to TSPA 1993. The result of the meeting was that the M&O will use the same source term that had been previously determined by interactions occurring between SNL and LLNL in February 1993. Also, a meeting was held in early-June 1993, to correlate the LLNL hydrothermal calculations with SNL thermal data to determine the hydrothermal profiles to be used in the TSPA 1993 source term.

A number of meetings were held at SNL and LLNL to couple the LLNL Yucca Mountain Integration Model source model to SNL transport models for the TSPA (both TOSPAC and WEEPTSA). There were a number of difficulties with this integration, but the collaboration went well and this interface between SNL programs should make future generations of the Yucca Mountain Integration Model easier to incorporate.

The calculations of waste-package lifetimes for the four emplacement configurations analyzed in TSPA 1993: 141 kW/ha (57 kW/acre) for the SCP-reference waste package design, vertical emplacement; 282 kW/ha (114 kW/acre) for the SCP-reference waste package design, vertical emplacement; 141 kW/ha (57 kW/acre) for a larger waste package, in-drift emplacement; and 282 kW/ha (114 kW/acre) for a larger waste package, in-drift emplacement were completed. The calculated range of lifetimes is from about 900 to over 10,000 years.

The SNL staff has also developed a source term that reflects the proper weighting of age and burnup for spent fuel and also includes glassified high-level waste for TSPA 1993. The spent-fuel inventory was built as for TSPA 1991, except that the waste stream that describes the proposed emplacement scheme will be used to determine fuel age and burnup. Data for glass form high-level waste were obtained from the "Characteristics Data Base" (DOE, 1987a). There will be two representations of the source term. The human intrusion source term will be composed of all of the inventory, while the aqueous flow and volcanism calculations will utilize indicator nuclides, as discussed in "Review of Radionuclide Source Terms Used for Performance Assessment Analyses" (Barnard, 1992).

The M&O developed a functional form for the dissolution rate of  $UO_2$  as a function of temperature, pH, and carbonate concentration. This function was obtained for use in the M&O source term calculations for TSPA 1993 using the Repository Integration Program code's engineered system module.



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The SNL staff attended an M&O-sponsored meeting in Richland, Washington, on the continuing development of the AREST source-term code. The plans and capabilities for the code (written by PNL for the M&O) were discussed. Currently, it is anticipated that AREST will have both low-level (process) model capability, as well as higher-level (performance assessment) features. Because of these ambitious requirements, coupled with low available funding, the code will not be available for some time. The waste package and near-field portions of the SNL features, events, and processes diagrams were also discussed. A staff member of PNL has characterized near-field environments in terms of amount and rate of moisture, oxygen, and heat around the waste package. This information is necessary to complete features, events, and processes diagrams.

The SNL staff also participated in the Technical Workshop on Near-Field Performance Assessment, at Cadarache, France, May 11-13, 1993. Attendees included representatives from the United States, Sweden, Switzerland, Germany, France, Finland, United Kingdom, and The Netherlands waste-disposal programs. The purposes of the meeting were to review the aspects of near-field performance assessment, to develop themes that should be pursued, and to identify areas common to the programs that might be appropriate for collaboration. Topics included near-field environment, releases, transport, modeling, and performance assessment integration. The workshop participants were split into interest groups to discuss the topics in detail and develop recommendations. Most of the emphasis was on the European programs (and their design and environmental conditions); consequently, most of the discussion was concerned with saturated repositories with bentonite backfill and reducing ground-water conditions. A member of the SNL staff was in the performance assessment integration group, therefore YMP interests were included in their recommendations. Areas of mutual interest included many of the scenario classes (e.g., near-field hydraulic, radiolytic, and chemical processes; volcanic processes; repository operations), some aspects of the geochemistry (e.g., alteration of near-field hydraulic properties by the engineered barrier system), glass-waste dissolution, and salt-repository characteristics. A survey and review document and a workshop summary are being prepared by the organizers to be published within a few months.

**Forecast:** A series of sensitivity studies will be performed on the results of TSPA 1993 that were obtained in FY 1993. The final documentation of the second cycle of the SNL contribution to the TSPA, as well as the M&O contribution, will be completed in early FY 1994. At this time, it is expected that TSPA 1993 modelers will make presentations on results of TSPA 1993 to other YMP participants to help guide site characterization studies, and also to other groups for information on progress in performance assessment. In addition, SNL and the M&O will cooperatively produce a document combining all elements of the DOE effort on TSPA 1993 in mid-FY 1994.

These activities are closely integrated with efforts described in Section 2.2.3.6 (geostatistical cross-correlation of parameters, stratigraphy), Section 2.4.1.16 (thermal history), Section 2.7.6 (scenarios for modeling, gas flow models, data sets), Section 2.7.5 (elicited parameters), and Section 2.7.5.2, Subactivity 1.6.2.2.2 (parameters for scaling, information on geochemistry, thermal effects validation experiments) by SNL, the M&O, LLNL, the USGS, Los Alamos, and LBL.

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A number of processes have been identified in TSPA 1991 and TSPA 1993 as potentially important to our understanding of the performance of the site. A number of laboratory validation studies and process modeling exercises describing these processes have reached a sufficient level of maturity to begin integration of the information into performance assessment calculations. Additional developmental work on existing tools is also required. This activity will incorporate the information from these studies into abstracted models that can then be used to expand and enhance the next cycle of TSPA.

Developmental activities are expected to include:

- Developing effective media models for flow through single fractures incorporating data on fingering and in-plane saturation processes described in Section 2.7.5.2, Subactivity 1.6.2.2.2.
- Developing and implementing a strategy for incorporation of nonisothermal processes into total-system simulations. The information for this effort will be provided in part by ongoing experimental and numerical efforts described in Sections 2.7.5.2 and 2.4.1.16.
- Developing an abstracted model for colloid transport of nuclides derived from detailed modeling efforts described in Section 2.7.5.1 with input from LLNL and Los Alamos.
- Including unit gradient method in TOSPAC to approximate two-dimensional streamlines using a one-dimensional code.
- Continued development of the detailed process level, AREST, and integrating level (Yucca Mountain Integration Model) source-term codes.

Contingent upon funding levels and YMP direction, the M&O and SNL may also begin initial problem definition for the next iteration of the TSPA in late FY 1994. Developmental studies performed in other performance assessment activities will form the basis for the next cycle of the TSPA. Also, the increased availability of data from site characterization activities will allow us to revise and expand the analyses performed during the first two cycles. This cycle will be the basis for the use of the total system in the Advanced Conceptual Design, and some of the analyses to be conducted during this cycle will be identified by examining the needs of that design phase.

### **2.7.7 Individual Protection (SCP Section 8.3.5.14)**

#### **2.7.7.1 Activity 1.2.1.1 - Calculation of Doses Through the Ground-Water Pathway**

No progress during the reporting period; this was an out-year activity. Related work is reported in Section 2.7.6.6 because ground-water pathway dose calculations are part of the TSPA 1993 exercise.

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**Forecast:** No activity is planned for FY 1994; however, see Section 2.7.6 for related work.

### **2.7.7.2 Activity 1.2.2.1 - Calculation of Transport of Gaseous Carbon-14 Dioxide Through the Overburden**

No progress during the reporting period; this was an out-year activity. Work related to this activity is reported under Section 2.7.6.3, Activity 1.1.3.1.2.

**Forecast:** No activity is planned for FY 1994. See Section 2.7.6.6, Performance Assessment Activity 1.1.5.1, for related work.

### **2.7.7.3 Activity 1.2.2.2 - Calculation of Land-Surface Dose and Dose to the Public in the Accessible Environment Through the Gaseous Pathway of Carbon-14**

The TSPA 1993 exercise includes calculations of  $^{14}\text{C}$  doses in the accessible environment, as was reported in Section 2.7.6.3, Subactivity 1.1.3.1.2.

**Forecast:** No activity is planned for FY 1994. See Section 2.7.6 for related work.

## **2.7.8 Ground-Water Protection (SCP Section 8.3.5.15)**

### **2.7.8.1 Analysis 1.3.1.1 - Determine Whether Any Aquifers Near the Site Meet the Class I or Special Source Criteria**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

### **2.7.8.2 Analysis 1.3.2.1 - Determine the Concentrations of Waste Products in any Special Source of Ground Water During the First 1,000 Years After Disposal**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

## **2.7.9 Performance Confirmation (SCP Section 8.3.5.16)**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

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**2.7.10 U.S. Nuclear Regulatory Commission Siting Criteria (SCP Section 8.3.5.17)**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

**2.7.11 Higher-Level Findings--Postclosure System and Technical Guidelines (SCP Section 8.3.5.18)**

No progress during the reporting period; this was an out-year activity.

**Forecast:** No activity is planned for FY 1994.

### CHAPTER 3 - SCHEDULE

In late November 1989, a new proposed Program schedule was announced in the Secretary's report to Congress (DOE, 1989). The new schedule was based on consideration of the duration required to obtain Yucca Mountain site access from the U.S. Nuclear Regulatory Commission, the State of Nevada, and others; and the work scope described in the SCP and the more-detailed study plans. In January 1990, the schedule presented in the Secretary's report to Congress was finalized by the Office of Civilian Radioactive Waste Management in the Program Cost and Schedule Baseline (DOE, 1990b). This Program Cost and Schedule Baseline was revised in March 1991, in November 1991, and again in September 1992. Factors external to the Program, including uncertainties associated with Program funding levels, and study plan review, continue to affect the Program schedule.

This section presents the schedule baseline for the Yucca Mountain Site Characterization Project (YMP) as of the end of this reporting period (September 30, 1993). More detailed schedules are maintained at the Yucca Mountain Site Characterization Project Office, in combination with work scopes and the funding needed to accomplish this work. Based on progress, funding, and re-baselining activities, as well as the Secretary's review of the Program,, a new schedule will be published in the near future.

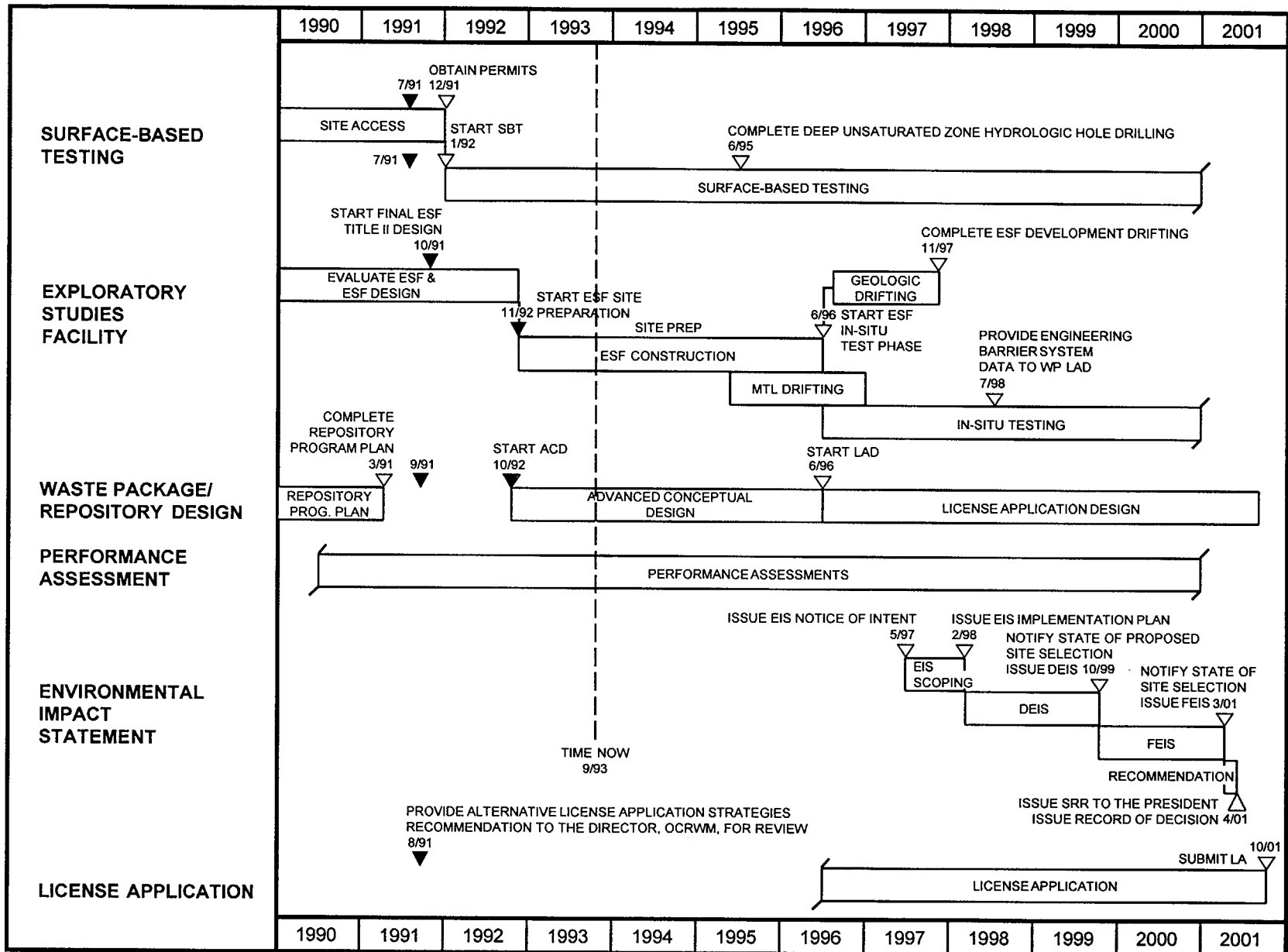
Table 3-1 presents the summary milestones for YMP. Figure 3-1 shows the relationship of the summary milestones to the major activities.

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Table 3-1. Summary Milestones <sup>a</sup>

Milestone	Baseline Date	Actual Date
<b><u>Surface-Based Testing</u></b>		
Obtain Permits	12/91	7/91
Start New Surface-Based Testing	1/92	7/91
Complete Deep Unsaturated Zone Hydrologic Hole Drilling	6/95	
<b><u>ESF</u></b>		
Start Final ESF Title II Design	10/91	10/91
Start ESF Site Preparation	11/92	11/92
Start ESF In Situ Test Phase	6/96	
Complete ESF Development Drifting	11/97	
Provide Engineering Barrier System Data to Waste Package License Application Design	7/98	
<b><u>Waste Package/Repository Design</u></b>		
Complete Repository Program Plan	3/91	9/91
Start Waste Package/Repository Advanced Conceptual Design	10/92	10/92
Start Waste Package/Repository License Application Design	6/96	
<b><u>Environmental Impact Statement</u></b>		
Issue EIS Notice of Intent	5/97	
Issue EIS Implementation Plan	2/98	
Notify State of Proposed Site Selection	10/99	
Issue Draft EIS	10/99	
Issue Final EIS	3/01	
Notify State of Site Selection	10/99	
Issue Record of Decision	4/01	
Issue Site Recommendation Report to the President	4/01	
<b><u>License Application</u></b>		
Provide Recommendation to the Director, OCRWM, on Alternative License Application Strategies for Review	8/91	8/91
Submit License Application to the NRC	10/01	

<sup>a</sup>Table shows approved Program Schedule Baseline and actual completion dates as of September 30, 1993. The baseline schedule is currently under review and will be revised and published in the near future.



3-3

LEGEND

- ▽ PROGRAM COST AND SCHEDULE BASELINE MILESTONE
- ▼ ACTUAL START/COMPLETION DATE

Figure 3-1. Site Characterization Summary Schedule

(This schedule is currently under review and will be revised and published in the near future)

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### CHAPTER 4 - EPILOGUE

This section provides a brief summary of key events that occurred after the close of the reporting period on September 30, 1993 and prior to final editing of this report.

On October 7, 1993, the U.S. Senate confirmed Dr. Daniel H. Dreyfus as the new Office of Civilian Radioactive Waste Management Director.

On October 27, 1993, the U.S. Congress approved an Office of Civilian Radioactive Waste Management budget for fiscal year 1994 at \$380 million. The Nuclear Waste Fund provided \$260 million; the Defense Nuclear Waste Disposal Account provided \$120 million.

The Nuclear Waste Technical Review Board report entitled "Underground Exploration and Testing at Yucca Mountain" was received by the Project in October 1993. The Project's response was submitted to U.S. Department of Energy/Headquarters on December 3, 1993, with the response to the Review Board scheduled for February 1994.

On November 18, 1993, the U.S. Department of Energy responded to the U.S. Nuclear Regulatory Commission concerns with respect to the Exploratory Studies Facility design process expressed in the Commission's letter dated August 20, 1993.



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### ACRONYMS, ABBREVIATIONS, AND SYMBOLS

ACNW	Advisory Committee on Nuclear Waste
AECL	Atomic Energy of Canada Limited
ASTM	American Society for Testing and Materials
ATM	Approved Testing Material
BLM	Bureau of Land Management
CRWMS M&O	Civilian Radioactive Waste Management System Management and Operating Contractor
DOE	U.S. Department of Energy
EPA	U.S. Environmental Protection Agency
ESF	Exploratory Studies Facility
FY	fiscal year
GSLIB	Geostatistical Software Library and User's Guide
HRL	Hard Rock Laboratory (Sweden)
ITE	Integrated Test Evaluation
LBL	Lawrence Berkeley Laboratory
LLNL	Lawrence Livermore National Laboratory
Los Alamos	Los Alamos National Laboratory
MC	Management Control
MGDS	Mined Geologic Disposal System
M&O	Civilian Radioactive Waste Management System Management and Operating Contractor
NAGRA	Swiss National Cooperative Society for the Storage of Radioactive Wastes
NAS	National Academy of Sciences
NRC	U.S. Nuclear Regulatory Commission
OCRWM	Office of Civilian Radioactive Waste Management
PNL	Pacific Northwest Laboratory
QA	quality assurance
QARD	Quality Assurance Requirements Document
REECo	Reynolds Electrical & Engineering Co., Inc.
RSN	Raytheon Services Nevada
SCP	Site Characterization Plan
SCPB	Site Characterization Program Baseline
SCP-CDR	Site Characterization Plan - Conceptual Design Report
SD	Geostatistical/Systematic Drilling Program
SNL	Sandia National Laboratories
TSPA	Total System Performance Assessment
TSw1	densely welded devitrified lithophysal-rich tuff
TSw2	densely welded devitrified lithophysal-poor tuff
USGS	U.S. Geological Survey
YMP	Yucca Mountain Site Characterization Project
YMPO	Yucca Mountain Site Characterization Project Office

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### ACRONYMS, ABBREVIATIONS, AND SYMBOLS (Continued)

#### Metric (SI) Units

°C	degree Celsius
cc	cubic centimeters (cm <sup>3</sup> )
cm	centimeter (= 10 <sup>-2</sup> m or 2.54 inches)
d	day
g	gram (= 0.3527 ounce)
h	hour
ha	hectare (= 2.48 acres)
Hz	hertz (cycles per second)
J	joule (kilogram-meter)
K	degree kelvin
kg	kilogram (= 10 <sup>3</sup> grams or 2.2046 pounds)
km	kilometer (= 10 <sup>3</sup> m or 0.6213 mile)
L	liter (= 0.2641 gallon)
MTU	metric tons of uranium
MTIHM	metric tons of initial heavy metal
m	meter (= 3.2808 feet)
mg	milligram (= 10 <sup>-3</sup> g)
mL	milliliter (= 10 <sup>-3</sup> L)
mm	millimeter (= 10 <sup>-3</sup> m)
µm	micrometer (= 10 <sup>-6</sup> m)
nm	nanometer (= 10 <sup>-9</sup> m)
Pa	pascal (also, MPa = megapascal, kPa = kilopascal)
S	siemens
s	second
V	volt
W	watt
kWh	kilowatt-hour
MWh	megawatt-hour
MWd	megawatt-day
GWd	gigawatt-day

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### ACRONYMS, ABBREVIATIONS, AND SYMBOLS (Continued)

#### Other (non-SI) Scientific/Engineering Terms and Units

bar	unit of barometric pressure
ca.	circa
cu. yd	cubic yard
ft	foot
gpm	gallons per minute
in	inch
ka	kiloannum (thousand years ago)
Ma	megannum (million years ago)
mi	mile
mil	1/1000th of an inch
mmol	millimolar
MN	meganeutons
pH	negative log of hydrogen ion concentration (acidity/alkalinity)
ppb	parts per billion
ppm	parts per million
psi	pounds per square inch
T	temperature
yr	year

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All technical reports and research products published by participating organizations on the YMP are generally available through the Office of Scientific and Technical Information (OSTI) at Oak Ridge, Tennessee. OSTI is the national center for dissemination of non-classified scientific and technical information prepared from research sponsored by DOE. The references cited in this section are available through OSTI, the open literature, or through proceedings volumes for symposia and technical conferences.

Copies of YMP reports and other documents published by DOE and the participating organizations, which are available through OSTI, can be ordered from:

National Technical Information Service  
U.S. Department of Commerce  
5285 Port Royal Road  
Springfield, VA 22161

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