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Civilian Radioactive Waste Management System
Management and Operating Contractor

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THERMAL LOADING STUDY FOR FY 1996
VOLUME I OF II

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November 8, 1996

Prepared for:

U. S. Department of Energy
Yucca Mountain Site Characterization Project
P.O. Box 98608
Las Vegas, Nevada 89193-8608

Prepared by:

TRW Environmental Safety Systems Inc.
101 Convention Center Drive
Las Vegas, Nevada 89109

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**THERMAL LOADING STUDY FOR FY 1996
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November 8, 1996

MR Hunt FOR O. J. GILSTRAP

M&O Quality Assurance Manager CONCURRENCE

11-22-96

Date

Steven F. Saterlie

Steven F. Saterlie, Study Manager and
Lead Document Preparer

11/22/96

Date

Richard D. Memory

Richard D. Memory, Systems Analysis
and Modeling Department Manager

11/22/96

Date

Richard C. Wagner

Richard C. Wagner, Systems Engineering
Office Manager

11/22/96

Date

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The major contributors and authors of the study were S.F. Saterlie (TRW), M. Reeves (IN), J.H. Lee (IN), E.R. Siegmann (IN), J.A. McNeish (IN), Y. Sun (MK), R.M. Nolting (MK), H. Yang (MK), M. Fortsch (FD), W.N. Shoemaker (FD), E.E. Ryder (SNL), F.J. Davis (SNL), T.A. Buscheck (LLNL), J.W. Carey (LANL), D.L. Bish (LANL), S.S. Levy (LANL), M.D. Rose (TRW), R.H. Bahney (FCF), and G. Danko (UNR).

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EXECUTIVE SUMMARY

This report documents the work conducted in a Thermal Loading Study over the period from October 1, 1995 through August 30, 1996. The primary objective of this study was to provide recommendations for Mined Geologic Disposal System requirements affected by thermal loading that will provide sufficient definition to facilitate development of design concepts and support life cycle cost determinations. The study reevaluated and/or redefined selected thermal goals used for design and are currently contained in the requirements documents or the *Controlled Design Assumptions Document* (CRWMS M&O 1996f). The study provided recommendations as to what, if any, actions (such as edge loading and limiting of the heat variability between waste packages) are needed and must be accommodated in the design. Additionally, the study provided recommendations as to what alternative thermal loads should be maintained for continued flexibility.

The thermal goals evaluated in the study were the not-to-exceed temperature of 200°C on the emplacement drift wall, the 350°C fuel cladding maximum temperature limit, and the not-to-exceed temperature limit of 115°C at the TSw2/3 interface. These goals were chosen for evaluation because it was questioned whether these criteria were valid to restrict the design. It was felt that sufficient information was available from tests to be able to quantify the effects on performance of changes in these goals. In addition, requirements were needed with regard to managing edge cooling of the potential repository and how the significant variations in package to package heat output should be handled.

Requirements [10 CFR 60, *Disposal of High-Level Radioactive Wastes in Geologic Repositories*, Section 21(c)(1)(ii)(D)], and the *Proposed Thermal Loading Strategy* (CRWMS M&O 1995a) direct that alternatives important to long term waste isolation, in this case alternative thermal loads, be considered. This study was tasked to examine what alternative thermal loads should be maintained to minimize Program risk, what is needed to ensure these alternative thermal loads are viable, and what constraints (schedule and cost) could be incurred on the system if a thermal loading decision is not made by specific dates.

The study used the latest available analytic tools and the latest measurements from underground and laboratory investigations to develop recommendations. However, in situ thermal tests have not been conducted and, for the most part, the analytic models used have not been validated. Therefore, in many cases significant uncertainty exists in the understanding of processes in the natural and engineered environment. As such, the approach taken in this study was to maintain a conservative defense in-depth approach at recommending system requirements.

The work documented in this technical report represents scoping analyses with the intention of facilitating the design process by providing requirements for design. However, much of the data and many of the models and codes used to support the development of these requirements are not qualified. Therefore requirements recommended by this study related to enhancing or preserving repository performance relative to a potential safety standard will be designated as *To Be Verified* (TBV).

Geochemical Thermal Goal. The *Site Characterization Plan* (DOE 1988) established a temperature goal for the TSw2/3 interface to remain less than 115°C in an effort to protect the

zeolites from mineralogic changes. Recent core measurements have found that the zeolitized layer varies in depth but in all cases is well below the TSw2/3 interface (more than 150 m below the potential repository), and 115°C has little relevance to potential mineralogic changes. Thus, it is recommended to delete this goal at the TSw2/3 interface and replace it with another goal as discussed below.

A process model to calculate the effects of dehydration of zeolites, resulting from elevated temperatures, was developed and coupled with a thermohydrologic model to determine whether repository performance would be impacted. The results of the calculations showed that insignificant impact on performance was predicted as a result of the dehydration of zeolites at thermal loads of either 20.5 or 28.4 kgU/m² (83 or 115 MTU/acre). However, mineralogic conversion of clinoptilolite (the most prevalent zeolite and the one which has significant sorptive properties for some radionuclides) to analcime, which has poor sorptive properties, was not considered. Natural analog studies have found that this irreversible reaction may take place somewhere in the range of 90 to 100°C in existing Yucca Mountain water chemistry (J-13 water). Thus, as a conservative, defense in-depth approach this study recommends placing a temperature criterion at the average top of the zeolitized layer beneath the potential repository area. Using this information and evaluations with other criteria, this study recommends that a not-to-exceed temperature limit of 90°C should be established at the average top of the zeolitized layer for the area in question. For the primary area this depth is 170 m based on the current Los Alamos National Laboratory Site Scale Geologic Model. The average depth of the zeolite layer beneath areas other than the primary area might be different. As additional information on zeolite compositions and locations becomes available, these criteria should be reviewed.

Maximum Allowable Thermal Loading. The geochemical thermal criteria of a not-to-exceed temperature limit of 90°C at the top of the zeolite layer will limit the thermal loading which can be accommodated in a given area. For the Primary Area which has an average depth of the top of the zeolite layer of 170 m beneath the repository horizon the thermal predictions indicate that the thermal load should not be more than about 22.2 kgU/m² (90 MTU/acre). For other reasons a decision could be made to exceed this thermal loading but some of the upper layer of zeolites may possibly undergo transition to analcime which does not have appreciable ability to sorb radionuclides. Only a portion of the zeolites, however, would undergo this transition. For example, if a decision is made to load the Primary Area at 24.7 kgU/m² (100 MTU/acre) then approximately 25 m of the upper layer of zeolites over approximately 75 percent of the repository area would be affected. Very preliminary calculations indicate that the possible loss of this 25 m could result in approximately a 100,000 year decrease in travel time through the CHn layer (zeroth order predictions indicate about 800,000 year travel time for Neptunium through 180 m thickness of zeolite bearing rock). Depending on the standard ultimately promulgated this may not be a critical issue but more information on zeolite concentrations, thicknesses, and a better understanding of the kinetics of zeolite alteration are needed to make such a decision. It should be noted that this current study only establishes limits on a thermal loading which should not be exceeded based on current criteria and knowledge and does not validate a particular thermal load as licensable. It should not constrain the current advanced conceptual design thermal load of 20.5 kgU/m² (83 MTU/acre).

Emplacement Drift Wall Criteria. Concerns about thermomechanical stresses in the host rock were recognized early in the program and a not-to-exceed thermal goal of 200°C was placed on rock

one meter from a borehole. This goal was subsequently expanded to limit the wall temperature for a horizontal emplacement drift. In this study, the thermomechanical impacts of exceeding this limit were analyzed. The results found that there is the potential for compressive failures at temperatures above 200°C, although it is currently anticipated that the rock mass behaves elastically even above 200°C. The interaction of the host rock and potential tunnel supports, such as steel sets or concrete, is important to consider. Calculations that included tunnel supports found potential problems, such as over-stress conditions at elevated temperatures. However, tunnel supports in the present Advanced Conceptual Design environment should perform adequately. While the use of jointed steel sets or thicker concrete liners would possibly mitigate failure, these are as yet untested. Additionally, the latest laboratory measurements of underground TSw2 samples found that significant increases in the thermal expansion coefficient occurred at temperatures above 200°C. These increases in the expansion coefficient were found to produce overstress conditions in the rock and tunnel supports. Thus, this study found no reason to change this limit and recommends that it be established as a criterion for design. The study also found that the stress calculations are sensitive to the choice of the coefficient of thermal expansion, Young's Modulus, and the Poisson Ratio, and thus it is recommended that once thermal tests are run these issues be readdressed prior to License Application. The study recommends retaining the not-to-exceed temperature criterion of 200°C on the emplacement drift wall.

Cladding Thermal Criteria. The *Site Characterization Plan* (DOE 1988) recommended a thermal goal of 350°C on the zircaloy cladding to preserve the cladding as an available barrier to radionuclide release. A probabilistic cladding degradation model was developed and total system performance calculations were conducted to examine the performance value of the potential cladding barrier. The calculations showed that the cladding barrier resulted in approximately two orders of magnitude reduction in total peak release rate to the accessible environment at 10,000 years and almost two orders of magnitude reduction at 1,000,000 years. The study also determined that cladding degradation was sensitive to temperature. When the fraction of rods whose temperature exceeded 350°C increased from 10 percent to 30 percent by increasing the initial center rod temperature by 50°C, the fraction of unzipped (grossly ruptured) clads increased by a factor of 8 (e.g., 0.5 vs 3.9 percent in unzipped clad fraction). This resulted in, approximately, an order of magnitude increase at 10,000 years and almost an order of magnitude increase at 1,000,000 years in the total peak release rate at the accessible environment. Thus, this study recommends that the requirement for a 350°C criterion on cladding be retained.

Credit for cladding performance, with sufficient level of confidence for License Application, would require that additional cladding processes not considered, such as stress corrosion cracking; long term corrosion radiolysis-induced acidic conditions; hydride reorientation; and degradation under static loads be evaluated. It is recommended that available cladding information be researched and a plan be developed to obtain licensing credit for cladding performance. At a minimum, cladding should be considered as an additional barrier in our compliance strategy to help qualitatively substantiate reasonable assurance of performance (10 CFR 60.10, *Purpose and Nature of Findings*).

Edge Loading. The edge of the potential repository will cool and rewet substantially faster than the center of the repository. Whether total system performance would be degraded as a result of this cooling was examined. The evaluations showed that some earlier, very low-level releases would occur as a result of edge cooling. However, the releases to the accessible environment were not

substantially changed at 10,000 or 1,000,000 years over the case with no edge cooling. Additionally, evaluations of the conditions that would be produced if the thermal load were increased in the edges to reduce cooling, found that the 200°C thermal criterion would be exceeded. Based on these results, the study recommends that no increased edge loading be considered.

Waste Stream Variability. Variability in waste package heat outputs of less than 1 kW to over 18 kW was found to exist for the incoming waste stream. Evaluations showed that this variability could cause as much as 50 to 100°C drift wall temperature differences within a distance of 10 to 20 meters (no ventilation, enclosed drifts). These large temperature differences result in thermomechanical problems (over-stress conditions) since the 200°C drift wall thermal criterion is exceeded in some areas (see discussion on emplacement drift wall). In addition, there are potential postclosure implications in that the evaluations indicate moisture is moved from the hotter to the cooler packages. The study recommends that the temperature variability in the potential repository be reduced to reduce these effects. Several thermal management methods were examined to evaluate methods to achieve a reduction in heat variability.

Varying the spacing of the waste packages provided some minor smoothing of the thermal profiles. However, the calculations indicated that close-spaced line loading (one-meter or less) would result in thermal criteria (drift wall and cladding) being violated for thermal loads of 20.5 kgU/m² (83 MTU/acre) and possibly even lower. Additionally, the logistics of ensuring an appropriate mix of waste packages did not appear to be supportable by the current waste stream. Thus, it is recommended that for Viability Assessment, the Advanced Conceptual Design spacing be maintained.

Ventilation of the emplacement drifts was examined and found to provide significant smoothing of the temperature distributions. Even low-flow natural ventilation of no more than between 0.1 and 1.0 m³/s was found to provide a significant amount of smoothing. The cost impacts of low-flow ventilation would be none to minimal. However, such a solution may have operational impacts which should be considered. Higher ventilation flows should not be considered since the cost impacts are large and the risks associated with the increased number of inlet shafts needed for higher ventilation may be significant.

Configuration of heat outputs of waste packages through selection of packages and/or assemblies, and through aging, was found to have the largest effect on reducing temperature variations. Selection of canisters to achieve some target heat output can reduce one-standard deviation of package heat output of PWR fuel from about 3 to 4 kW to about 1 kW or less. This solution involves establishing some lag storage, but the costs associated are estimated to be about \$45M (about 0.4 percent of Mined Geologic Disposal System costs).

The study determined that the temperature variations along the emplacement drift that result from the currently planned emplacement waste stream are too large and can give rise to thermomechanical over-stress conditions and conditions where moisture is moved from hotter to cooler packages. The study found that the most reduction in heat variations could be obtained with either ventilation (a flow of 1 m³/s or less is suggested) or through package selection/aging. A requirement for limiting the heat variations during emplacement needs to be established.

Alternative Thermal Loadings. Analyses with as yet unverified models have indicated that the design focused thermal loading of 20.5 kgU/m² (83 MTU/acre) may meet requirements, at least for 10,000 years. Because of the lack of verification, there has been no confirmation that a high thermal loading may not negatively impact natural barriers or that coupled processes on a mountain scale can be understood in the time frame of the tests. Thermal tests are underway to provide information to help verify the analytic models. Additionally, the repository performance objectives and design criteria may be revised as a result of the current Environmental Protection Agency deliberations on Yucca Mountain standards. Thus, alternatives need to be considered to mitigate the risk that the thermal tests could discover some undesirable effects or other performance objectives could be imposed.

The study evaluated alternate thermal loadings and recommends that, as a minimum, an additional thermal loading of 8.9 kgU/m² (36 MTU/acre) be considered. The evaluations found that additional area (at least up to a total of 12.2 km² (3015 acres)) may exist by using expansion area to the north of the primary area and other optional expansion areas. This total potential area could provide for emplacing 70,000 MTU at a loading of as low as 5.7 kgU/m² (23 MTU/acre). The cost of characterizing and emplacing all of this additional area, should it be necessary, was found to be no more than a 2.5 percent increase in Mined Geologic Disposal System costs. If it is determined that other waste package designs and/or materials may be needed at alternating loadings, the costs would need to be reevaluated.

The study recommends that this alternative thermal loading be pursued at a relatively low level of effort until sufficient results from thermal testing are available to predict with confidence that the tentatively chosen high thermal loading will support the repository in meeting its performance objectives. These results are expected to be available by the end of 1999. The scope of the effort to maintain the alternative thermal loading can be limited to a low level of design work, an additional performance assessment case, and development of a plan for characterizing additional area, if required. Further, it is recommended that the adequacy of performance at 8.9 kgU/m² should be assessed. These minimal costs are believed to be supportable and prudent to prepare for the contingency that the relatively high thermal loading case might be determined to be unacceptable. Management may choose to continue to pursue the alternative thermal loading design even further into the future, balancing the additional cost of maintaining the option and the (hopefully) increasing confidence in the adequacy of high thermal loading against the significant delays should low thermal loading later be found necessary.

A firm decision on thermal loading should be made as soon as practical after sufficient thermal testing results are available, as it would take time to characterize additional potential emplacement areas and to revise the licensing basis to be presented to the U.S. Nuclear Regulatory Commission in the License Application if the alternative thermal loading must be used. Also, it is very desirable, from a licensing standpoint, to have thermal loading issues resolved prior to License Application submittal to minimize the likelihood of a licensing issue emerging on this subject.

If the alternative (lower) thermal loading is found to be needed at a time too close to planned License Application submittal to characterize additional area without delaying License Application, the Program may choose to submit the License Application at the lower thermal loading and somewhat reduced capacity using the previously characterized area. The additional area needed to emplace

70,000 metric tonnes uranium at the lower thermal loading could then be characterized at a later date, to be followed by an amendment to the License Application.

Summary. This study recommends thermal requirements for the repository design. A conservative approach, emphasizing the defense in-depth concept, was used in developing the recommendations. The study also provided rationale to limit the thermal loading in the primary area to no more than 22.2 kgU/m² (90 MTU/acre). Once thermal test measurements are available, some of these issues will need to be reevaluated for License Application.

The study recommends that the following requirements be established, retained, and/or changed:

Delete the requirement [CDA EBD RD 3.7.G.3] to limit the TSw3 (basal vitrophyre) maximum temperature to less than 115°C.

Delete the requirement [CDA DCSS 025] to limit the CHn maximum temperature to less than 115°C.

Establish a not-to-exceed temperature of 90°C for the zeolitized tuff in the Calico Hills unit. This temperature limit is to be established at the average depth of the top of the zeolitized tuff beneath a given potential emplacement area (e.g., this temperature limit would be at a depth of 170 m beneath the upper block of the Primary Area). The average depth of the top of the zeolitized layer for other potential areas remains to be established. (TBV)

Retain the not-to-exceed emplacement drift wall temperature of 200°C. (TBV)

Retain the not-to-exceed cladding temperature of 350°C. (TBV)

CONTENTS

Page

1.	INTRODUCTION	1-1
1.1	STUDY OBJECTIVE	1-1
1.2	SCOPE	1-1
1.3	BACKGROUND	1-2
1.4	REPORT ORGANIZATION	1-4
2.	REQUIREMENTS AND STANDARDS	2-1
2.1	QUALITY ASSURANCE	2-1
2.2	DESIGN REQUIREMENTS	2-4
2.3	INPUTS AND ASSUMPTIONS	2-8
3.	SELECTED THERMAL GOALS REEVALUATION	3-1
3.1	INTRODUCTION	3-1
3.2	EVALUATION OF THE THERMOCHEMICAL GOAL	3-1
3.2.1	Geochemical Background	3-2
3.2.2	Development of Geochemical Inputs	3-4
3.2.3	Thermohydrologic Calculations	3-5
3.2.4	Overview of Natural Analog Studies Pertinent to Clinoptilolite Stability	3-12
3.2.5	Identification of a Layer for Establishing a Performance Criteria	3-19
3.2.6	Summary	3-22
3.3	NEAR-FIELD THERMOMECHANICAL PERFORMANCE	3-23
3.3.1	Evaluations of Mechanical Effects Resulting from Heating and Thermal Gradients	3-24
3.3.2	Thermomechanical Evaluations of Tunnel Support and Emplacement Drift Stability	3-30
3.3.3	Summary	3-45
3.4	CLADDING PERFORMANCE CONTRIBUTION TO WASTE CONTAINMENT	3-47
3.4.1	Cladding Degradation Models	3-48
3.4.2	WP Degradation	3-50
3.4.3	Probabilistic Cladding Failure Calculation	3-58
3.4.4	RIP Simulation	3-73
3.4.5	Summary	3-90
4.	EDGE LOADING EVALUATIONS	4-1
4.1	THERMOHYDROLOGIC CALCULATIONS OF NON-UNIFORM AMLs	4-1
4.2	THERMOMECHANICAL EVALUATIONS	4-2
4.3	TOTAL SYSTEM PERFORMANCE ASSESSMENTS	4-2
4.4	SUMMARY	4-5

CONTENTS (Continued)

	Page
5. WASTE STREAM VARIABILITY	5-1
5.1 INTRODUCTION	5-1
5.2 THERMAL MANAGEMENT WITH WP SPACING	5-5
5.3 THERMAL MANAGEMENT WITH VENTILATION	5-13
5.4 THERMAL MANAGEMENT THROUGH SURFACE ACTIVITIES	5-31
5.5 SUMMARY	5-43
6. ALTERNATE THERMAL LOADS	6-1
6.1 ALTERNATE THERMAL LOADS FOR INVESTIGATION	6-1
6.2 ESTIMATES OF USABLE EMPLACEMENT AREA	6-2
6.3 COST ANALYSIS	6-7
6.4 WASTE PACKAGES	6-10
6.5 DECISIONS POINTS	6-14
6.6 SUMMARY	6-16
7. CONCLUSIONS	7-1
8. REFERENCES	8-1
9. ACRONYMS	9-1

APPENDIXES

APPENDIX A	TECHNICAL BASIS FOR EVALUATION OF THERMAL GOALS BELOW THE POTENTIAL NUCLEAR WASTE REPOSITORY AT YUCCA MOUNTAIN	A-1
APPENDIX B	THERMAL-MECHANICAL EVALUATION OF THE 200°C DRIFT WALL TEMPERATURE GOAL	B-1
APPENDIX C	EVALUATION OF GROUND STABILITY AND SUPPORT	C-1
APPENDIX D	COUPLED VENTILATION AND HYDROTHERMAL EVALUATIONS	D-1
APPENDIX E	HEAT FLOW AND TEMPERATURE CALCULATIONS FOR CONTINUOUSLY VENTILATED EMPLACEMENT DRIFTS	E-1
APPENDIX F	THERMAL MANAGEMENT USING AGING AND BLENDING	F-1
APPENDIX G	WASTE STREAM EVALUATIONS	G-1

FIGURES

Page

3.2-1	Isobars Depicting the Estimated Depth of the Zeolitized Layer Below the Potential Repository in Meters	3-6
3.2-2	Effect of Clinoptilolite (Cpt) on Drift-Centerline Temperatures at Specified Times	3-10
3.2-3	Effect of Clinoptilolite (Cpt) on Drift-Centerline Temperatures at Specified Times	3-11
3.2-4	Effects of Clinoptilolite (Cpt) at 100 m Below Repository	3-13
3.2-5	Effects of Clinoptilolite (Cpt) at 186.3 m Below Repository	3-14
3.2-6	Effects of Clinoptilolite (Cpt) on the Top of the Clinoptilolite Layer	3-15
3.2-7	Effects of Clinoptilolite (Cpt) at 186.3 m Below Repository	3-16
3.3-1	(a) Instantaneous Coefficient of Thermal Expansion Data from NRG 5 and NRG 6, (b) Nominal and Bounding Thermal Expansion Data	3-26
3.3-2	Example of Gradients Examined in Study	3-27
3.3-3	Maximum Principal Stresses for a Drift Temperature of 200°C and a μ of 1.0	3-29
3.3-4	Maximum Principal Stresses for a Drift Temperature of 225°C and a μ of 1.0	3-29
3.3-5	Geometry and Boundary Conditions for Thermomechanical Modeling Using FLAC	3-35
3.3-6	Temperatures Histories of Drift Wall for 83, 100 and 115 MTU/acre: (a) 9.21 kW/package; (b) 14.2 kW/package	3-37
3.3-7	Factors of Safety Contours and Plasticity Indicators around Opening with Steel Sets Ground Support for RMQ=3, 83 MTU/acre and 9.21 kW/package: (a) 10 Years after Emplacement; (b) 50 Years after Emplacement; (c) 100 Years after Emplacement	3-39
3.3-8	Factors of Safety Contours and Plasticity Indicators around Opening with Steel Sets Ground Support for RMQ=3, 100 MTU/acre and 14.2 kW/package: (a) 10 Years after Emplacement; (b) 50 Years after Emplacement; (c) 100 Years after Emplacement	3-40
3.3-9	Axial Forces in Concrete Liner Ground Support for RMQ=3, 83 MTU/acre and 9.21 kW/package: (a) 10 Years after Emplacement; (b) 50 Years after Emplacement; (c) 100 Years after Emplacement	3-41
3.3-10	Axial Forces in Concrete Liner Ground Support for RMQ=3, 100 MTU/acre and 14.2 kW/package: (a) 10 Years after Emplacement; (b) 50 Years after Emplacement; (c) 100 Years after Emplacement	3-42
3.4-1a	10,000-year temperature history of the WP surface for the case of 20.5 kg U/m ² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)	3-53
3.4-1b	100,000-year temperature history of the WP surface for the case of 20.5 kg U/m ² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)	3-53
3.4-1c	10,000-year relative humidity history of the WP surface for the case of 20.5 kg U/m ² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)	3-54

FIGURES (Continued)

		Page
3.4-2	Cumulative fraction of WPs that failed for the case of 20.5 kg U/m ² (83 MTU/acre) thermal loading, no backfill, and high infiltration rate (0.3 mm/yr)	3-55
3.4-3	Representative pitting histories for 25 WPs for the case of 20.5 kg U/m ² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)	3-55
3.4-4	Abstractions for the RIP implementation for the case of 20.5 kg U/m ² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)	3-56
3.4-5	Approximation of the WP surface temperature in the repository edge for the case of 20.5 kg U/m ² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)	3-57
3.4-6	Approximation of the WP surface relative humidity in the repository edge for the case of 20.5 kg U/m ² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)	3-57
3.4-7	Comparison of cumulative fraction of WPs that failed in the repository edge with the fraction in the repository interior for the case of 20.5 kg U/m ² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)	3-59
3.4-8	Representative pitting histories for 25 WPs in the repository edge for the case of 20.5 kg U/m ² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)	3-59
3.4-9	Abstractions for the RIP implementation for the WPs in the repository edge for the case of 20.5 kg U/m ² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)	3-60
3.4-10	The temperature history of the center pin in a WP for the base case of 20.5 kg U/m ² thermal loading, no backfill and high infiltration rate (0.3 mm/yr)	3-61
3.4-11	Radial distribution of pin temperature across WP at 0.8 years. Radial Index 1 is the center and 13 is the outer-most edge of the WP	3-62
3.4-12	Distribution of peak cladding temperatures with the initial center pin temperature of 276 or 325°C	3-62
3.4-13	Estimated pin failures at different initial center pin temperatures using the Peehs model	3-64
3.4-14	The effect of reduced EFs on the pin failure estimation using the Peehs model ...	3-64
3.4-15	Comparison of the cladding failure estimations at different initial center cladding temperatures using the Peehs model and Chin model	3-65
3.4-16	Fraction of unzipped cladding as a function of WP failure times at two initial center pin temperatures	3-66
3.4-17a	10,000-year total release rate history at the accessible environment using expected values	3-75
3.4-17b	10,000-year ⁹⁹ Tc release rate history at the accessible environment using expected values	3-76

FIGURES (Continued)

Page

3.4-17c	10,000-year ^{237}Np release rate history at the accessible environment using expected values	3-76
3.4-18a	1,000,000-year total release rate history at the accessible environment using expected values for the stochastic simulation parameters	3-77
3.4-18b	1,000,000-year ^{99}Tc release rate history at the accessible environment using expected values for the stochastic simulation parameters	3-78
3.4-18c	1,000,000-year ^{237}Np release rate history at the accessible environment using expected values for the stochastic simulation parameters	3-78
3.4-19	CCDF of the 10,000-year total normalized cumulative release to the accessible environment	3-79
3.4-20	CCDF of the 1,000,000-year total normalized cumulative release to the accessible environment	3-80
3.4-21	10,000-year total dose history at the accessible environment using expected values of the stochastic simulation parameters	3-81
3.4-22	1,000,000-year total dose history at the accessible environment using expected values of the stochastic simulation parameters	3-81
3.4-23	CCDF of the 10,000-year total peak dose at the accessible environment	3-82
3.4-24	CCDF of the 1,000,000-year total peak dose at the accessible environment	3-83
3.4-25	10,000-year total release rate histories at the accessible environment using expected values for stochastic simulation parameters to compare the effects of 50°C higher initial cladding temperature	3-84
3.4-26	1,000,000-year total release rate histories at the accessible environment using expected values for stochastic simulation parameters to compare the effects of 50°C higher initial cladding temperature	3-85
3.4-27	10,000-year total dose histories at the accessible environment using expected values for stochastic simulation parameters to compare the effects of 50°C higher initial cladding temperature	3-85
3.4-28	1,000,000-year total dose histories at the accessible environment using expected values for stochastic simulation parameters to compare the effects of 50°C higher initial cladding temperature	3-86
3.4-29	CCDFs of the 10,000-year total peak doses at the accessible environment to compare the effects of 50°C higher initial cladding temperature	3-87
3.4-30	CCDFs of the 1,000,000-year total peak doses at the accessible environment to compare the effects of 50°C higher initial cladding temperature	3-87
3.4-31	CCDFs of the 10,000-year total peak dose comparing the cases for a standard at 30 km	3-88
3.4-32	CCDFs of the 1,000,000-year total peak dose comparing the cases for a standard at 30 km	3-89
4-1	CCDF of the 10,000-year Total Peak Dose at the Accessible Environment	4-4
4-2	CCDF of the 1,000,000-year Total Peak Dose at the Accessible Environment	4-4
5.1-1	Relative Humidity Calculations for Several Different WPs for the ACD Design ...	5-2
5.1-2	Predictions of Functions of Failed Packages for Several Different WPs for the ACD Design	5-3

FIGURES (Continued)

	Page
5.1-3 Moisture Flux on the Drift Wall at the DHLW Locations for the ACD Design for a) 400 Years and b) 100,000 Years	5-4
5.2-1 WP Types and Spacings for the Cases Considered	5-9
5.2-2(a) Multiple WP Peak Temperatures for the ACD Spacing Case	5-10
5.2-2(b) Multiple WP Surface Temperatures for the ACD Spacing Case	5-10
5.2-3 Multiple Drift Wall Temperatures for ACD Spacing Case	5-11
5.2-4 Multiple WP Peak Temperatures for the 1-meter Spacing Case	5-11
5.2-5 Multiple Drift Wall Temperatures for the 1-meter Spacing Case	5-12
5.3-1 Drift Wall Temperatures for the High Flow (10m ³ /s) Ventilation Case	5-15
5.3-2 Drift Wall Temperatures Using a Conduction Only Module for a High Flow (10m ³ /s) Ventilation Case	5-17
5.3-3 Drift Wall Temperatures for the Moderate Flow (1m ³ /s) Ventilation Case	5-18
5.3-4 Drift Wall Temperatures for the Low Flow (0.1m ³ /s) Ventilation Case	5-19
5.3-5 Integrated Moisture Flux for the High Flow (10m ³ /s) Ventilation Case	5-20
5.3-6 Integrated Moisture Flux for the Moderate Flow (1m ³ /s) Ventilation Case	5-21
5.3-7 Integrated Moisture Flux for the Low Flow (0.1m ³ /s) Ventilation Case	5-22
5.3-8 Drift Wall Temperatures for Multiple Heat Packages with No Ventilation	5-23
5.3-9 Drift Wall Temperatures for Multiple Heat Packages with Low Flow (0.1m ³ /s) Ventilation	5-25
5.3-10 Drift Wall Temperatures for Multiple Heat Packages with High Flow (10m ³ /s) Ventilation	5-26
5.3-11 Drift Wall Temperatures for Multiple Heat Packages for Looped Ventilation of 10m ³ /s for 30 Years and 0.1m ³ /s Thereafter	5-28
5.3-12 Drift Wall Temperatures for Multiple Heat Packages for Axial Heat Pipes on the WPs	5-29
5.3-13 Drift Wall Temperatures for Multiple Heat Packages for Thermal Rock Bolts	5-30
5.4-1 Average and one-Standard Deviation WP Heat Outputs for Case 1 OFF; PWR Fuel	5-35
5.4-2 Average and one-Standard Deviation WP Heat Outputs for Case 1 OFF; BWR Fuel	5-36
5.4-3 Average and one-Standard Deviation WP Heat Outputs for Case 1 YFF; PWR Fuel	5-37
5.4-4 Fine Blending of WP Heats for Case 6 OFF; PWR Fuel	5-38
5.4-5 Fine Blending of WP Heats for Case 6 OFF; BWR Fuel	5-39
5.4-6 Pictorial Concept of Surface-Storage Interactions for the Various Study Cases ...	5-41
5.4-7 Surface Repository Cost Variations from the Base Case	5-43
6.2-1 Estimate of Maximum Available Emplacement Area	6-4

TABLES

	Page
3.2-1 Hydration Parameters for Na-Cpt	3-7
3.2-2 Energy Parameters for Na-Cpt	3-8
3.2-3 Rock Peak Temperatures at Different Locations	3-22
3.3-1 Drift and WP Spacings Used in Analysis	3-31
3.3-2 Results from ANSYS Models for Different Thermal Loads and Package Heat	3-38
3.3-3 Results from FLAC Models for Concrete Liner Ground Support	3-43
3.3-4 Results from FLAC Models for Steel Sets Ground Support	3-44
3.4-1 Clad Unzipping Times for Various Temperatures	3-66
3.4-2 Effect of WP Failure Distribution on Clad Unzipping	3-68
3.4-3 Cladding Degradation Model Results for RIP Implementation for WP Groups in the Repository Interior for the Case of 83 MTU/acre, No Backfill, and High Infiltration	3-68
3.4-4 Cladding Degradation Model Results for RIP Implementation for WP Groups in the Repository Edge for the Case of 83 MTU/acre, No Backfill, and High Infiltration	3-69
3.4-5 Cladding Degradation Model Results for RIP Implementation for WP Groups in the Repository Interior with Higher Initial Center Cladding Temperature (325°C) for the Case of 83 MTU/acre, No Backfill, and High Infiltration	3-70
3.4-6 Input Summary for Clad Degradation Analysis	3-71
3.4-7 Summary of Cladding Degradation Analysis Results	3-72
5.3-1 Differential numbers of shafts and costs of ventilation between various cases and the base case with no ventilation	5-31
5.4-1 Cost Differences for Surface Thermal Management Options	5-40
6.2-1 Maximum Emplacement Area Available	6-5
6.2-2 Usable Area Needed For Emplacement	6-5
6.2-3 Total Area Needed	6-6
6.2-4 Required Length of Drifting ACD WP Spacing	6-7
6.2-5 Required Length of Drifting Line-Load WP Spacing	6-7
6.3-1 Historical Costs Allocation Table	6-8
6.3-2 Historical D&E Costs Attributed to Site Suitability Determination	6-9
6.3-3 Development and Evaluation Costs Attributed to Site Suitability Determination ...	6-9
6.3-4 Development and Evaluation Costs Attributed to Site Suitability Determination ...	6-9
6.3-5 Development & Evaluation Summary	6-10
6.3-6 Primary Area ACD Land Usage	6-10
6.4-1 ACD 1996 - Design Base Summary	6-11
6.4-2 Area Characterization Cost Factors	6-13
6.4-3 Advanced Conceptual Design Cost Summary (Million FY 1995 Dollars)	6-13
6.4-4 Cost Delta from ACD - Summary	6-14

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1. INTRODUCTION

1.1 STUDY OBJECTIVE

This document reports the work conducted in a Thermal Loading Study over the period from October 1, 1995 through August 30, 1996 and meets deliverable number TR150120. The study is a continuation of the FY 1993 and FY 1994/FY 1995 Thermal Loading System Studies and is built on the framework of those efforts. The study continues the system study role taken in the 1993 effort to provide a structured, detailed analyses that will form the technical basis for ultimately making a decision as to what thermal loading should be established in the potential repository. This effort concentrated primarily on developing recommendations for design requirements related to thermal goals and thermal management techniques for emplacing and, if necessary, aging spent nuclear fuel (SNF).

The thermal loading in the proposed repository can impact the system in a number of areas (e.g., receipt of waste, repository size and design, engineered barrier design and performance [including waste package (WP) size], and natural barrier performance). The ultimate objective of the thermal loading system study will be to develop the technical basis for making a thermal loading decision to support License Application and design. The primary objective of the FY 1996 study is to provide recommendations for requirements that will provide sufficient definition to facilitate development of design concepts and support life cycle cost determinations. The study will reevaluate and/or redefine select thermal goals that are currently being used by design as required based on technical analysis and/or measured data. The study will provide a recommendation as to what actions, if any (such as edge loading), are needed and must be accommodated in the design. Recommendations will be developed to establish requirements on emplacement, which will minimize any potential performance impacts resulting from fuel or WP variability of heat output. Additionally, the study will provide recommendations as to what alternative thermal loads should be maintained to minimize Program risk, what is needed to ensure these alternative thermal loads are viable, and what constraints (schedule and cost) could be incurred on the system if a thermal loading decision is not made by various dates.

1.2 SCOPE

Study activities for this effort were primarily related to the Mined Geologic Disposal System (MGDS) Thermal Loading Study for the proposed repository at Yucca Mountain, Nevada. Activities that impact functions external to the "Dispose of Waste" function were coordinated with the Office of Civilian Radioactive Waste Management through the Management and Operating Contractor (M&O) Vienna Systems Analysis group.

The scope of this effort encompassed a wide range of activities and involved a number of different organizations within the Office of Civilian Radioactive Waste Management. It involved analytic calculations of thermohydrologic, thermomechanical, and thermochemical performance of the natural and engineered barriers at the proposed repository at Yucca Mountain. The basis for the calculations was the latest available data and the source of the data and the assumptions used will be clearly defined. Based on these analyses and associated trade studies performed, the effort developed recommendations for requirements.

The study was managed by the Systems Analysis and Modeling Department with key technical support provided by the following organizations:

- Subsurface Design
- Surface Design
- WP Design
- Performance Assessment
- Scientific Programs
- Regulatory and Licensing
- University of Nevada Reno
- National laboratories to include:
 - Lawrence Livermore National Laboratory
 - Los Alamos National Laboratory
 - Sandia National Laboratories (SNL).

1.3 BACKGROUND

The ability to meet the overall performance requirements for the proposed MGDS at Yucca Mountain, Nevada requires the two major subsystems (natural barriers and engineered barriers) to positively contribute to containment and radionuclide migration retardation. In addition to the postclosure performance, the proposed repository must meet certain preclosure requirements of safety, retrievability, operability, and also must take into consideration cost and schedule. The thermal loading strategy chosen for such a repository may significantly affect both the postclosure and preclosure performance of the proposed repository. Additionally, NUREG 1466 specifies that demonstrating that the system performance of the proposed repository complies with the regulations in 10 CFR 60.133, will require that the coupled thermal, mechanical, hydrological, and chemical (T-M-H-C) aspects of the repository performance be considered. To address the thermal loading issues of the repository, an initial systems study was conducted in FY 1993. One result of this study, among others, was to provide recommendations to narrow the range of thermal loading to less than or equal to 24.7 kgU/m² (100 metric tonnes uranium (MTU)/per acre).

In the absence of a promulgated standard, and due to the current dearth of data that limits our ability to make confident performance predictions, it was necessary to establish goals for the system early in the program. It was believed that meeting those criteria/goals should result in adequate (i.e., has the ability to meet the standards that will ultimately be required) performance of the repository and the natural and engineered barrier systems, and that the criteria could be used to evaluate and rank thermal loading options. The *Site Characterization Plan* (SCP, DOE 1988) established a set of necessary criteria by developing thermal goals. In 1993 the DOE commissioned an effort to reevaluate these thermal goals and the results were reported in the *Site Characterization Plan Thermal Goals Reevaluation Report* (CRWMS M&O 1993). These reevaluated thermal goals were used in the previous thermal loading study. Currently, a number of the thermal goals have been included in the requirements documents. Three of these goals, the 350°C cladding temperature, the 200°C emplacement wall temperature, and the 115°C TSw2/3 interface temperature appear to be providing some design constraints.

As our understanding of the processes occurring in the mountain improve we began to have the capability of making total system performance assessments. This allows us to move away from reliance on thermal goals. Since there will be some unknowns in the processes that can occur, it is likely that we can never move completely away from all thermal goals which would become thermal criteria.

Developing verified/validated analytic models to assist in developing an understanding of the performance of the engineered and natural barriers out to long times with reasonable assurance requires thermal testing data. Measurements will be needed at various scales to understand both near-field and mountain scale processes. Laboratory data, in situ thermal test data (short term and long term), and natural analog studies are needed to obtain the necessary measurements. Some laboratory and natural analog studies are currently underway. Test planning is being done to establish the most robust in situ testing which will meet the Program Objectives. To help focus the test planning, the FY 1994/FY 1995 Thermal Loading Study conducted a number of sensitivity studies. Based on those studies, recommendations for testing and/or specific measurements to be taken were developed to aid the test planning.

During the period of this study, the Experimental Studies Facility Thermal Test construction began which included a single heater test that is scheduled to start in September 1996. A drift scale test which focuses on coupled processes is scheduled to start in late 1997.

Some thermal management will be needed in the proposed repository to meet requirements. The FY 1994/FY 1995 Thermal Loading Study performed a preliminary examination of some of these thermal management issues. For example, a coupled thermohydrologic and ventilation model was developed to predict the amount of heat (sensible and latent heat of vaporization) and moisture that can be removed by ventilation. Fuel variability could result in developing 'hot' and 'cold' (cooler) spots in the repository. The impacts of this fuel variability were examined and found to be significant. Additionally, the study found that cooling at the repository edges could significantly degrade the performance of the WPs in the outer edges of the repository over the performance anticipated in the center of a high thermal loaded repository. Increasing the density of WPs at the edges may mitigate this effect but the increased density will exceed thermal goals. Additional edges may ultimately occur in the design if there are regions in the potential repository where decisions are made not to emplace waste due to a determination that there is rock that does not meet the requirements for emplacement and/or areas that may contain possible fast flow paths.

A selection of the thermal loading for licensing has not been made by the Project. However, recently a near term thermal strategy decision was established in an effort to focus design activities. That strategy is to focus current design activities on a reference design thermal load that will permit emplacement of at least the statutory maximum (70,000 MTU) within the primary repository area. Based on that, the Program is considering designs for a thermal loading of 19.8 to 24.7 kgU/m² (80 to 100 MTU/acre). In addition, as a working hypothesis, the strategy will maintain prudent levels of flexibility (contingencies) by including alternative areal mass loadings (AMLs).

Implementation guidance in the form of requirements to be able to adequately complete Viability Assessment designs is needed. For example, guidance is needed on how to handle emplacement of WPs that can have significantly different power outputs. Projected power outputs can vary from as

little as less than 1 kW for the cooler boiling water reactor (BWR) packages to as high as the design basis waste package heat output of almost 18 kW (CRWMS M&O 1996a). Some of the defense high-level wastes (DHLW) might have even lower power output. An evaluation is needed as to how performance might be impacted by having cooler WPs or groups of cooler WPs in a repository that is trying to use heat to mobilize water and dry out the repository horizon. This FY 1996 Thermal Study examined this question and provides recommendations for requirements that can be established as to what power variations should be allowed in a given area of the repository and when (in time) variations that exceed those levels become important. Additionally, the study will provide recommendations as to what techniques might be used to mitigate fuel variability and how cost effective those techniques may be.

The study examined whether edge cooling could impact performance. Based on performance, operability, retrieval, and other issues, the study established recommendations for requirements as to how edge loading might be implemented in such a way that long term performance could be improved without degrading preclosure performance to a significant degree. The study concentrated on examining the outer edges although there will be numerous internal edges that may need to be considered to some extent.

As indicated above, certain thermal goals that have been established as design requirements appear to be having some impact on the ability of the design to meet these goals. These goals are the 350°C cladding temperature, the 200°C emplacement wall temperature, and the 115°C TSw2/3 interface temperature. The study evaluated these goals and provides recommendations as to whether or not a particular goal should be deleted, kept as is, or changed based on current technical reasons.

The study also identified, based on analysis, which alternate thermal loads should be kept under consideration by the Program. In particular, the study examined what is needed to make these alternate thermal loads viable and the costs associated with establishing the viability. As a part of this effort the study identified when decisions are needed to narrow the range of thermal loads to avoid constraining the Program schedule and/or increasing the costs significantly.

The affected organizations that would benefit from the results of this study are the design organizations (subsurface, surface, waste package materials, and WP design). Also affected are the Systems Engineering Requirements group, Performance Assessment, Scientific Programs Organization and Regulatory and Licensing. Coordination, support, and integration of activities, as needed, were done throughout the study with the design organizations, Performance Assessment, and the national laboratories.

1.4 REPORT ORGANIZATION

The report organization follows the outline in the Technical Document Preparation Plan as follows:

- The Executive Summary provides a top-level description of the study and the results
- Section 1 provides the study objective, background, scope, and organization of the report

- Section 2 documents the requirements and standards to include quality assurance (QA) requirements, any requirements used or evaluated, and the inputs and assumptions considered
- Section 3 provides the analysis and recommendations for the thermal goals reevaluation
- Section 4 discusses the evaluation of edge loading and provides conclusions
- Section 5 provides the analyses done to establish recommendations as to what requirements need to be implemented to either limit or manage the amount of heat output variability that may occur
- Section 6 discusses alternate thermal loadings
- Section 7 provides the study conclusions and recommendations
- Section 8 provides the references, standards, and regulations
- Section 9 contains the acronym list.

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2. REQUIREMENTS AND STANDARDS

2.1 QUALITY ASSURANCE

The QA program applies to the development of this technical document. *QAP-2-0, Control of Activities, Activity Evaluation, Perform System Studies*, B00000000-01717-2200-00086 REV 02, dated 12/11/95, was completed (CRWMS M&O 1995d). Although a *QAP-2-3, Classification of Permanent Items*, classification analysis has not yet been performed, the *QAP-2-0* activity evaluation determined that the work performed to develop a system study report is quality affecting because it impacts items that are on the *Q-List* (DOE 1994a) by direct inclusion. This study report, as appropriate, provided recommendations for requirements to be included in the *Repository Design Requirements Document* (RDRD, DOE 1994b) and the *Engineered Barrier Design Requirements Document* (EBDRD, DOE 1994c). Appropriate procedures, *QAP-3-5, Development of Technical Documents*, in particular, were used in the preparation, review, approval, and if necessary, the revision of the report. Accordingly, a Technical Document Preparation Plan [*Technical Document Preparation Plan for the FY 1996 thermal Loading Study Report*, B00000000-01717-4600-00058 Rev. 02, August 9, 1996] for this document was developed, issued, and utilized to guide its preparation. Other applicable procedural controls not specifically discussed in the Technical Document Preparation Plan are listed in the above mentioned *QAP-2-0*. There are no applicable determinations of importance evaluations in accordance with *NLP-2-0 Determination of Importance Evaluation*.

Data and/or computational codes of indeterminate quality were used in this study. A portion of the existing site data was collected or developed prior to the approval of a QA program. Also, current scoping results from analyses conducted were used and identified in this study. Any data of indeterminate quality were identified as such in the report. Data developed in accordance with an approved QA program were utilized when available. Some computer codes were used in this study that were not controlled in accordance with *QAP-SI* series procedures (see below). The results of any computer programs not controlled by *QAPs* were also identified. Steps are being taken to ensure the codes comply with the appropriate quality procedures. As such, as additional data is obtained under procedures subject to *Quality Assurance Requirements and Description*, DOE/RW-0333P, requirements and computer codes are validated it may be necessary to review these results to determine what impact the new results might have and if any changes may be warranted in the conclusions.

The work documented in this study represents scoping analyses with the intention of facilitating the design process by providing requirements for design. Much of the data and many of the models and codes used to support the development of these requirements are not qualified. The quality status of the data and codes is addressed in each section of the text. It is important to note that neither a legal standard nor regulation related to repository long-term performance exists. Therefore, it was not the purpose of this study to confirm the adequacy of the repository design compared to a performance standard, but rather to assess the appropriateness of preserving various thermal limits on the design, assessing the potential advantages of thermal management options, and identifying an alternative thermal loading. Any requirements recommended by this study related to enhancing or preserving repository performance relative to a safety standard will be designated as TBV. For these requirements, it is recommended that an aggressive program be undertaken to qualify the data,

models, and software necessary to allow verification of the requirements. For those requirements that are not related to enhancing or preserving repository performance relative to safety, no such verification is required because they are not relied on to ensure repository performance. Therefore, it is not necessary to contain within this report the listings of all input and output files for the computer analyses conducted in support of this study. As a result, this document contains the appropriate level of documentation related to the use of computer software, per QAP-3-5. Use of any data or conclusions from this analysis for input into documents supporting procurement, fabrication, or construction is required to be controlled as TBV in accordance with the appropriate procedures.

Data and assumptions that are identified in this document are for preliminary design and shall be treated as unqualified. Computer codes are employed in this study that have not been controlled in accordance with QAP-SI series procedures. The resulting data from any computer programs not controlled by QAPs will be unqualified. The computer codes used in the work conducted in support of this study are listed by section number of this report as follows:

Section 3.2

TOUGH2, Version 1.0 of March 1991 developed by Pruess with T2.FOR Module replaced by T2CG1.F Version 1.1 April 1993. The code was used in conjunction with a processor code, CLIN, developed by Intera in May 1996 to include the geochemical aspects as discussed in Section 3.2. The code runs on a PC using a SALFORD compiler. The software does not currently have a configuration control number. The code is unvalidated but was used over the range for which it was designed and was appropriate for the application.

GEOMESH, last updated March 19, 1996, was developed by Los Alamos National Laboratory, and runs on a SUN Sparc10 workstation. Some qualified data went into the development of this code but the code has not been validated. The software does not currently have a configuration control number. The code was used over the range for which it was designed and was appropriate for the application.

Section 3.3

JAC2D, Version YMP 1.0, October 26, 1992. This thermomechanical code developed by Sandia National Laboratories runs on a SUN Unix workstation. The code has been verified and controlled under QAIP-3-2 and QAIP-19-1, which are SNL procedures subject to QARD requirements. The code control number is 110.67. The code is used over the range for which it has been verified as stated in Work Agreement WA-0213 and the code is appropriate for the application.

FLAC, Version 3.22, 1993 (CSCI #20.93.3001-AAu3.22). The code has been verified and validated. The code runs on IBM PC. The code was run over the range that it has been validated for. This code is appropriate for the application.

ANSYS Version 5.1 (CSCI #30003 V5.1 HP). The code was run on a Hewlett Packard 9000 series 735 workstation. The software has been qualified and this is described in *Software Qualification Report for ANSYS Version 5.1HP* Rev. 00 (CRWMS M&O 1995e), CSCI: 30003 V5.1HP,

DI: 30003-2006. The Life Cycle Plan and the QAP-SI series procedures for the code are described in *Life Cycle Plan for ANSYS Version 5.1HP* Rev. 00 (CRWMS M&O 1995f), CSCI: 30003 V5.1HP, DI: 30003-2007. The code was run over the range that it has been validated for and the code is appropriate for the application.

Section 3.4

RIP - Repository Integrating Program, Version 4.04, November 1995. This code runs on a PC. It has not been validated although Golder, the developer, has it under configuration control. The code was used over the range for which it was designed and it is appropriate for the application.

FEHM, May 7, 1996. Developed by Los Alamos National Laboratory and runs on an HP9000 workstation. This code has not been validated nor is it configuration controlled. The code was used over the range for which it was designed and is appropriate for the application.

WAPDEG developed by INTERA. This code runs on an HP9000 workstation. The code has not been validated nor is it configuration controlled. The code was used over the range for which it was designed and is appropriate for the applications.

CLADDING PROCESS MODEL, May 1996. The process model is a FORTRAN subroutine linked into a statistical code called SAMPLE (a 1975 code). The description of the subroutine is found in Section 3.3. The code runs on an IBM PC. It has not been validated nor configuration controlled. The code was used over the range for which it was designed and is appropriate for the applications.

Section 4.1

VTOUGH, developed by Lawrence Livermore National Laboratory based on the TOUGH2 code. The code runs on an IBM RISC6000 Powerserver Model 375. The software does not currently have a configuration control number. The code is unvalidated but was used over the range for which it was designed and was appropriate for the application.

Section 5.2

Nonisothermal Unsaturated-Saturated Flow and Transport (NUFT), Version 4-16-96b, 1996. Developed by Lawrence Livermore National Laboratory and runs on an IBM RISC6000 Power server Model 375. This code has not been verified nor is it configuration controlled. The code was used over the range for which it was designed and is appropriate for the applications.

ANSYS Version 5.1, (CSCI #30003 V5.1 HP) The code was run on a Hewlett Packard 9000 series F35 workstation. The software has been qualified and this is described in [Software Qualification Report for ANSYS Version 5.1HP (CSCI: 30003 V5.1HP), DI Number: 30003-2006 REV 01, CRWMS M&O]. The Life Cycle Plan and the QAP-SI series procedures for the code are described in [Life Cycle Plan for ANSYS Version 5.1HP (CSCI: 30003 V5.1HP), DI Number: 30003-2007 REV 01, CRWMS M&O]. The code was run over the range that it has been validated for and the code is appropriate for the application.

Section 5.3

NUFT, Version 4-16-96b, 1996. Developed by Lawrence Livermore National Laboratory and runs on an IBM RISC6000 Powerserver Model 375. This code has not been validated nor is its configuration controlled. The code was used over the range for which it was designed and is appropriate for the applications.

MTECS, June 1996. This is the Mackay Thermal Enhancement and Climate Simulation model developed by Mackay School of Mines, University of Nevada, Reno. The code runs on an IBM PC. The code has not been validated nor is its configuration controlled. The code was used over the range for which it was designed and is appropriate for the applications.

Section 5.4

WSM, Version 3.3, February 1995, run on Pentium 90 PC using OS2. The code has been baselined under Configuration Control Number A00000000-00811-1200-20014. The code has not been validated but was used over the range for which it was designed and was appropriate for the application.

2.2 DESIGN REQUIREMENTS

The input requirements and many of the assumptions for this study were obtained from the RDRD (DOE 1994b), the EBD RD (DOE 1994c), and the *Controlled Design Assumptions Document* (CDA Document) (CRWMS M&O 1996f). These documents contain a number of requirements which impact design as a function of the thermal environment in the engineered and natural environment. A number of the analyses conducted in this study were intended to either provide technical justification for the choice of some of the requirements or, as appropriate, to develop justification to recommend a change to the requirement. This section presents the applicable requirements and discusses whether analyses were conducted in this study which may impact these requirements.

The following assumption will be used as the basis for establishing the preclosure period of 100 years in the calculations.

The repository will be designed to permit waste retrieval for up to 100 years after the initiation of waste emplacement. [CDA Key 016]

The following assumption addresses many of the reasons why a thermal loading decision is needed (with sufficient technical validation) and why alternative AMLs are needed to mitigate risks and was best phrased in the *Mined Geologic Disposal System Requirements Documents* (MGDS-RD, DOE 1996a) as follows:

Assumption on Heat Management. The continuing heat generation of waste packages after emplacement may require management during the preclosure period. The thermal load on the geologic setting may require management to avoid adverse effects on its waste isolation capability. The thermal load may determine the amount of waste that may be emplaced in a given repository area. Thermal load management techniques may involve: (1) blending the

waste (i.e., mixing SNF or HLW of different thermal outputs in Multi-purpose Canisters (MPCs) and waste packages); (2) partially filling MPCs and waste packages; (3) selecting the age (or thermal characteristics) of waste to be accepted for emplacement; (4) temporary storage of waste for cooling prior to emplacement; (5) waste emplacement configurations; (6) ventilation options; (7) repository horizon options; or some combination of these.

Current repository design activities focus on a reference design thermal load that will permit emplacement of at least 70,000 MTU within the primary repository area (See 3.7.2.1.D), and produce dry conditions around the WPs. The current working hypothesis is that a reference AML of 80-100 MTU per acre (commercial spent fuel) should produce an average areal thermal loading of about 100 kW per acre at the time of waste emplacement, and will satisfy both criteria. This approach is expected to maintain prudent levels of flexibility by including alternative AMLs through design options and through operational parameters. As laboratory and field test data and more refined analysis become available, a preferred, specific thermal load will be selected.

Risks associated with this approach, such as unexpected and undesirable site responses, will be mitigated by maintaining design and operational flexibility to accommodate a range of AMLs, and by pursuing a performance confirmation program to validate preclosure predictions, to increase confidence in postclosure predictions.

The assumption used in developing this MGDS-RD regarding the extent of any blending of SNF or HLW that may be required is limited to blending that can be accomplished through management of the waste stream. Limited blending of SNF can be accomplished at the Monitored Retrievable Storage and MGDS. If significant blending is required, this could have a major impact on the Monitored Retrievable Storage and MGDS design and operations, as well as use of MPCs in the system; or it may require negotiations with Purchasers, should blending of wastes loaded into MPCs at Purchaser sites be recommended. These issues will be the subject of system studies. If these studies show that changes in system design requirements are necessary, this document will be revised.[MGDS-RD 3.1.5.E]

Thermal Loads. The underground facility shall be designed so that the performance objectives will be met taking into account the predicted thermal and thermomechanical response of the host rock, and surrounding strata, and groundwater system. [10CFR60.133(I)] [RDRD 3.7.5.E.7]

The following requirements, in part, make it necessary for the natural and engineered barriers to function together within the thermal environment to ensure that satisfactory waste isolation is achieved.

Mission Requirement. The design of the repository segment shall provide for the disposal of SNF and civilian and DHLW such that the public health and safety and the environment are protected. [NWPA 42USC10131(a)(4)] [NWPA 42USC10131(b)(1)] [1985 Presidential Memo]

The disposal system shall be designed to provide a reasonable expectation, based upon performance assessments, that the cumulative releases of radionuclides to the accessible environment for 10,000 years after disposal from all significant processes and events that may affect the disposal system will have a likelihood of less than one chance in 10 of exceeding the quantities calculated according to Table 1 of Appendix A of 40CFR191; and have a likelihood of less than one chance in 1,000 of exceeding ten times the quantities calculated according to Table 1 of Appendix A of 40CFR191. <TBV> [40CFR191.13(a)] [RDRD 3.2.1.6.C]

Under normal operations and anticipated occurrences, the annual dose equivalent to any real individual who is located beyond the controlled area shall not exceed 25 mrem to the whole body, 75 mrem to the thyroid, and 25 mrem to any other organ as a result of exposure to planned discharges of radioactive materials, radon and its decay products excepted, to the general environment; direct radiation from repository operations; and any other radiation from uranium fuel cycle operations within the region.

<TBV> [10CFR60.111(a)] [40CFR191.03(a)(1)] [RDRD 3.2.2.1.D.1]

The Engineered Barrier Segment shall be designed to ensure that releases of radioactive materials from the Engineered Barrier Segment, and then through the geologic setting to the accessible environment following permanent closure, conform to applicable environmental standards for radioactivity established by the Environmental Protection Agency with respect to both anticipated and unanticipated processes and events. [EBDRD 3.7.B] [10CFR60.112]

The Engineered Barrier Segment shall be designed, assuming anticipated processes and events affecting the geologic setting, so that containment of radioactive material within the waste packages will be substantially complete for a period to be determined by the U.S. Nuclear Regulatory Commission (NRC) but not less than 300 years nor more than 1,000 years after permanent closure of the geologic repository <TBV>. [10CFR60.113(a)(1)(ii)(A)] [EBDRD 3.7.D]

This requirement has been modified in the CDA Document as the EBS shall be designed, assuming anticipated processes and events, so that containment of radioactive material within the waste packages will be substantially complete for 1000 years (with less than 1 percent of the waste packages failing with 1000 years after permanent closure of the geologic repository) and with a mean waste package lifetime well in excess of 1000 years. [10CFR60.113(a)(1)(ii)(A)] [CDA EBDRD 3.7.D]

The Engineered Barrier Segment shall be designed, assuming anticipated processes and events, so that the release rate of any radionuclide from the Engineered Barrier System following the containment period shall not exceed one part in 100,000 per year of the inventory of that radionuclide calculated to be present at 1,000 years following permanent closure, or such other fraction of the inventory as may be approved or specified by the NRC; provided, that this requirement does not apply to any radionuclide that is released at a rate less than 0.1 percent of the calculated total release rate limit. The calculated total release rate limit is defined to be one part in 100,000 per year of the inventory of radioactive waste, originally emplaced in the underground facility, that remains after 1,000 years of radioactive decay. [10CFR60.113(a)(1)(ii)(B)] [EBDRD 3.7.E]

Although possibly subject to modification if some form of interim storage is established, the analysis performed in this study, except for some modification in Section 5 where storage options are examined, uses the following requirement on waste receipt rates.

The repository shall be capable of receiving waste according to the schedule shown in Table 3-3 of this document. [10CFR60.3(a)] [NWP 42USC10222(a)(5)] [RDRD 3.2.1.2.B]

The total amount of fuel considered for emplacement in the proposed repository at Yucca Mountain is based on the current requirement.

Assuming the Monitored Retrievable Storage facility is located more than 50 miles from the repository, no quantity of SNF and solidified HLW resulting from the reprocessing of such a quantity of spent fuel containing in excess of 70,000 metric tons of heavy metal shall be emplaced in the repository until such time as a second repository is in operation. [RDRD 3.2.1.2.A] [NWP 42 USC 1013)(d)]

CDA Document Key Assumption 003 provides for a total of 63,000 MTU of SNF to be emplaced in the repository.

CDA Document Key Assumption 005 provides for a total of 7000 MTU of HLW to be emplaced.

Some of the thermomechanical evaluations and considerations for tunnel support are based on a requirement for underground openings.

Openings in the underground facility shall be designed to reduce the potential for deleterious rock movement or fracturing of overlying or surrounding rock. [10CFR60.133(e)(2)] [RDRD 3.7.5.E.2]

Thermal effects need to be considered on WPs.

The design of waste packages shall include but not be limited to consideration of the following factors: solubility, oxidation/reduction reactions, corrosion, hydriding, gas generation, thermal effects, mechanical strength, mechanical stress, radiolysis, radiation damage, radionuclide retardation, leaching, fire and explosion hazards, thermal loads, and synergistic interactions. [10CFR60.135(a)(2)] [EBDRD 3.7.1.B]

The study examined the limits that should be placed on the Zircaloy cladding and evaluated the impact on total performance.

Limit the fuel cladding temperature to less than 350°C. [CDA DCWP, 001]

The current design layouts for the potential repository geometry, layout, and depth were established to satisfy the following.

The orientation, geometry, layout, and depth of the underground facility, and the design of any engineered barriers that are part of the underground facility shall contribute to the containment and isolation of radionuclides. [10CFR60.133(a)(1)] [RDRD 3.7.5.E.3]

The EBD RD (DOE 1994c) originally had a requirement for boreholes to keep the temperature 1 m into the drift in a borehole to less than 200°C to avoid deleterious thermomechanical effects [EBDRD 3.7.G.2]. Based on previous work (CRWMS M&O 1993), the criteria was changed to keep the emplacement drift wall temperature below 200°C. Evaluation of this criterion was conducted in this study. This requirement, which was documented in the CDA is as follows.

Keep emplacement drift wall temperatures <200°C. [CDA EBD RD 3.7.G.2]

The EBD RD had a requirement to limit the predicted thermal response of the host rock [EBDRD 3.7.G.3]. Evaluation of this criteria was conducted in the study. This requirement, which was documented in the CDA is as follows.

Limit the TSw3 (basal vitrophyre) maximum temperature to less than 115°C. [CDA EBD RD 3.7.G.3]

Alternates to major design features should be considered.

An assessment shall be provided to document the predicted effectiveness of engineered and natural barriers, including barriers that may not be themselves a part of the geologic repository operations area, against the release of radioactive material from the WP to the environment. The analysis will also include a comparative evaluation of alternatives to the major design features that are important to waste isolation, with particular attention to the alternatives that would provide longer radionuclide containment and isolation. [RDRD 3.3.1.H] [10CFR60.21(c)(1)(ii)(D)]

2.3 INPUTS AND ASSUMPTIONS

This section identifies the reference case, the major input conditions for the study, and the assumptions used. The primary parameters used (such as WP size, emplacement tunnel dimensions, and general repository layout) are described below. In many cases specific input parameters and/or assumptions for a given analytic model or for a particular option are discussed in the pertinent section of the report. The origin of the inputs and their quality will be identified where appropriate. However, in some cases where these inputs have been used in previous analyses, the reader will be directed to the appropriate references for the supporting information. The following identifies the basic assumptions and inputs used in the study.

Thermal Loading. The thermal load in this report will be referred to in terms of an area mass density of SNF. The units of the area mass density are generally kilograms Uranium (taken in this report to be equivalent to kilograms initial heavy metal) per square meter (kgU/m^2) or, alternatively, MTU/acre. The area mass density is used since it tends to be most representative of long-term, mountain-scale performance (Buscheck et al. 1994). Another method of identifying the thermal load is in terms of an area power density (kW/acre) because it influences the early-time (first few hundred years), drift scale environment.

The reference thermal loading for these calculations was 20.5 kgU/m² (83 MTU/acre). Other thermal loads were considered necessary for evaluations of alternate thermal loads or to determine when potential thermal effects may arise.

WP. A difference between this study and previous thermal studies is that a MPC was not being considered. Instead, a single large WP for PWR and BWR assemblies, and a single canister for DHLW were used. The WP dimensions are given below (CRWMS M&O 1996a).

Fuel Type	Number of Assemblies/ Pour Canisters	Package Length (m)	Package Diameter (m)
PWR	21	5.335	1.629
BWR	44	5.335	1.626
DHLW	5	3.680	1.709

Waste Stream. For various scenarios the fuel selection criteria followed an oldest fuel first (OFF) or a youngest fuel first with fuel age greater than 10 years (YFF(10)). Burnups and fuel ages are identified in the pertinent sections.

Subsurface. The reference case is the case established in the *Mined Geologic Disposal System Advanced Conceptual Design Report* (ACD Report, CRWMS M&O 1996a). The proposed repository horizon location at Yucca Mountain has been identified as the welded, lithophysae-poor, ash-flow tuffs in the Topopah Spring Tuff of the Paintbrush Group. This rock is unsaturated but the pores are filled with 80 to 85 percent water. The repository location, defined as the Primary Area and described in the ACD Report (CRWMS M&O 1996a), consists of emplacement primarily in the upper block with some emplacement in the lower block. Other emplacement areas were considered in the alternate thermal loads evaluation but the details of these choices and the assumptions are identified in Section 6 of this report.

The repository depth below the surface of the mountain varies across the repository area. However, for many of the thermal-hydrologic calculations an average depth of 343 m was chosen. The differences will be identified where this depth differs from this value in the analysis.

The subsurface repository considers emplacement of WPs in horizontal emplacement drifts. These emplacement drifts have a diameter of 5 m. The WP spacings varied from about 5 m to about 19 m depending on the package mass loading. The drift spacings in all cases were 22.5 m. In this analysis some of the calculations used different WP spacings and drift spacings and where this was done it will be identified in the pertinent section.

Rock Properties. In some cases, for specific evaluations, properties were selected using data obtained from recent subsurface and surface drilling programs and any associated laboratory testing. Where this was done the information will be identified and the quality will be reported. All other inputs were taken from the *Reference Information Base* (DOE 1995b).

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3. SELECTED THERMAL GOALS REEVALUATION

3.1 INTRODUCTION

The SCP defined a set of thermal goals with the intent to ensure that the engineered barrier system assists the geologic setting in meeting performance objectives for waste isolation, and allows for safe handling and storage and facilitates retrieval. These thermal goals were developed based primarily on expert elicitation with little information available. These thermal goals were reevaluated (CRWMS M&O 1993) again using expert elicitation and available laboratory data in 1993. To focus design, some of these thermal goals were identified as requirements in the EBDRD. As more information becomes available from underground exploration and testing it is appropriate to reexamine these thermal goals, which are really surrogate criteria for performance.

Several thermal goals are currently constraining the design. Test information from underground samples and, in some cases, enhanced modeling capability exist to reevaluate these goals. Based on this, the study conducted a reevaluation of three selected thermal goals, the 115°C goal at the TSw2/3 interface; the 200°C emplacement drift wall goal; and the 350°C goal for the spent fuel cladding. The 115°C not to exceed thermal criterion at the TSw2/3 interface was established to prevent mineralogic changes to the zeolites in the Topopah Spring basal vitrophyre and the Calico Hills nonwelded (CHn) unit (CRWMS M&O 1993). Meeting these criterion limits the thermal load that can be attained to about 20.5 kgU/m² (83 MTU/acre) and to some extent limits the area that can be used for emplacement at the higher thermal loadings. The not-to-exceed 200°C criterion for the emplacement drift wall was to limit thermomechanical effects which might cause tunnel stability problems (i.e., rockfall). These criteria limit the thermal load that can be achieved, the WP spacing, and the heat output of a specific WP. The not to exceed 350°C cladding goal was to protect from rupture the zircaloy cladding which was deemed to be a possible additional barrier to prevent or limit the dissolution and transport of radionuclides. Meeting this criterion can impact the thermal load possible, the type and time that backfill might be emplaced, and the waste package design.

To reevaluate the above thermal goals, where possible, process models were developed and evaluations of Total System Performance Assessment (TSPA) were performed to examine the impact on total releases to the accessible environment. However, in some cases the connection to performance is as yet unknown. In these cases the performance was evaluated using a couple of methods such as the effect on duration of boiling and relative humidity of the WP environment when the WP temperature drops below boiling, or thermomechanical response of the host rock and evaluations of potential rock and/or tunnel support failure. The discussions of these evaluations are contained in the following subsections.

3.2 EVALUATION OF THE THERMOCHEMICAL GOAL

A thermal goal of 115°C was set for the Topopah Spring basal vitrophyre (TSw3) and for the underlying Calico Hills nonwelded (CHn) unit. The rationale for these goals is described in the SCP (DOE 1988) and the *Site Characterization Plan Thermal Goals Reevaluation* (CRWMS M&O 1993). The temperature limits were intended to limit mineralogic changes which could be induced by repository heating and that might have chemical and physical effects that could be detrimental to waste isolation. Additionally, questions concerning the impact on the hydrology as a result of

mineral changes have been raised. Dehydration of the zeolites can produce substantial quantities of water and irreversible mineral alteration may increase the porosity of the rock which could effect ground water travel time. The purpose of this section is to address a number of these questions dealing with the mineralogic alterations which may result as a consequence of heating and the impact that these may have on waste isolation. The task used results of laboratory measurements of samples taken from core samples from the surface drilling program and subjected them to heat and natural analog studies.

An objective of this study was to evaluate the need for a thermal criteria to protect the zeolites beneath the repository, a potential natural barrier to radionuclide transport. These analyses were done to determine the impact on performance, if any, of the effect of heating on the zeolitized, nonwelded, and partially welded ash flow tuffs beneath the potential repository at Yucca Mountain. The effort examined potential mineralogic alterations which could have potential impacts on waste isolation. Primarily, the effort focused on the dehydration of the zeolites and the effect this additional water may have on the duration of boiling and the saturation at the potential repository horizon. Laboratory and natural analog studies were used to develop estimates of the mineralogic changes as a function of temperature and time which were then used as inputs to the calculations. The evaluations of the effect of heating on the zeolites were performed by incorporating the geochemical interactions in a thermohydrologic code. The thermohydrologic code was then used to estimate the movement of water, the temperature changes, and the saturation changes at the potential repository horizon.

Many of the samples used in the laboratory work were from nonqualified core samples. However, the guidelines for the experiments did not require that the material be pedigreed Yucca Mountain core. The experiment only required that the material be of known mineralogy and composition. Both the data collection and data analysis were carried out using quality affecting procedures under an approved quality program. The TOUGH2 (Pruess 1991) code is not qualified nor has it yet been verified to any extent with measurements. This verification with qualified experimental data is needed to confirm this analysis.

3.2.1 Geochemical Background

The CHn unit consists of glassy and variably zeolitized nonwelded and partially welded ash flow tuffs and bedded tuffs extending vertically downward to the water table from the basal vitrophyre in the overlying TSw unit. The CHn is a natural geochemical barrier to radionuclide transport because major portions of the unit, designated CHnz, contain abundant clinoptilolite, a zeolite with high sorptive capacities for Cs and Sr (Meijer 1990). Clinoptilolite may provide significant retardation even with only slight preferential sorption of some radionuclides. For example, Robinson, et al. (1995) examined the effect of the presence of clinoptilolite on the travel time of Np to the water table. By assuming that Np was only weakly sorbed by zeolitic Calico Hills units and not sorbed by any other rock units, it is shown that travel times were delayed by a factor of about 10. The loss of clinoptilolite from the Calico Hills unit might therefore result in significantly decreased travel times for Np. Clinoptilolite also has good sorptive properties for such radionuclides as Am, Pu, and U. Although Am is relatively short lived (a half life of about 430 years), the other radionuclides have much longer half lives and would affect the 10,000 year dose (CRWMS M&O 1995c). Thus the zeolites in the CHnz layer could possibly reduce dose over some time periods

(10,000 to several hundred thousand) and would provide a barrier for potential early releases. The unsaturated CHnz is a potential hydrologic barrier as well, with higher matrix porosity and lower fracture abundances than the densely welded TSw (Lappin, et al. 1982).

The long-term stability of clinoptilolite in the potential repository may be important to the performance of a repository but difficult to assess quantitatively. Geologic emplacement of high-level radioactive waste will heat the rocks due to heat produced by the radioactive decay of the waste. Studies on the effects of repository-induced heating include research on the dehydration behavior of clays and zeolites in tuffs (Bish 1984, 1988a, b) and on the hydrothermal stability of tuffs (Blacic et al. 1986; Duffy 1983a, 1983b). In an analysis of the thermal constraints on radioactive waste isolation in zeolitic tuffs, Smyth (1982) concluded that the reaction of clinoptilolite to analcime would begin at about 105°C based on data summarized by Iijima (1975), thereby giving rise to volume reductions and significantly reducing the cation sorptive capacity of the rocks (Vaughan 1978). Analcime has little or no cation exchange capability, particularly compared to clinoptilolite. This indicates that analcime has reduced radionuclide sorption compared to clinoptilolite. [Little information is available comparing the sorptivity of clinoptilolite and analcime but the cation exchange is discussed in Gottardi and Galli (1985).] Smyth advised constraining the maximum temperature in zeolitized tuff to 85°C to prevent reaction. Smyth's paper initiated the long-standing programmatic concern with the effects of repository-induced heating on the zeolitic rocks at Yucca Mountain.

A reasonable fraction of rock below the potential repository is composed of zeolites, primarily clinoptilolite. Approximately 50 percent of the rock is zeolites although different layers can vary from 10 to over 70 percent by weight (CRWMS M&O 1996b). The average volume fraction of rock that is composed of clinoptilolite is about 35 percent (see Table A-10 in Appendix A). The transformation of the abundant clinoptilolite to analcime in rocks underlying the host rock at Yucca Mountain would give rise to large decreases in volume leading to increased rock porosity and probably permeability. The reaction would also yield large amounts of water and greatly reduce the total cation-exchange capacity of the zeolite barrier (Vaniman and Bish 1995). However, the temperature at which the clinoptilolite-to-analcime reaction might occur and the rate of the reaction are difficult to assess experimentally. The reaction is thought to occur in nature at temperatures below 200°C, where reaction rates are very slow. Laboratory research on the long-term effects of heating Yucca Mountain tuffs to relatively low temperatures (<250°C) has been hampered by the slow reaction kinetics, and laboratory experiments either have not reproduced the assemblages observed in Yucca Mountain (Duffy 1983a, 1983b) or only do so at higher temperatures that speed reactions and potentially change reaction mechanisms (Knauss and Beiriger 1984). Furthermore, the reaction is known to be affected greatly by water compositions¹. Because of this one must turn to natural analogs for information on potential alteration over long time scales. Natural analog information will be addressed below.

¹ Found in article accepted for publication by *Clays and Clay Minerals*, written by S.J. Chipera and D. L. Bish, titled "Equilibrium Modeling of Clinoptilolite-Analcime Equilibria at Yucca Mountain, Nevada."

3.2.2 Development of Geochemical Inputs

The details of the geochemistry of clinoptilolite were developed by Los Alamos National Laboratory and are described in detail in Appendix A of this report. This information primarily came, as indicated above, from laboratory and natural analog studies. Many of these studies are still preliminary in nature. A brief overview of the geochemistry issues used to develop analytic predictions of the behavior of zeolites with heating used in the thermohydrologic model is provided in this section.

Hydration and dehydration of clinoptilolite may have significant consequences for the stability of clinoptilolite and for the hydrology of Yucca Mountain. Dehydration will destabilize clinoptilolite relative to less hydrous mineral assemblages (albite and analcime); release significant amounts of water; have a significant impact on the heat transport; and result in porosity changes due to changes in molar volume. The experimental data necessary to assess all of these factors have been obtained by Bish² and others.

The equilibrium water contents of clinoptilolite as a function of temperature were determined by Carey and Bish² and are discussed in more detail in Appendix A. The experiments performed show that clinoptilolite hydrates and dehydrates reversibly at temperatures less than or equal to 215°C. Equilibration times for hydration and dehydration of clinoptilolite appear to be on the order of an hour, thus the kinetics of hydration/dehydration do not appear to be relevant to processes at Yucca Mountain. In addition, there are no discontinuities in the dehydration behavior at the boiling point of water. Based on these results and estimates of the thermodynamics of hydration, the equilibrium constant for the amount of water released in dehydration as a function of temperature can be found (see Appendix A). The analytic expressions describing this behavior were incorporated in the TOUGH2 thermohydrologic code.

Possibly as important as the amount of water released during dehydration is the thermodynamics of the process that requires heat to perform the dehydration. This potential additional heat sink beneath the potential repository could possibly result in reducing the duration of boiling at the repository horizon for conditions of a high thermal loading which will drive the dehydration process. The energetics of hydration and dehydration of clinoptilolite have been measured calorimetrically³ and the results show (see Appendix A) that the energetic requirements to dehydration increase as dehydration proceeds. These energetics were also included in the TOUGH2 code.

Developing the thermodynamic properties of zeolites (e.g., clinoptilolite) at Yucca Mountain is a particularly challenging problem because of the extensive compositional variation that occurs in the natural material. The composition of clinoptilolite and isostructural heulandite at Yucca Mountain is highly variable, with Si/Al ratios between 3 and 5; exchangeable cation compositions that are combinations of Na⁺, K⁺, and Ca²⁺; and significant variation in water content (Broxton et al. 1987).

² Found in article in press, *American Mineralogist* by J.W. Carey and D.L. Bish 1996 titled "Equilibrium in the Clinoptilolite-H₂O System."

³ Found in article submitted to *Clays and Clay Minerals* by J.W. Carey and D.L. Bish 1996 titled "Calorimetric Measurement of the Enthalpy of Hydration of Clinoptilolite."

Equations to estimate the Gibbs free energy of formation of analcime as a function of Si/Al ratio were developed, primarily, using natural analog studies. The natural analogs were used to estimate the effect of repository-induced alterations; however, the zeolitic reactions also appear to be affected by fluid compositions (including the activity of water). Use of Yucca Mountain as a natural analog assumes that the future fluid compositions at the site as a result of thermal effects will be approximately those that were present during the initial alteration ~11 Myr ago. Given these caveats, the data from Yucca Mountain suggest that conversion of clinoptilolite to analcime could occur at temperatures above about 100°C. The kinetics of these reactions are discussed in more detail in work done by Bish et al. 1996. These estimates were used to develop bounding calculations of the conversion of clinoptilolite to analcime and the resulting changes in the porosity of CHn in Appendix A. However, because of the uncertainty associated with these predictions and the time scale over which such mineralogic alterations might occur, the alteration of clinoptilolite to analcime was not included in the thermohydrologic calculations, only the dehydration of clinoptilolite was considered. More work is needed in this area to establish the kinetics of the clinoptilolite to analcime conversion.

The 115°C thermal goals were placed on the TSw2/3 interface and the top of the CHn unit as convenient reference points, and due to the fact that at the time of the SCP there was only very limited information as to where the zeolites were located. Additional information has been gained from the surface drilling program in the last few years, which has helped identify the locations of the zeolitized layers and the depths of those layers. The zeolites are found at distances that are substantially below the TSw2/3 interface. Figure 3.2-1 (Robinson et al. 1995) provides contour estimates of the approximate distance that the top of the zeolitized layer is below the potential repository horizon. Although the Primary Area of the potential repository is not shown on this contour plot, the coordinates of the corners show that, based on the ACD Report (CRWMS M&O 1996a), the north-south limits of the repository are about the north-south limits of the contour map. The east-west edges of the potential repository are roughly equivalent on the east side and the repository edge is about 200 m inside of the western bound of the contour map. The zeolite depth below the potential repository varies from about 130 m in the southwestern corner to about 210 m in the eastern portion of the block.

3.2.3 Thermohydrologic Calculations

To examine the effects of clinoptilolite (abbreviated at times on the figures as Cpt) on the water and energy balance, a process model was developed to evaluate the effect of dehydration of the clinoptilolite under the influence of heating. This process model was coupled with the thermohydrologic code TOUGH2 (Pruess 1991). The calculations only considered clinoptilolite since this is the predominate zeolite in the CHnz unit and is the primary attribute with potential for sorbing radionuclides. For specified changes in temperature and pressure, the process model determines changes in the hydration and energy levels of clinoptilolite. These changes then entered the thermohydrologic analyses as source terms. Not considered in the calculations were the kinetics of altering clinoptilolite to analcime and the impact this alteration might have on increasing the porosity and hence the permeability.

Distance from Repository West of Ghost Dance Fault to First Zeolitic Unit of Calico Hills

Figure 3.2-1. Isobars Depicting the Estimated Depth of the Zeolitized Layer Below the Potential Repository in Meters

Hydration of Clinoptilolite. To characterize the hydration state at vapor-pressure P_v and temperature T , we use the following equation from Carey (1993):

$$-R \ln K_{ideal} = \frac{\Delta\mu_w^0}{T_0} + \Delta H_w^0 (1/T - 1/T_0) + W_{w1} \theta/T + W_{w2} \theta^2/T - 3R (\ln(T/T_0) + (T_0/T - 1)) \quad (3.2-1)$$

Here $R=8.31456 \text{ J/mol/}^\circ\text{K}$ is the ideal gas constant, $T_0=298.15 \text{ }^\circ\text{K}$ is the reference temperature, and θ is the fractional hydration. Table 3.2-1 defines the remaining parameters and presents their values for sodium-exchanged clinoptilolite (Na-Cpt), the most abundant clinoptilolite at the Yucca Mountain Site.

Table 3.2-1. Hydration Parameters for Na-Cpt

Parameter	Definition	Value
$\Delta\mu_w^0$	Gibbs Free Energy	-55,080
ΔH_w^0	Specific Enthalpy	-99,593
W_{w1}	Mixing Parameter	74,649
W_{w2}	Mixing Parameter	-32,111

The equation

$$K_{ideal} = \left(\frac{\theta}{(1-\theta)f_{H_2O}} \right) \quad (3.2-2)$$

defines the equilibrium constant in terms of hydration fraction and fugacity. We approximate fugacity by the relation $f \approx P_v$ with the vapor pressure expressed in bars. Combining Equations 3.2-1 and 3.2-2 gives a transcendental equation which is solved iteratively to obtain the fractional hydration θ as a function of temperature and vapor pressure.

To calculate the rate $G_w[\text{kg/s}]$ of fluid injected into, or withdrawn from, the flow system, the clinoptilolite process model considers a time interval $\Delta t=t_2-t_1$ across which the fractional hydration changes by an amount $\Delta\theta=\theta_2-\theta_1$. The desired element-specific rate is:

$$G_w = VM_w N_w \rho_{Cpt} \Delta\theta/\Delta t \quad (3.2-3)$$

where $V=[m^3]$ is the volume of an element containing clinoptilolite, $M_w= 18.016 \times 10^{-3} \text{kg/H}_2\text{O-mol}$ is the mass of a mole of water, $N_w=23.9 \text{ H}_2\text{O-mol/Cpt-mol}$ is the maximum level of hydration for Na-Cpt, and $\rho_{Cpt}=277.74 \text{ Cpt-mol/m}^3$ represents the areal density $2.35 \times 10^{11} \text{ Cpt-mol/8.30} \times 10^6 \text{ m}^2$ (Carey 1993) divided by a model thickness of 102 m.

The enthalpy associated with rate $G_w[\text{kg/s}]$ is defined by:

$$E_w = U_w + \bar{P}/\rho_w \quad (3.2-4)$$

Here the internal energy U_w and density ρ_w of water are computed by a stand-alone version of the TOUGH2 subroutine COWAT for average values of pressure $\bar{P}$ and temperature $\bar{T}$ within time interval $\Delta t=t_2-t_1$.

Energetics of Clinoptilolite. The change in the enthalpy of hydration $\Delta H_H=[\text{J/H}_2\text{O-mol}]$ which occurs during time interval Δt is given by:

$$\Delta H_H = \Delta H_H^0(\theta_2 - \theta_1) + W_{H1}(\theta_2^2 - \theta_1^2)/2 + W_{H2}(\theta_2^3 - \theta_1^3)/3 + 3R(\bar{T} - T_0)(\theta_2 - \theta_1) \quad (3.2-5)$$

where Table 3.2-2 defines the parameters (Carey 1993) and R is the ideal gas constant.

Table 3.2-2. Energy Parameters for Na-Cpt

Parameter	Definition	Value
ΔH_H^0	Specific Enthalpy	-88,326
W_{H1}	Mixing Parameter	41,853
W_{H2}	Mixing Parameter	0

Using parameter values, also given in Table 3.2-2, we calculate the rate $G_H[\text{J/s}]$ of energy withdrawal from, or injection into, the flow system for Na-Cpt:

$$G_H = -VN_w \rho_{Cpt} \Delta H_H / \Delta t \quad (3.2-6)$$

Explicit Coupling to TOUGH2. From calculated values of pressure and temperature at adjacent restart times, the clinoptilolite process model calculates TOUGH2 source-sink terms G_w , E_w , and G_H using the relations given in Equations 3.2-3, 3.2-4, and 3.2-6. Then, assuming relatively slowly varying clinoptilolite behavior, these rates are applied to TOUGH2 as source-sink terms for each restart interval.

Conceptual Model of the Thermohydrologic Analyses. To characterize the thermohydrological effects of clinoptilolite, the study considered the same drift-scale model used in the *Thermal Loading Study for FY 1995* (CRWMS M&O 1996b, Section 3.5). This model assumes that a large 21 PWR capacity (8.75 MTU) WP is emplaced at a depth 343.1 m below ground surface, suspended within a closed (unventilated), air-filled drift having a radius of 3.81 m. This is a larger drift than the other calculations but it will not effect the results since we are primarily looking at mountain scale effects. At 568.1 m below ground surface, the water table locates the top of a 1,000 m saturated zone.

At 1,568 m below ground surface, the bottom boundary is held at a constant pressure of 9.8 MPa and a constant temperature of 53.5°C. The former is an appropriate static pressure for 1,000 m of water overlain by 568.1 m of air within the unsaturated zone. The latter, when reduced by the surface temperature, represents an appropriate geothermal gradient for the area. The top boundary is held at average ambient conditions of 86 kPa and 13°C with an average annual infiltration rate of 0.05 millimeters/year (mm/yr) (CRWMS M&O 1995b and Flint and Flint 1994). In addition, the humidity of the surface air is held at a value slightly less than 100 percent. Though inappropriate for a desert climate, a humidity of this magnitude reduces vapor losses through the surface to levels which are appropriate for the area (CRWMS M&O 1995b). Placed symmetrically about the WP, vertical no-flow boundaries define a system with lateral dimensions of one drift spacing by one waste-package spacing.

To the basic model described above, a clinoptilolite layer was added. At 102 m, the thickness of the layer is consistent with the volume and area values given in Table A10 of Carey (1993). To achieve bounding levels of hydration and energy, however, the top of the layer was placed at a depth of 94.3 m below the WP in the model. The depth contours of Robinson et al. (1995), reproduced in Figure 3.2-1, place the clinoptilolite layer at substantially larger depths below the potential repository. Thus, these calculations are conservative in that respect.

Results. The discussion to follow describes the effects, if any, of the presence or absence of clinoptilolite on repository performance. Effects of the repository thermal pulse on the zeolite layer are discussed in the natural analog Section (3.2.4). Calculations to examine the effect of clinoptilolite on the potential repository performance (temperature, saturation, and duration of boiling) were conducted at two thermal loads of 20.5 and 28.4 kgU/m² (83 and 115 MTU/acre).

Figures 3.2-2 and 3.2-3 show temperature profiles as a function of depth in the mountain for three times, 100; 1,000; and 5,000 years for the 20.5 kgU/m² case, and 100; 1,000; and 10,000 years for the 28.4 kgU/m² case. Recall that the potential repository is located at a depth of 343 m and the zeolitized nonwelded and partially welded ash flow tuffs extend from about 440 to 540 m below the potential repository. The plots compare predictions for the base case which does not consider dehydration of clinoptilolite with the case where liquid and energy changes as a result of clinoptilolite dehydration are calculated. As can be seen from the figures, negligible differences occur in the temperatures of both thermal loads. As expected, the presence of the water produced by the clinoptilolite dehydration and the energy consumed in that dehydration tend to result in very slightly cooler conditions throughout the mountain, but most pronounced (still negligible) below the potential repository. Although not shown here, liquid saturations show little difference between the cases with and without clinoptilolite at either thermal loading.

Figure 3.2-2. Effect of Clinoptilolite (Cpt) on Drift-Centerline Temperatures at Specified Times

Figure 3.2-3. Effect of Clinoptilolite (Cpt) on Drift-Centerline Temperatures at Specified Times

Figures 3.2-4 and 3.2-5 show the temperature, liquid saturation, and hydrated fraction (see Equation 3.2-2) as a function of time in the upper layer (about 100 m below the potential repository horizon) and in a layer 88 m deeper in the zeolitized layer respectively for the 20.5 kgU/m² case. Similarly, Figures 3.2-6 and 3.2-7 show similar parameters plotted at those two locations for the 28.4 kgU/m² case. The plots compare the calculated effects of considering dehydration (with clinoptilolite) with those in which dehydration does not occur (without clinoptilolite). An examination of the figures shows that the predicted temperatures reach about 90°C after about 1,000 years for the 20.5 kgU/m² case at the top of the zeolitized layer and, as expected, the deeper layer (186.3 m below the repository) does not get much over 80°C and at times beyond 2,000 years. The saturations of the upper zeolitized layer show some drying from ambient but the deeper layer shows little change from ambient. The upper layer shows some slight differences between the two cases considered (with and without clinoptilolite) while the deeper layer shows negligible differences. Additionally, the hydrated fraction shows a reduction indicating that, even though temperatures are below boiling, some dehydration is occurring.

For the higher thermal loading of 28.4 kgU/m², the temperature of the upper zeolitized layer exceeds boiling and reaches about 105°C while the deeper layer does not exceed 90°C. The saturation profile undergoes significant drying with some differences between the two cases. However, the deeper layer, due to the fact that it doesn't exceed 90°C sees little changes in saturation. These results indicate that, although a relatively high thermal loading is employed, primarily only the upper layer of zeolites in the CHn is impacted.

3.2.4 Overview of Natural Analog Studies Pertinent to Clinoptilolite Stability

Because of the difficulties in experimentally reproducing the clinoptilolite-to-analcime reaction, we have examined the possibility of using natural geologic systems as analogs to the conditions that might be expected near a high-level radioactive waste repository at Yucca Mountain. The use of such analogs is based on the presence of rock sequences containing clinoptilolite grading into analcime, coupled with information on the temperatures and timing of past mineral reaction. This section provides a brief overview of some of the natural analog findings. More detail can be found in Appendix A and the referenced literature.

We have used clinoptilolite occurrences in rocks at Yellowstone National Park to provide information on the compositional and temperature effects on clinoptilolite stability. In addition, we have used the large amount of mineralogical information available from Yucca Mountain cores. Bish (1989) and Bish and Aronson (1993) studied the clay mineralogy of tuffs from Yucca Mountain, Nevada, in order to understand the alteration history of the rocks and to predict potential future alterations. Bulk-rock samples and clay-mineral separates from three drill holes at Yucca Mountain (USW G-1, USW G-2, and USW GU-3/G-3) were studied using X-ray powder diffraction, and supporting temperature information was obtained using fluid inclusion data from calcite. Samples from these drill holes appear to be representative of the zeolites found throughout the primary area. A site scale geologic model has been developed based on information from these three drill holes and other available drill holes and survey data (Robinson et al. 1995) and the site scale model discusses the consistency and thickness of the zeolite layers.

Figure 3.2-4. Effects of Clinoptilolite (Cpt) at 100 m Below Repository

Figure 3.2-5. Effects of Clinoptilolite (Cpt) at 186.3 m Below Repository

Figure 3.2-6. Effects of Clinoptilolite (Cpt) on the Top of the Clinoptilolite Layer

Figure 3.2-7. Effects of Clinoptilolite (Cpt) at 186.3 m Below Repository

The core samples used were taken from drill holes cores that were not obtained under qualified procedures. The laboratory analyses were done under existing Los Alamos National Laboratory Quality Procedures but, at the time, those procedures were not certified by the Yucca Mountain Project. Thus the data are, to some extent, of indeterminate quality. These measurements could be brought under control of existing quality procedures. A discussion of the details of the test is found in Bish (1989).

The predominant clay minerals in the Yucca Mountain tuffs are interstratified illite/smectite (I/S), with minor amounts of chlorite and interstratified chlorite/smectite. The I/S reactions observed as a function of depth are similar to those observed for pelitic rocks; I/S transforms from R=0 interstratifications through R=1 and R>3 interstratifications where R is the number of interstratifications to illite in USW G-2 and to R>3 I/S in USW G-1. The R=0 I/S clays in USW GU-3/G-3 have not significantly transformed. Both I/S geothermometry and fluid inclusion data suggest that the rocks at depth in USW G-2 were subjected to post-depositional temperatures of at least 275°C, those in USW G-1 reached 200°C, and rocks from USW GU-3/G-3 probably did not exceed 90 to 100°C. Thus, at Yucca Mountain, mineralogical data can be used to provide paleotemperatures to which the rocks have been subjected. The I/S studies established the temperatures and, based on looking at the zeolites associated with these I/S, we can infer the temperatures range where mineral reactions occurred. Based on these evaluations it can be concluded that in the range of 90 to 100°C there is a potential for clinoptilolite to undergo alteration to analcime.

Meijer⁴ reviewed a variety of natural geological and geochemical analogs to repository-induced alteration at Yucca Mountain. Of four potential sites in the continental U.S., he concluded that the Yellowstone caldera most closely duplicates the details of the volcanic rocks at Yucca Mountain and the conditions anticipated in the potential repository. The Yellowstone caldera is an active hydrothermal system in silicic ash-flow tuffs, and considerable data on present-day water compositions and temperatures are available. This situation contrasts with most other potential natural analogs for which temperatures and water compositions must be approximated from geological and geochemical information. Zeolites are common in many drill holes at Yellowstone, and clinoptilolite is the most common zeolite, followed by mordenite, and analcime.

Yellowstone rocks that coexist with acid waters usually contain clay minerals rather than zeolites. This suggests that development of lower pH waters in and around the repository horizon would destabilize zeolites. In the neutral to alkaline waters in Yellowstone rocks, zeolites coexist with clays and K-feldspars, and K-feldspars, analcime, and quartz appear to represent a stable higher temperature assemblage. Meijer concluded that this assemblage resulted from the interaction of clinoptilolite/mordenite-bearing rocks with thermal waters of low aqueous silica activity. At temperatures above about 165°C, K-feldspar, mordenite, and quartz often coexist. Clinoptilolite and K-feldspar usually coexist only with cristobalite rather than quartz and always at temperatures <165°C. Thus, in the Yellowstone system, clinoptilolite appears to have an upper temperature stability limit of about 165°C.

⁴ Found in unpublished Los Alamos National Laboratory report by A. Meijer (1987) titled *Investigations of Natural Geologic and Geochemical Analogs in Relation to a Potential Nuclear Waste Repository at Yucca Mountain, Nevada*.

Due to the potential nonequilibrium conditions at Yellowstone and the water chemistry differences with Yucca Mountain, another natural analog was considered to obtain information on zeolite alterations. Valuable data concerning possible zeolite reactions in tuffs at Yucca Mountain can be obtained by examining the changes in bulk mineralogy with depth at Yucca Mountain and correlating these changes with the I/S reactions and the estimated paleotemperatures documented by Bish (1989) and Bish and Aronson (1993). Important variations in mineralogy with depth in a number of drill holes at Yucca Mountain include the gradation from unaltered volcanic glass to clinoptilolite $\pm$ mordenite to analcime and finally to authigenic albite. This sequence was first emphasized for these tuffs by Smyth (1982), who related these mineralogic changes to those documented by Iijima (1975, 1980). Smyth correlated the temperatures at which some of these reactions occurred (clinoptilolite-analcime, analcime-albite) to the aqueous Na concentration. In contrast, Kerrisk (1983) conducted reaction-path calculations of mineral formation in tuffs near Yucca Mountain and concluded that aqueous silica activity was the controlling variable in the mineral evolution.

A recent thermodynamic modeling of potential zeolite reactions was conducted by Chipera and Bish⁵ at Yucca Mountain, with conclusions that temperature, relative cation abundances, and silica activity are all important factors in determining clinoptilolite-analcime equilibria. Increased Na⁺ concentrations in either clinoptilolite or the fluid phase, increased clinoptilolite K⁺ concentration, increased temperature, and decreased aqueous silica activity all stabilize analcime relative to clinoptilolite, assuming present-day Yucca Mountain water compositions. However, increased Ca²⁺ concentrations in clinoptilolite (i.e., heulandite) will stabilize clinoptilolite with respect to analcime. The models suggest that the geochemical factors controlling the reaction of clinoptilolite to analcime are more complex than those inferred in the Yellowstone natural analog study.

Using the results of Chipera and Bish⁵, assuming well J-13 water as the analog chemistry from Yucca Mountain water, clinoptilolite should remain stable with respect to analcime if temperatures in the clinoptilolite-bearing horizons do not significantly exceed 100°C. Even if temperatures rise significantly (e.g., to 150°C), not all clinoptilolite should alter to analcime, consistent with the observations from Yellowstone. Perhaps more importantly, thermodynamic modeling suggests that some Yucca Mountain clinoptilolites, particularly those rich in Ca and Al, will remain stable at elevated temperatures, even with an aqueous silica activity at quartz saturation.

The reaction of clinoptilolite to analcime at Yucca Mountain coincides with the appearance of significant amounts of calcite and minor amounts of chlorite and interstratified chlorite/smectite. The increase in calcite with depth is contrary to what is observed in pelitic rocks (e.g., Hower et al. 1976), reflecting either the differences in mineral assemblages or perhaps an increase in CO₂ with depth (Zen 1961) that may have been contributed by geothermal fluids. It is likely that the breakdown of clinoptilolite provided the source of at least some of the Mg for chlorite formation and the source of some of the Ca for calcite formation, although the formation of one or both of these minerals may have been associated with the hydrothermal fluids circulating at the time of alteration. The clinoptilolite probably also provided the source for at least some of the K in the deeper I/S clays and some or all of the Na for analcime and albite.

⁵ Found in article accepted for publication by *Clays and Clay Minerals*, written by S.J. Chipera and D.L. Bish 1996 titled "Equilibrium Modeling of Clinoptilolite-Analcime Equilibria at Yucca Mountain, Nevada."

Both Yellowstone caldera and Yucca Mountain appear to be reasonable natural analogs to repository-induced thermal alterations. The temperatures at which zeolite reactions occur are affected by fluid composition (including the activity of water). Water compositional data from Yellowstone suggest that acid water would destabilize clinoptilolite. Use of Yucca Mountain as a natural analog assumes that future fluid compositions at the site will be approximately the same as those present during the alteration about 11 Myr ago. This is probably a reasonable assumption, as fluid-inclusion waters are dilute. However, although present-day waters are also dilute, waters surrounding the repository environment may vary significantly from the present composition, particularly if they are concentrated by evaporation. Given these caveats, the I/S data from Yucca Mountain suggest an upper temperature stability of 90 to 100°C for clinoptilolite, 100 to 130°C for mordenite, and 175 to 200°C for analcime. Natural analog information from Yellowstone rocks suggest that clinoptilolite may exist to about 165°C but it appears to be in the process of still reacting and coming to equilibrium. The discrepancy between Yucca Mountain and Yellowstone inferences probably reflects both differences in water compositions and kinetic effects. The assemblages at Yucca Mountain have equilibrated over millions of years, whereas the Yellowstone assemblages are probably still actively reacting which could, in part, explain the higher temperatures than what was found in Yucca Mountain. This situation would have the effect of causing clinoptilolite to appear to be stable to higher temperatures.

3.2.5 Identification of a Layer for Establishing a Performance Criteria

The preceding section indicated that above a temperature of 90 to 100 °C the zeolite layer may potentially alter to analcime which has much poorer sorption properties for radionuclides than does clinoptilolite. But where should the criteria be placed? Four possible options were considered. One option was to put the temperature limit at the top of the zeolite layer wherever that layer might be. This option would require that we know where the zeolite layer is everywhere in the Primary Area which would be difficult to accomplish without developing a number of additional drillholes in the Primary Area. Additionally, this would involve having a variable thermal load across the repository with possibly less than 80 MTU/acre in the west and up to 100 MTU/acre in the east. This would not be very practical. Another option considered is to establish the temperature limit at a depth of about 130 m which is the shallowest depth anywhere in the Primary Area (beneath the emplacement area) that the zeolites are estimated to occur. This would insure no alteration of the zeolites. However, this depth occurs in a very narrow strip in the far southwestern portion of the Primary Area and appears to be overly conservative. Another option is to place the temperature limit on the average depth of the top of the zeolite layer in any given area. For the Primary Area this average depth, based on a numeric average, is about 170 m. It should be noted that, based on Figure 3.2-1 and the Los Alamos National Laboratory model, the depth of the top of the zeolites below the repository horizon (emplacement area) varies from about 130 m in the southwestern edge of the Primary Area to about 210 m in the east. However, a qualitative examination of Figure 3.2-1 and using an overlay of the emplacement area (not shown here) indicates that only about 25 to 30 percent of the emplacement area would have zeolites which are shallower than 170 m. This would imply that potential alteration could occur in these areas if the temperature reached 90 °C at 170 m and more will be said about this below. A fourth option considered was to place the 90 °C limit at a depth of about 195 m. If 90 °C is reached at this level then there is a potential to damage some portion of the zeolites to an average depth of about 25 m over about 50 to 75 percent of the Primary Area. This option, however, allows the thermal load of up to 100 MTU/acre which is consistent with

the upper limit of the current design focus. A "zeroth order" evaluation of the impact of these last two options is provided below.

A question that must be addressed is whether the alteration of a portion of volume of zeolites could adversely impact performance. This can only be answered in a qualitative manner at this time. For illustration purposes a simple example is shown below as to how the transport of Np might be affected. The following assumptions were made:

- A. A linear, equilibrium K_d model is valid for Np transport.
- B. The zeolites occupy one-half of the unsaturated zone thickness of 360 m beneath the repository and the water table (i.e., zeolites are 180 m thick).
- C. Np is only sorbed (retarded) in zeolites.
- D. Analcime does not sorb Np.
- E. The retardation factor (K_d) in the zeolites is 20 (CRWMS M&O 1995c).
- F. The conservative tracer velocity is 5 mm/yr (assuming a single continuum).

Using these assumptions, a "zeroth" order estimate of the travel time can be made.

The travel time to the water table for Np through the entire unaltered layer of zeolites would be:

$$(180\text{m}/0.005\text{m/yr}) + (180\text{m}/(0.005\text{m/yr}/20)) = 756,000 \text{ years}$$

The travel time to the water table for Np passing through zeolites which had the top 20 m altered to analcime (most of the western edge of the repository is at a minimum of 150 m above the zeolites) would be:

$$(200\text{m}/0.005\text{m/yr}) + (160\text{m}/(0.005\text{m/yr}/20)) = 680,000 \text{ years}$$

Thus, this simple approach indicates that approximately a 10 percent decrease in travel time would occur for a small portion of the potential repository. This is minor and should not result in any significant increases to the accessible environment. No difference will be discernable at 10,000 years and negligible difference at 1,000,000 years.

An average depth of 170 m, as indicated above, would have zeolites closer to the repository horizon than 170 m in about 25 to 30 percent of the area. Much of this area is along an edge of the repository and there will be lateral transport of heat at the edges which will result in somewhat cooler temperatures than would occur in the center of the repository. Calculations were done with the ANSYS code for an 83 MTU/acre repository which estimated the amount of edge cooling as a function of depth. Although not shown here, the calculations indicated that the 90 °C temperature is not exceeded at depths larger than about 130 m at locations in the emplacement area which are

within 250 m of the edge. This would imply that less than about 10 percent of the area would have the potential for alteration of the zeolites. This in itself is a somewhat conservative estimate since thermohydrologic calculations would estimate somewhat lower temperatures (five to ten degrees). Thus, it would appear that setting the limit at 170 m would result in little potential impact to performance. For the case in which the limit is set at 195 m the edge cooling would also reduce the area impacted. However, there would still be roughly between 30 to somewhat over 50 percent of the area which could have potential alteration. At an average depth of 25 m this would translate into a decrease in travel time of approximately 100,000 years for Np. While this may not significantly impact performance the amount of alteration is significantly larger than the other.

The natural analog studies indicate that clinoptilolite could begin altering to analcime if the temperature is within the range of 90 to 100°C. A conservative criteria would be to establish a not to exceed limit of 90°C on the zeolite layer. However, this could overly constrain the problem if it is too conservative. Thermal predictions were done with ANSYS for four thermal loads (83, 90, 95, and 100 MTU/acre) and these results are shown in Table 3.2-3. These calculations can be used to show that the maximum thermal load which can be emplaced and not exceed the 90°C limit is about 22.2 kgU/m² (90 MTU/acre). These predictions indicate that the temperature profiles at a depth of 170 m are slowly changing and there is little difference between a 90 MTU/acre and a 100 MTU/acre thermal load (the former reaches 90°C at 170 m while the latter reaches about 93°C at the same depth). If one were to want to exceed 100 MTU/acre then other criteria would be violated. Thus, there are additional reasons to limit the thermal load to 100 MTU/acre. This would allow additional flexibility in emplacing waste in the primary area. It should also be noted that the calculations provided in Table 3.2-3 were for the center of the repository and at the edges there is heat loss in the lateral direction (edge cooling). Thus, even if the distances are somewhat less than 170 m at the edges it is unlikely that the temperatures will reach those predicted by ANSYS and thus the alterations will not likely occur.

Establishing a not-to-exceed temperature limit of 90°C on the average top of the zeolite area will provide the most conservative limit that will insure that the zeolites do not alter to analcime. For the Primary Area the average top of the zeolite layer is about 170 m beneath the repository horizon. This option of using the average depth of the top of the zeolite layer appears to allow for very little alteration of the zeolite layer. The other options either provided the possibility of some zeolite alteration, were overly conservative, or represented an impractical solution which would require significant measurements to implement. The selected option appears reasonably conservative.

Parameters:

Thermal Loads:	40, 83, 90, 95 and 100 MTU/acre
WP Initial Heat Outputs:	9.21 kW/pk
Drift Diameter:	5.0 meters
Drift Spacing:	22.5 and 45.0 meters
Package Spacing:	19.85, 19.12, 17.65, 16.72 and 15.88 meters
Package Diameter:	1.802 meters
Package Length:	5.682 meters
Emplacement Mode:	Center-in-drift
TSw2 Lower Contact:	30 m from drift center

Table 3.2-3. Rock Peak Temperatures at Different Locations

Distance from Drift Center (meters)	83 MTU/acre		90 MTU/acre	
	Rock Peak Temperature (°C)	Time to Peak (years)	Rock Peak Temperature (°C)	Time to Peak (years)
2.5	147.7	64	155.5	64
30	124.1	518	129.7	517
40	117.2	783	122.1	769
50	112.1	1250	116.0	1250
60	107.6	1750	111.3	1750
70	104.4	2041	107.8	2041
80	101.8	2768	104.8	2518
90	99.8	3518	102.4	3268
100	98.0	4000	100.5	4041
120	94.9	4791	97.2	5041
140	92.0	5041	94.2	5541
160	89.3	5541	91.5	6000
180	87.0	5666	89.1	6041
200	84.8	5896	86.8	6291
Distance from Drift Center (meters)	95 MTU/acre		100 MTU/acre	
	Rock Peak Temperature (°C)	Time to Peak (years)	Rock Peak Temperature (°C)	Time to Peak (years)
30	133.3	517	137.1	534
40	125.2	764	128.4	775
50	118.7	1268	121.5	1356
60	113.7	1768	116.2	1750
70	109.9	2041	112.1	2000
80	106.8	2768	108.6	2518
90	104.3	3268	105.9	3268
100	102.2	4041	103.8	4291
120	98.8	5268	100.2	5541
140	95.7	6000	97.1	6268
160	92.9	6291	94.2	6644
180	90.5	6541	91.8	6890
200	88.10	6791	89.3	7023

3.2.6 Summary

A process model considering the dehydration and rehydration of zeolites was developed and incorporated in the TOUGH2 thermohydrologic code to evaluate potential impact on repository performance. Predictions of changes in temperature, duration of boiling, and liquid saturation were

compared between the cases with and without zeolites. The results of the calculations show negligible changes in the repository environment when zeolite dehydration is considered over the base case which did not include any zeolite dehydration effects. Natural analog studies were also reviewed in the study and the results of these studies found that alteration of clinoptilolite to analcime (a less sorptive mineral) may occur at temperatures above 90 to 100°C. These mineralogic changes appear to be irreversible and could degrade the ability of this natural barrier to sorb some radionuclides. The results indicate that a not-to-exceed temperature limit of 90°C should be placed on the average depth of the top of the zeolites beneath the repository. This average depth is about 170 m in the Primary Area although only about 25 to 30 percent of the area would be at depths that are less than 170 m and of that probably less than 10 percent would exceed 90 °C as a result of edge cooling. This limits the thermal loading to about 90 MTU/acre in the Primary Area. Higher thermal loads could be accommodated if the decision is made to allow for the possibility that some portion of the zeolites may undergo alteration with some decrease in travel time for the radionuclides through the CHn layer. Thermal loads above 100 MTU/acre violate other thermal goals/criteria. Additional information on zeolite alterations, locations and depths of zeolites, and better temperature predictions should be obtained. The above criteria supplements the 115°C thermal goal.

3.3 NEAR-FIELD THERMOMECHANICAL PERFORMANCE

The SCP recognized that thermally induced stresses in the rock could result in local rock failure and placed a temperature limit of 200°C at 1 m into the rock for a WP emplaced in a vertical borehole. When the concept changed to emplacement of large WPs in a horizontal emplacement drift the near-field thermomechanical goal was reexamined under the auspices of the 1993 Thermal Loading Study. Based on preliminary work and expert elicitation, a recommendation was made (CRWMS M&O 1993) to establish a thermal limit of 200°C on the emplacement drift wall. The original limit for boreholes was adopted in the EBD RD (DOE 1994c) [EBDRD 3.7.G.2] and the CDA Document (CRWMS M&O 1996f) updated this for horizontal emplacement drifts (see Section 2 of this report). The purpose of this section is to reexamine this thermal limit using updated rock property measurements and laboratory measurements of the thermal expansion coefficient from samples taken from the repository horizon.

The principle thermomechanical concern in the SCP was the issue of potential failure of a large volume of host rock which could possibly crush or damage the waste container and frustrate retrieval. The concern was based on the fact that phase transitions of silica polymorphs (tridymite and cristobalite) were believed to occur at temperatures above about 200°C. More recent work done by Oversby (1993) confirmed that the α - β cristobalite transition occurs above this temperature and can result in a significant increase in the thermal expansion coefficient. Laboratory measurements of expansion coefficients of samples from the potential repository horizon have been made by SNL and calculations made with those expansion coefficients will be discussed in this section.

More recently concerns have been raised about the coupling between the thermomechanical effects and the thermal-hydrologic effects. The issues raised for the near field are the potential opening of fractures resulting in increased flow of water to the WPs upon cooling or the potential sealing of fractures with precipitate produced when the moisture in the fractures boils. Both effects must be understood based on a combination of testing and modeling to ensure that the near-field performance can be predicted. Also of serious concern is the impact that thermomechanical effects might have

on the far field such as the Paint Brush Tuff layer (PTn), which some have dubbed the "tin roof" since it appears to substantially limit infiltration. Preliminary predictions (DOE 1994d) have indicated the potential for stressing this layer with the subsequent possibility of introducing fractures in the layer. This analysis will not address the thermomechanical coupling with the hydrology of the mountain. Instead the effort will only focus on the near-field tunnel stability issues. Further work on the coupling issues must await results from the thermal tests and the development of a large scale thermomechanical model.

Near-field thermomechanical predictions of rock stresses were done by Sandia National Laboratories in support of this effort. The primary issue being addressed with these calculations is not only what temperature limit should be placed on emplacement drifts but whether or not a temperature limit alone is sufficient. Specifically, the effort examined whether or not the magnitude of temperature gradient which might exist can produce deleterious mechanical effects that could impact rock stability. The first part of this section will discuss those results.

Since tunnel supports are likely to be used even in the emplacement drifts, it was necessary to examine the thermomechanical performance of the tunnel support, rock interface. The use of tunnel supports could stabilize the rock face in emplacement drifts even to temperatures above where the rock would normally fail. However, if the thermal expansion coefficients of the tunnel supports are significantly different than those of the host rock then differential stresses may be produced. In addition to the thermomechanical issues are the cost issues. While a tunnel support may be conceived which could stabilize rock at reasonably high temperatures, the cost to build and emplace such support may be prohibitive. This section will primarily examine the thermomechanical effects of a tunnel which has various kinds of tunnel support. The cost issues, will only be addressed in a qualitative fashion.

In both sets of calculations center-in-drift emplacement was assumed. Non center-in-drift emplacement has been considered to facilitate backfill emplacement. However, the latest project position is that, at this time, backfill is not needed. Thus, this appears to be a reasonable assumption.

The codes used in this section (JAC2D, UDEC, and FLAC) have been subject to the appropriate quality affecting procedures for qualification of computer codes. The input data primarily were obtained from the *Reference Information Base* (DOE 1995b) which was obtained under quality affecting procedures. Some parameters still need to be obtained in situ during appropriate tests. Thus, the estimates obtained in this section are the best that could be obtained at the time and have appropriate qualifications attached.

3.3.1 Evaluations of Mechanical Effects Resulting from Heating and Thermal Gradients

This investigation is intended to provide guidance towards establishing bounds on the allowable temperatures and temperature gradients near an emplacement drift based on predicted structural responses to imposed thermal fields. The details of the calculations and many of the specific results can be found in Appendix B.

The effort attempted to examine the sensitivity of a modeled emplacement drift to various temperatures and temperature gradients. As such, it was not necessary to generate specific thermal

profiles that could be directly linked to a specific thermal design. Instead, the thermal component was generated independent of any specific repository design but the shapes of the thermal gradients used were consistent with expected responses around a central emplacement drift.

The structural response of the host rock in the emplacement drift was obtained using the JAC2D model (Biffle and Blanford 1994) which is a qualified code. The majority of the calculations performed used the elastic constitutive model in the JAC2D code, however, limited comparison runs were also made using a jointed-rock model. Due to symmetry only half the 5 m diameter drift and half the space between drifts needed to be modeled and this required 5271 nodes as discussed in more detail in Appendix B. The boundary conditions and material properties (Young's Modulus, Poisson's Ratio, and density) used in the calculations are provided in Appendix B. These values either came from the *Reference Information Base* (DOE 1995b) or from stratigraphic information reported for drill hole USW G-4. Body forces consistent with a domain composed of TSw2 rock were also applied.

The coefficient of thermal expansion was obtained from available site specific thermal expansion data for samples from North Ramp Geologic (NRG) drill holes 5 and 6 [see Technical Data Information Forms (TDIFs) 303285 and 304353]. Some additional discussion concerning the measurements can be found in Appendix B, however, for ease of discussion the nominal and bounding values used in the calculations are reproduced in Figure 3.3-1. An examination of the figure shows that above about 200°C the instantaneous coefficient of thermal expansion begins to display a significant increase. It should be noted that the cool down sample data show a hysteresis (the heating was taken to 400°C). These data still, however, show a significant increase in expansion coefficient above 200°C although one could even conclude this increase occurred at about 160 or 170°C. The oven dried NRG 6 data appeared to be most representative of the majority of the expansion coefficient data and thus was selected as the baseline for use in these evaluations.

To approximate the relatively steep near-field thermal gradients that are anticipated during preclosure times, an algorithm was created to generate imposed temperature fields and gradients. The algorithm is based loosely on the solution of the time-dependent, one-dimensional cylindrical heat conduction equation and uses a simple exponential solution to the Bessel functions (Wylie and Barrett 1982). The imposed temperature is thus determined as a function of distance, r , from the center of the drift as:

$$T = T_{\text{ambient}} + (T_{\text{drift}} - T_{\text{ambient}}) e^{\left[\mu \left(1 - \frac{r}{R_o} \right) \right]} \quad (3.3-1)$$

where R_o is the drift radius, T_{drift} is the temperature at the drift wall, T_{ambient} is the initial ambient temperature within the rock mass, and μ is the multiplier to impose different gradients. Figure 3.3-2 shows four different temperature gradients generated for a drift wall temperature of 225°C and an ambient rock temperature of 25°C. These are likely only representative of early times during preclosure, since later times will see the gradients diminish as the heat moves out into the rock. As μ decreases, the imposed thermal profiles become more similar in shape to later-time host-rock responses.

Figure 3.3-1. (a) Instantaneous Coefficient of Thermal Expansion Data from NRG 5 and NRG 6, (b) Nominal and Bounding Thermal Expansion Data

Figure 3.3-2. Example of Gradients Examined in Study

To establish whether or not the potential for failure of the rock mass around an emplacement drift exists, it is necessary to compare the thermomechanical predictions of stress and strain against some form of failure criteria. This is generally difficult to do without in situ measurements since it can depend on the type of rock, where that rock is located, the assumptions used, and the type of tunnel supports, among other things. The calculations in this subsection assumed unsupported rock. Evaluations of tunnel support effects are discussed in a subsequent subsection. Based on this, a compressive failure criterion for the TSw2 rock-mass was developed using the approach described by Hardy and Bauer (1991). This approach uses the intact rock strengths, the rock-mass quality indices, and two empirical rock-mass strength criteria proposed by Hoek and Brown⁶, and Yudhbir and Prinzl (1983). A power law relationship of the form:

$$\sigma_1 = A + B\sigma_3^C \quad (3.3-2)$$

was developed by fitting the resulting average strength envelopes to describe the strength-confinement response; where σ_3 is the confinement pressure or overburden; A, B, and C are fitted constants, and σ_1 is the rock-mass compressive strength. Additional details of this evaluation including the coefficients used which were developed from North Ramp Geologic site data (DOE 1995b, [TDIF 303849]) can be found in Appendix B. A rock mass category of 3 (Hardy and Bauer 1991) was chosen to represent nominal conditions expected for the potential repository at the Yucca Mountain. Based on this the compressive strength for rock around the tunnel opening is estimated to be 56 MPa. Tensile failure in the rock was also evaluated and this is discussed in Appendix B.

A variety of calculations were made for the different thermal gradients and the results are presented in Appendix B. The results indicate that for wall temperatures of 200°C (or less) no tensile failure or compressive failure are predicted in the modeled domain for any of the thermal gradients modeled. An example of the results is shown in Figure 3.3-3 for the thermal gradient where μ in Equation 3.3-1 was 1.0. For this case the maximum stress was about 51 MPa which is less than the criteria above and so no significant compressive failure near the drift is predicted.

Another set of calculations was done in which the drift wall temperature was raised to 225°C. As with the previous case, no tensile failure is predicted for those simulations. However, applying the compressive failure criterion results in an increase in predicted compressive failure zones for all gradients examined. Although temperature appears to be the primary driver for rock reaching the failure criteria, once those criteria are exceeded the sharper the gradient the more failure predicted (see Appendix B). An example of this is shown in Figure 3.3-4 for the case of μ equal to 1. The figure shows that the rock around the opening and some distance into the rock exceeds the criteria of 56 Mpa.

The sensitivity to changes in various parameters was examined in this effort. Several parameters such as the coefficient of thermal expansion, Poisson's Ratio, and Young's Modulus are currently

⁶ Found in unpublished manuscript by E. Hoek and E. T. Brown (1988). From the Canadian Rock Mechanics Symposium, np. titled, "The Hoek-Brown Failure Criterion- A 1988 Update."

Figure 3.3-3. Maximum Principal Stresses for a Drift Temperature of 200°C and a μ of 1.0

Figure 3.3-4. Maximum Principal Stresses for a Drift Temperature of 225°C and a μ of 1.0

uncertain to some extent. These parameters were varied over a range of values to see what effect these changes might have on the predictions of rock failure. Figure 3.3-1 indicates the range of values that are likely to exist in the coefficient of thermal expansion (maximum and minimum values were plotted). The results of calculations with the range of coefficients of thermal expansion show that the relative amounts of compressive failure increase with higher expansion coefficients for a drift temperature of 225°C (Figure 3.3-4). At a drift wall temperature of 200°C the higher coefficient of thermal expansion produces predictions showing maximum principal stresses generated which are close to the compressive failure limit (Figure 3.3-3).

Available data from boreholes indicates that a range of Poisson's Ratio from 0.10 to 0.40 have been observed in the TSw2 rock. The results of the thermomechanical calculations show that an increase in Poisson's Ratio results in an increase in the magnitude of the induced stresses (see Appendix B). This indicates that there is some sensitivity to Poisson's Ratio.

To examine the sensitivity to changes in Young's Modulus, cases were run using a range of elastic moduli. An analysis of available site data (Brechtel et al. 1995) indicates that the TSw2 rock-mass elastic modulus can vary from 6.37 to 23.51 GPa, depending on rock mass category. These calculations were done for a uniform temperature of 225°C. The results indicate that the range of Young's Modulus can produce an increase in the x-component stresses of a factor of 3.7 which indicates a sensitivity to Young's Modulus. Given that the factor of safety is small for most of the cases where the drift wall temperature is 200°C, this indicates that minor increases in the assumed modulus could result in the generation of compressive failure zones around the drift.

Results. The results of the sensitivity studies show that the predicted stresses in the rock surrounding the drift are sensitive to changes in the coefficient of thermal expansion, the Young's Modulus, and Poisson's Ratio. The factor of safety is small for drift wall temperatures of 200°C and minor increases could generate compressive failure zones even at these temperatures. Further evaluation of the potential for rock failure are done in the following subsection considering the presence of tunnel supports.

The results of the thermomechanical analysis of unsupported emplacement drifts indicates that, while compressive failure is exacerbated by the temperature gradients, the potential failure of the rock is dependent primarily on temperature. Based on these calculations and the assumptions inherent in them it would appear that imposing a not-to-exceed temperature criteria of 200°C on the drift wall is still valid. This appears reasonable since, although no calculations were done between 200 and 225°C, the 200°C limit is conservative and will not constrain the existing design.

3.3.2 Thermomechanical Evaluations of Tunnel Support and Emplacement Drift Stability

Thermomechanical analyses were performed for evaluation of the 200°C rock temperature criterion in repository design. The analyses was accomplished using numerical modeling with the ANSYS and FLAC programs. Three different thermal loads, 20.5, 24.7, and 28.4 kgU/m² (83, 100 and 115 MTU/acre), with two values of WP initial heat output, 9.21 and 14.2 kW/package, were assumed in the modeling. Rock temperatures were calculated with the ANSYS program, while displacements and stresses in rock due to in situ and thermal loads were evaluated with FLAC for continuous rock masses. The details of this analysis are documented in Appendix C and summarized below.

3.3.2.1 Inputs

Modeling inputs include geologic information, thermal/mechanical properties, repository layout design parameters, ground support types, in situ stress, thermal loads, and temperature histories. Sources for this information, mainly CRWMS M&O and CRWMS M&O/Sandia reports, are referenced. Some of these data are qualified sources and some are not; however, these data are considered the most appropriate data for the modeling that was performed.

In Situ Stress. Components of the in situ-stress state at the approximate depth of the repository are given in Appendix C. These stresses, caused by the weight of the overlying geologic units, lateral confinement, and past stress history, are the initial stress condition for modeling. The vertical normal stress σ_v is considered equal to the weight of the overlying rock and is expressed as

$$\sigma_v = - \sum_{i=1}^n \rho_i g Y_i \quad (3.3-3)$$

where ρ_i = the average density of i th layer rock, kg/m³
 g = the gravitational acceleration, m/s²
 Y_i = the average thickness of i th layer rock, m
 n = number of overlying rock layers

The magnitude of the horizontal stress σ_h is expressed as a function of the vertical stress and given as the horizontal-to-vertical stress ratio K . Ranges of the horizontal and vertical stresses are tabulated (see Table C-1) in Appendix C. In summary, an average vertical stress of 7.0 MPa and a horizontal stress of 3.5 MPa were calculated for the proposed repository horizon.

Thermal Loads. Thermal loads of 20.5, 24.7, and 28.4 kgU/m² (83, 100 and 115 MTU/acre) are used in modeling. Drift spacings and WP spacings associated with these thermal loads are listed in Table 3.3-1, based on the horizontal in-drift emplacement mode and the AML approach. WP initial heat outputs of 9.21 (OFF average fuel) and 14.2 kW (YFF 10 year old fuel) per package are assumed as representatives for the average and extreme cases.

Table 3.3-1. Drift and WP Spacings Used in Analysis

Spacing	Thermal Load (kgU/m ²)		
	20.5	24.7	28.4
Drift (m)	22.5	22.5	22.5
WP (m)	19.12	15.88	13.81

Thermal and Mechanical Rock Properties. Thermal and mechanical properties for the Yucca Mountain strata are listed in Tables C-3 through C-6 in Appendix C. The mechanical properties are given for rock mass quality categories (RMQ) ranging from 1 to 5. The RMQ categories, first presented by Hardy and Bauer (SNL 1991) and used for Exploratory Studies Facility (ESF) analyses (CRWMS M&O 1995o) represent the distribution of rock properties for a given rock unit. Each category is associated with a frequency of occurrence of a certain range of Q-values. For example, category RMQ=3 for rock unit TSw2 has a typical Q-value of 1.91 for which rock properties have been derived and ground support categories have been developed (Table C-6). Also, category RMQ=3 is considered representative of the most frequently occurring range of Q-values and is thus used as a reference case for this study. The thermal expansion coefficients (see Table C-4) used in this analysis were based on a 1995 work by SNL and have been used in recent work by Subsurface Design. These values have trends similar to the expansion coefficients used in the SNL work reported in this section (see Figure 3.3-1 but the coefficients are somewhat less at temperatures above about 150°C. These values could have some affect on the results. The thermal expansion coefficient used in the previous subsection are based on more recent analysis (DOE 1995b, TDIFs 303285 and 304353) and would provide more conservative results but the calculations in this subsection should still be representative and will have appropriate trends.

Layout Parameters. Horizontal center-in-drift emplacement is the reference emplacement mode, based on preliminary assessments of WP design and repository criteria and requirements (CDA Key Assumption 011). The current conceptual layout shows emplacement drift excavation by tunnel boring machines, which produce drifts with a circular cross section. The 5.0-m diameter drift used in the stability analyses was chosen based on WP size, emplacement equipment size, and invert and ground support considerations. WP length and diameter are assumed to be 5.68 m and 1.80 m, respectively, based on the CDA (EBDRD 3.7.1.J.1). These two parameters were used in numerical modeling with ANSYS to determine rock-mass temperature distributions.

Ground Support Types. Ground support materials considered for emplacement drifts consist primarily of rock bolts, welded wire mesh, shotcrete, and structural steel sets. Two ground support types were assumed for these analyses and are used as examples to provide guidance in determining likely support behavior:

- Concrete lining, 200 mm thick
- Structural steel sets, W5×19, spaced at 1.2 m intervals

Parameters and properties used to characterize the ground support elements include cross-sectional area, elastic modulus, strength, and moment of inertia for both concrete liner and steel sets. Values for these parameters, grouped by ground support type, are listed in Appendix C (Table C-7).

3.3.2.2 Numerical Modeling

Computer Programs. Two commercially available computer programs, ANSYS (ANSYS 1995) and FLAC (described below), were used for the numerical analysis of rock temperature and opening stability. The release of the ANSYS program used in the thermal analysis is Revision 5.2. ANSYS Revision 5.1 has been verified and validated according to the QAP-SI-series of CRWMS M&O

Computer Software Quality Assurance procedures, but Revision 5.2 has not been verified and validated. The FLAC code, Version 3.22, on the other hand, is approved for design use in accordance with the QA procedures and carries the appropriate CSCI number (given below).

FLAC (Fast Lagrangian Analysis of Continua) is a two-dimensional explicit finite difference code that simulates the behavior of structures built of soil, rock, and other materials that are subjected to static, dynamic, and thermally induced loads (Itasca 1993). Modeled materials respond to applied forces or boundary restraints according to prescribed linear or non-linear stress/strain laws, and undergo plastic flow when a limiting yield condition is reached. FLAC is based on a Lagrangian calculation scheme, especially suited for modeling large displacements, and has several built-in constitutive models that permit the simulation of highly non-linear, irreversible responses typical of many geologic materials. The FLAC program was initially developed by Dr. Peter Cundall and Itasca Consulting Group, Inc. in 1986. The program version used to analyze opening stability is Version 3.22 (CSCI # 20.93.3001-AAu3.22), which has been verified and validated in accordance with applicable CRWMS M&O procedures.

Yield Criterion. The Mohr-Coulomb yield criterion was used in the analysis to judge whether or not the rock mass experiences failure. The criterion is defined as

$$\tau = c - \sigma_n \tan \phi \quad (3.3-4)$$

where τ = shear stress on a failure or yield plane, Pa
 σ_n = normal stress on a failure plane (tensile stress is positive), Pa
 c = cohesion, Pa
 ϕ = friction angle, degrees

The yield criterion is used to represent the rock mass strength in FLAC. The ratio of Mohr-Coulomb strength to rock stress (strength/stress ratio) is evaluated for every element and is especially useful in assessing rock mass stability in the vicinity of the drift. An element is considered to perform satisfactorily when its strength/stress ratio is larger than 1.0 and is thought to fail structurally if the strength/stress ratio is equal to or less than 1.0.

The concept of factor-of-safety was used as the criterion to assess ground support performance under in situ stress and thermal loads. The factor-of-safety for ground support components is defined as the ratio of material strength to stress or force. A ground support component is in a stable state when its strength/stress (or force) ratio is larger than 1.0 and is of structural failure if the strength/stress ratio is equal to or less than 1.0.

Initial and Boundary Conditions. Initial stress condition in the analysis is assumed to be consistent with the in situ stress given above and in Appendix C. Initial temperature in the thermal/mechanical units is based on a rock temperature at the ground surface of 18.7°C and a rock thermal gradient as described in Appendix C.

Boundary conditions for the thermomechanical model with FLAC are illustrated in Figure 3.3-5. The half-drift-spacing geometry is appropriate for the thermomechanical model because the model is symmetric along a vertical plane through the center of the drift. The model dimension in the vertical dimension is the entire thickness of the TSw2 unit. As shown by the bar-and-roller symbols along the sides and bottoms of the models (Figure 3.3-5), displacements in the horizontal direction on two vertical boundaries and in the vertical direction at the TSw2 lower boundary are zero (or fixed). Overburden stress is applied to the TSw2 upper contact, which is free to move vertically. The surface of the drift is stress and constraint free.

Rock temperatures after waste emplacement are time-dependent and were evaluated with the ANSYS program. Due to limitations of the thermal options in the FLAC code, rock temperature distributions are calculated based on the boundary temperature histories obtained from the thermal analyses with ANSYS. Based on thermal symmetry, the vertical model boundaries are prescribed as adiabatic, or zero heat flow, boundaries.

3.3.2.3 Thermally-Induced Opening and Ground Support Behavior

Two-dimensional modeling for emplacement drifts has been carried out with ANSYS (ANSYS 1995) and FLAC. Thermally-induced displacements and stresses in the rock mass and in ground support elements were calculated for up to 150 years after waste emplacement.

Temperature histories of the drift wall and TSw2 boundary contacts due to the thermal loads of 20.5, 24.7, and 28.4 kgU/m² (83, 100 and 115 MTU/acre) from waste emplacement for the initial heat outputs of 9.21 and 14.2 kW/package, respectively, were calculated with the ANSYS code (a total of 6 cases). The heat transfer mechanism in modeling with ANSYS involves both radiation and conduction, and the thermal radiation process is simulated explicitly. Thermal analyses for FLAC models calculate time-dependent temperature distributions resulting from boundary temperature inputs, and the heat transfer mechanism involved is limited to conduction only. Coupled thermomechanical analyses with FLAC have been performed for a period of 150 years after waste emplacement. This period of time, called the overall thermal time, is divided into a number of thermal time steps. At each thermal time step, the temperature distributions are determined first, and stress and displacement fields around the supported drift opening, strength-to-stress ratios, and axial forces or moments if applicable in ground supports are then obtained by conducting a quasi-static mechanical analysis. Owing to temperature dependence of thermomechanical properties of rock, such as specific heat and thermal expansion coefficient, each thermal time step has been further divided into a number of sub-thermal time steps. At the beginning of each sub-thermal time step, the values of specific heat and thermal expansion coefficient are updated for every zone based on its corresponding temperature and the temperature dependence of the properties (see Appendix C).

Depending upon mechanical properties and the magnitude of thermomechanical loads, the continuous rock model used in FLAC may behave elastically or elasto-plastically. The Mohr-Coulomb failure criterion is used in the analysis to judge whether or not the stress level reaches the yield limit, which varies with the RMQ categories. In this analysis, only the RMQ category of 3 was selected to evaluate the rock mass response to the elevated temperatures after waste emplacement.

Figure 3.3-5. Geometry and Boundary Conditions for Thermomechanical Modeling Using FLAC

Rock Temperature. Two-dimensional analysis with ANSYS shows that average peak temperatures experienced on the drift wall, as shown in Figure 3.3-6a, are about 146°C, 166°C, and 183°C for an average initial heat output of 9.21 kW/package and the thermal loads of 20.5, 24.7, and 28.4 kgU/m², respectively. With a higher value of WP initial heat output of 14.2 kW/package, the average peak temperature on the drift wall, as shown in Figure 3.3-6b, go up to about 197°C, 227°C, and 254°C for the thermal loads of 20.5, 24.7, and 28.4 kgU/m², respectively. This case is somewhat unrealistic since it assumes all of the waste packages in a drift are 14.2 kW but it was done to establish higher drift wall temperatures for the purposes of evaluating the thermomechanical effects. A high value of initial heat output of 14.2 kW/package results in the maximum rock temperatures at or above 200°C, while an average value of initial heat output of 9.21 kW/package causes the rock temperatures to reach to about or above 150°C but below 200°C. Table 3.3-2 summarizes the results from temperature calculation with ANSYS, and indicates that rock peak temperatures occur at about 50 to 65 years after waste emplacement for all cases considered. Information on temperature gradients is presented in Appendix C but in summary of that work, after the peak temperature is reached, the variation in rock temperature between the drift wall and pillar center is only about 10 to 30°C, depending on the thermal loads and WP initial heat outputs.

Drift Closure and Rock Mass Yield. Thermally-induced vertical and horizontal drift closures were calculated for emplacement tunnels supported with the two types of ground supports. The details of the calculations and plotted closures are presented in Appendix C. The results determined that the net vertical elongations were about 4 to 6 mm for the average package and were 7 to 9 mm for the larger heat package. Horizontal closures were about 10 to 15 mm and 17 to 26 mm for the 9.21 and 14.2 kW/package respectively.

As can be seen from these results, horizontal closures for the 9.21 kW/package case are about 60 to 76 percent of those for the 14.2 kW/package case, while vertical closures for the 9.21 kW/package case are about 55 to 67 percent of those for the 14.2 kW/package case. These numbers by themselves do not tell us much about the possibility of problems. What is more important is the differential closure between two locations in proximity. Unfortunately since these were two-dimensional calculations this type of information could not be obtained. Thus the above information only provides some indications that significant increases in closures occur as we approach and exceed 200°C temperatures on the drift wall. For example concrete has a yield limit for greater than 0.3 percent change in dimensions. For a tunnel liner this would be a change of about 15 mm in any direction. As indicated above the horizontal closures exceed this at temperature above 200°C. Additionally, similar significant increases are observed in drift closures as we go from a thermal load of 20.5 to 28.4 kgU/m².

An indication of drift stability was obtained from calculations of the time histories of the principal stresses (major and minor) in the drift crown of the emplacement drift. It is noteworthy that the differences in compressive stresses between the cases with the two packages is no more than 13 to 16 percent even though the heat output of the hotter package is more than 50 percent hotter. Potential rock mass yield is indicated by 3.3-7a, 3.3-7b, and 3.3-7c, which give strength-to-stress-ratio contour plots and failure surface envelopes at 10, 50 and 100 years after emplacement (thermal load of 20.5 kgU/m² (83 MTU/acre), initial heat output of 9.21 kW/package, steel sets ground support and RMQ= 3). Note that the peak rock temperature for this case is about 146°C, well below 200°C. The plots of strength-to-stress ratios indicate potential rock yield to a depth of about 60 cm

(a)

(b)

Figure 3.3-6. Temperatures Histories of Drift Wall for 83, 100 and 115 MTU/acre: (a) 9.21 kW/package; (b) 14.2 kW/package

Table 3.3-2. Results from ANSYS Models for Different Thermal Loads and Package Heat Outputs

Initial Heat Output (kW/package)	9.21			14.2		
Thermal Load (kgU/m ²)	20.5	24.7	28.4	20.5	24.7	28.4
Drift Wall Peak Temperature (°C)	146	166	183	197	227	254
Temperature at Center-of-Pillar at 100 yr (°C)	134	150	164	176	201	224
Time to Peak (years)	64	57	57	57	56	52

from the periphery of the drift (Figures 3.3-7a through 3.3-7c). In addition, Figures 3.3-7b and 3.3-7c show an increasing strength-to-stress ratio into the rock away from the drift wall, then a decrease, then a constant value as the line of symmetry (i.e., the center of the pillar) between the drifts is approached. Strength also decreases as the confining stress in the pillar decreases. Beyond 50 years, the strength-to-stress ratio in the majority of the pillar is at or above a value of 4.0. When the rock temperature exceeds 225°C (thermal load of 24.7 kgU/m² (100 MTU/acre), initial heat output of 14.2 kW/package, ground support steel sets for RMQ=3), potential rock mass yield is indicated in Figures 3.3-8a through 3.3-8c, which illustrate strength-to-stress-ratio contour plots and failure surface envelopes at 10, 50, and 100 years after waste emplacement. At 50 years, the potential rock mass yield, as shown in Figure 3.3-8b, may occur to a depth of about 2 m from the periphery of the drift. The overall patterns of strength-to-stress-ratio contours are similar to those for the case with the maximum rock temperature below 200°C.

Maximum major and minor principal stresses at the drift crown for 20.5, 24.7, and 28.4 kgU/m² and concrete lining ground support are about the same magnitude as those for the steel set ground support for RQM=3, which means that the strength-to-stress ratios of rock mass with the ground support concrete lining are similar to those with the steel sets. The results indicated that there was no tensile failure.

Ground Support Loads. Calculations were done to determine the axial forces (axial refers to the axis of a circular member, that is circumferential in the drift coordinate system) in 200-mm thick concrete liner, for 20.5 kgU/m² (83 MTU/acre) and 9.21 kW/package, at 10, 50 and 100 years after waste emplacement, are presented in Figures 3.3-9a through 3.3-9c for concrete liner ground support with RMQ=3. Axial forces increase with time; depending on location, the concrete liner may be in tension or compression. All concrete liners begin in compression, but the portion along the sidewalls quickly changes to tension and remains in tension. Figures 3.3-10a and 3.3-10b show the maximum axial forces for the 24.7 kgU/m² (100 MTU/acre) and 14.2 kW/package at 10, 50, and 100 years after waste emplacement. These axial stresses are about twice as large in this latter case when the wall temperature reaches 225°C (exceeds 200°C) than in the former lower heat output WP case. It is indicated that at 20.5 kgU/m² and 9.21 kW/package, the stresses in concrete liner increase with time, and remain below the compressive strength of 34.5 MPa during the preclosure period. The maximum compressive axial stress for 20.5 kgU/m² and 9.21 kW/package occurs, as shown in Table 3.3-3, at about 150 years after emplacement and is about 88 percent of the compressive strength of

(a)

(b)

(c)

Figure 3.3-7. Factors of Safety Contours and Plasticity Indicators around Opening with Steel Sets Ground Support for RMQ=3, 83 MTU/acre and 9.21 kW/package: (a) 10 Years after Emplacement; (b) 50 Years after Emplacement; (c) 100 Years after Emplacement

(a)

(b)

(c)

Figure 3.3-8. Factors of Safety Contours and Plasticity Indicators around Opening with Steel Sets Ground Support for RMQ=3, 100 MTU/acre and 14.2 kW/package: (a) 10 Years after Emplacement; (b) 50 Years after Emplacement; (c) 100 Years after Emplacement

(a)

(b)

(c)

Figure 3.3-9. Axial Forces in Concrete Liner Ground Support for RMQ=3, 83 MTU/acre and 9.21 kW/package: (a) 10 Years after Emplacement; (b) 50 Years after Emplacement; (c) 100 Years after Emplacement

(a)

(b)

(c)

Figure 3.3-10. Axial Forces in Concrete Liner Ground Support for RMQ=3, 100 MTU/acre and 14.2 kW/package: (a) 10 Years after Emplacement; (b) 50 Years after Emplacement; (c) 100 Years after Emplacement

34.5 MPa. As illustrated in Appendix C, axial stresses in the concrete liner for the RMQ category of 3 exceed the compressive strength of 34.5 MPa at about 70 years for 24.7 kgU/m² and 9.21 kW/package, about 30 years for 28.4 kgU/m² and 9.21 kW/package, about 20 years for 20.5 kgU/m² and 14.2 kW/package, about 15 years for 24.7 kgU/m² and 14.2 kW/package, and about 10 years for 28.4 kgU/m² and 14.2 kW/package.

Table 3.3-3. Results from FLAC Models for Concrete Liner Ground Support

Ground Support: 200 mm Concrete Liner			
Heat Output (kW/package)	9.21		
Thermal Load (kgU/m ²)	20.5	24.7	28.4
Max. Compressive Axial Stress in Concrete (MPa)	-30.5 (150) ¹	-35.4 (150) ¹	-39.7 (150) ¹
Ratio of Concrete Liner Compressive Strength to Compressive Axial Stress	1.1 (150) ¹	1.0 (150) ¹	0.9 (150) ¹
Heat Output (kW/package)	14.2		
Thermal Load (kgU/m ²)	20.5	24.7	28.4
Max. Compressive Axial Stress in Concrete (MPa)	-44.2 (150) ¹	-53.4 (150) ¹	-64.1 (150) ¹
Ratio of Concrete Liner Compressive Strength to Compressive Axial Stress	0.8 (150) ¹	0.6 (150) ¹	0.5 (150) ¹

¹ Time in years after emplacement to reach a maximum value during preclosure.

Both tensile and compressive stresses are developed in concrete liner at all three thermal loads considered. Though compressive stresses are below the strength of 34.5 MPa for 20.5 kgU/m² and 9.21 kW/package, tensile stresses for all cases considered are of a similar magnitude and may result in tensile failures. For steel, the tensile and compressive strengths are similar, but for concrete, the tensile strength is usually between zero and 10 percent of its compressive strength.

It is noted that if a concrete liner with a high compressive strength, for example 50 MPa, is used, its maximum compressive axial stress may remain below the yield limit as long as the rock temperature stays below 200°C. If the rock temperature exceeds 200°C, however, the concrete liner may experience overstress even with the high compressive strength of 50 MPa.

Appendix C presents the results of similar calculations of the axial stresses in steel sets (W5x19) induced by thermal effects in an emplacement drift. The results of those evaluations predict stresses well in excess of the estimated strength of steel of 248 MPa. These results are summarized in Table 3.3-4 and show ratios of compressive strength to compressive axial stress which are all less than one. It is noted that overstress in steel sets may be caused by the way with which steel sets are modeled in the FLAC program. FLAC simulates steel sets by assuming that they are bounded with

Table 3.3-4. Results from FLAC Models for Steel Sets Ground Support

Ground Support: 1.2 m Spacing W5 x 19 Steel Sets			
Heat Output (kW/package)	9.21		
Thermal Load (kgU/m ²)	20.5	24.7	28.4
Horizontal Closure (mm)	10.41 (150) ¹	13.7 (150) ¹	14.7 (150) ¹
Vertical Closure (mm)	-3.9 (150) ¹	-4.9 (150) ¹	-5.8 (150) ¹
Max. Major Principal Stress at Crown (MPa)	-32.1 (150) ¹	-34.6 (70) ¹	-36.4 (50) ¹
Max. Minor Principal Stress at Crown (MPa)	-2.9 (150) ¹	-3.2 (70) ¹	-3.5 (50) ¹
Max. Compressive Axial Stress in Steel Sets (MPa)	-309.0 (150) ¹	-387.1 (150) ¹	-465.0 (150) ¹
Ratio of Compressive Strength to Compressive Axial Stress for Steel Set	0.8 (150) ¹	0.6 (150) ¹	0.5 (150) ¹
Heat Output (kW/package)	14.2		
Thermal Load (kgU/m ²)	20.5	24.7	28.4
Horizontal Closure (mm)	16.7 (150) ¹	20.9 (150) ¹	25.9 (150) ¹
Vertical Closure (mm)	-6.5 (150) ¹	-7.7 (150) ¹	-9.0 (150) ¹
Max. Major Principal Stress at Crown (MPa)	-37.4 (50) ¹	-39.3 (50) ¹	-41.2 (40) ¹
Max. Minor Principal Stress at Crown (MPa)	-3.6 (50) ¹	-3.9 (50) ¹	-4.2 (40) ¹
Max. Compressive Axial Stress in Steel Sets (MPa)	-535.3 (150) ¹	-707.8 (150) ¹	-915.1 (150) ¹
Ratio of Compressive Strength to Compressive Axial Stress for Steel Set	0.5 (150) ¹	0.4 (150) ¹	0.3 (150) ¹

¹ Time in years after emplacement to reach a maximum value during preclosure.

rock perfectly, and no relative sliding or normal displacement occurs between steel sets and rock surface. This assumption is conservative when compared to reality. However, the analysis presented here for steel sets with FLAC is still useful in that it shows the relationship of potential stresses among the different scenarios (different thermal loads and WP heat outputs) even if the magnitude of the stresses is overstated. For the cases in which the temperatures exceeded 200°C, the axial stresses were about 75 percent to almost a factor of 100 percent larger than the cases which had the lower temperatures (the 9.21 kW/package cases). An effort is currently being made by using the ANSYS program to model the interaction between steel sets and rock mass such that the relative sliding or normal displacement is allowed with the use of interface or gap elements, which connect the steel sets elements to those of rock but allow them to move relatively in both normal and tangential directions. Preliminary results with this approach indicate that decrease of stresses in steel sets is substantial, but it is too early to draw any definitive conclusion on this matter.

3.3.3 Summary

Thermomechanical evaluations were done with two different codes to determine whether or not the current emplacement drift wall temperature criteria of 200°C is a valid criteria. In the first set of evaluations, unsupported drifts and their response to both temperature and temperature gradients were examined. In the second set of evaluations, the response of the rock was examined when tunnel supports (steel sets or concrete liner) were present. Additionally, the stresses in the tunnel supports was also examined. These evaluations used codes which have been qualified under Computer Software Quality Assurance procedures.

Input data to numerical analyses reflect the best documented information currently available on elastic properties, strength parameters, thermal properties, in situ stresses, and thermal loads. These properties and their time dependent behavior, if any, have been considered in modeling as realistically as possible. Careful attention was also given to mesh refinement and boundary conditions in order to minimize the effect of mesh dimensions on finite element numerical output.

The results of the evaluations done for the unsupported tunnels found that at temperatures above 200°C there is potential for rock failure. While larger temperature gradients appear to exacerbate the situation, the results indicate that it is primarily temperature and not temperature gradient which produces the high stresses in the rock. Additionally, sensitivity studies found that the calculations are relatively sensitive to the parameters such as thermal expansion coefficient, Young's Modulus, and Poisson Ratio used. If these parameters increase significantly, the temperature at which potential failure occurs could be changed.

In the second set of evaluations 5-meter-diameter emplacement drifts were analyzed using both ANSYS (ANSYS 1995) and FLAC codes under combinations of static and thermal loading conditions. Only one set of material properties for average rock mass state (RMQ=3) was considered. Concrete liner and steel sets were incorporated in numerical models as candidate ground support for the drift. The main objective of the analysis is to examine the response of emplacement drifts to the elevated temperature, especially above 200°C, under long-term thermal loading, so that the drift stability can be assessed.

Under the thermal loads of 20.5, 24.7, and 28.4 kgU/m² (83, 100, and 115 MTU/acre), the drift experiences higher horizontal closure than vertical closure. In fact, the drift will elongate vertically. The maximum horizontal closure detected is 14.7 mm for the rock temperature below 200°C and 25.9 mm for the rock temperature above 250°C, while the maximum vertical elongation is 5.8 mm for the rock temperature below 200°C and 9.0 mm for the rock temperature above 250°C. Potential rock mass yield at temperature below 200°C may occur to a depth of about 60 cm from the periphery of the drift. At temperature above 225°C, the potential rock mass yield may occur to as deep as about 2 m. These values indicate that though the normal components of the stress state have increased significantly, rock mass behaves essentially elastically even with the rock temperature exceeding 200°C.

Overstress in cast in place concrete liner and steel sets at elevated temperatures both below and above 200°C due to long-term thermal loads is possible. Maximum compressive axial stresses in 200-mm thick concrete liner exceed its compressive strength for all cases except for the 20.5 kgU/m² and 9.21 kW/package case in which the peak rock temperature is about 146°C. Regardless whether the temperature is somewhat below or above 200°C under thermal loads, the tensile load in concrete liners is high enough for tensile cracks to develop, eventually reducing the effectiveness of the concrete liner. Light steel sets are also shown to exceed their yield strength in tension and in compression. In this respect, high thermal loads indicate the need for structurally flexible support systems such as precast concrete lines.

However, the overstress indicated in the concrete lining and steel sets is due in part to the assumption of full bonding with the rock. This assumption is conservative, especially when steel sets and precast concrete segments are used. Any air gap between lining and rock wall may allow rock to deform without inducing high stresses in lining so that overstress in ground supports may be very limited. In addition, a literature survey regarding the thermomechanical properties of Hanford concrete exposed to long-term elevated temperature (Portland 1981) indicates that concrete may experience a decrease in Young's modulus and creep deformation at elevated temperature. The Young's modulus of concrete when subjected to heating at 232°C (450°F) may drop to as low as 30 percent of that measured with unheated concrete. So, it can be predicted that the stress in the concrete lining will be substantially lower if these considerations are taken into account in modeling. Given the large conservatism associated with the existing modeling, it is the opinion of design that there is no significant concern at the present time for the design of the ground supports at the ACD thermal loading. Further study is under way using the best available information on the thermomechanical properties of ground support materials and analysis.

The model used in this analysis had a number of limitations. There is no coupling with the hydrologic flow in the rocks which may not be that important since the high temperatures would tend to dry out the rock. There is also no consideration of small scale rock heterogeneity, and microcrack formation. The FLAC model has limitations but these were considered acceptable since the study was primarily concerned with overall stability of larger rock blocks. These issues should certainly be investigated as the results of the thermomechanical tests are obtained.

The study found that, based on the latest available measurements, the TSw2 tuff rock undergoes relatively dramatic increases in the coefficient of thermal expansion when the rock temperature exceeds 200°C. These increases may be due to phase changes in some of the rock minerals. The

increases in coefficient of thermal expansion may also trigger rock deformation, which may, in turn, produce high stresses in ground support elements such as concrete liner or steel sets unless the ground support systems are structurally flexible to be capable of adjusting to the thermally-induced rock deformation. These issues need to be considered in the design of the emplacement drifts, the design of the tunnel supports, and the selection of the thermal load.

The calculations found that the potential exists for rock failure at temperatures above 200°C. Including tunnel supports found similar results although it is not clear that concepts could not be found for higher temperatures, but they don't exist now. Probably the most compelling reason to remain below 200°C is the changes in the thermal expansion coefficients which occur around that value. Thus, there does not appear to be reason to recommend changing the not-to-exceed wall temperature of 200°C. This analysis dealt primarily with preclosure effects. Another analysis (CRWMS M&O 1996d) found that the frequency of rock fall and the size of the rocks was not sufficient to result in postclosure problems.

3.4 CLADDING PERFORMANCE CONTRIBUTION TO WASTE CONTAINMENT

Performance of spent fuel cladding is currently a significant uncertainty in the performance assessment of the engineered barrier system and the total repository system of the potential repository. While no specific performance allocation currently applies to the cladding, it is a high performance material that may contribute significantly to waste containment and isolation, including limiting water contact of the SNF. The Waste Package Design Concept Assumptions of the recent CDA (CRWMS M&O 1996f) and the requirements documents [MGDS-RD 3.7.3.3.B.2 (DOE 1994a)] (see Subsection 2.2) limit the spent fuel cladding temperature to less than 350°C to allow/preserve the option for Zircaloy cladding to perform as a barrier to radionuclide release. Nominal cases of previous TSPAs conservatively assumed cladding failure occurred immediately after WP failure. The purpose of this part of the study was to assess the potential impact of cladding on performance. This section presents the results of those efforts.

To assess the contribution of cladding performance to the repository performance, it is necessary to estimate cladding degradation in expected near-field conditions. Then, the estimated cladding failure which determines the spent fuel waste available for release is incorporated into a repository total system performance model. The objectives of this task were two-fold: development of a probabilistic modeling tool to calculate cladding degradation by utilizing the cladding degradation models and data available in the literature; and evaluation of the cladding contribution to the waste isolation in the potential repository. The Repository Integration Program (RIP), a total system performance assessment model, was used to simulate performance of the potential repository.

The data used in this section were not collected under the Program's QA program. Additionally, the process models developed have not been qualified although in many cases the models have been checked against measurements taken. The Repository Integration Program was developed by Golder Associates using their own in-house quality controls but the program has not been qualified under existing Yucca Mountain Program guidelines. Thus, the recommendations developed in this section should be considered as needing to be verified.

3.4.1 Cladding Degradation Models

This section discusses the cladding degradation models included in this study. More complete discussion of cladding degradation modes and their models are given by Rothman (1984), Pescatore et al. (1989), and Pescatore and Cowgill (1994).

3.4.1.1 Creep Rupture

DOE sponsored the development of a cladding creep rupture model by Chin and Gilbert (1989). This model was developed for studying temperature limits of cladding based on various theoretical failure mechanisms. The dominant failure mechanism is void formation and decohesion at grain boundaries. In earlier clad failure analyses for this program Santanam et al. 1992 and McCoy⁷ used the Chin model. Another clad creep model was developed by Peehs and coworkers in Germany (Peehs and Fleish 1986). The German model is an empirical fit of stress versus strain to a single set of experiments and assumes that the clad creeps as a function of stress, temperature, and time. The Peehs model was used in Germany for licensing of spent fuel storage facilities (Peehs and Fleish 1986). In the Peehs model, a conservative value for a strain at which pin failure occurs must be selected (see Subsection 3.4.3.3).

Pescatore and Cowgill (1994) compared the Chin and Peehs models and recommended use of the Peehs model because of a lack of experimental conformation of Chin's work (void formation at crystal boundaries in strain tests has not been observed). Thus, the Peehs model is employed in this analysis. The model is expressed as follows

$$\epsilon = A \left[\frac{B}{T} - \frac{\ln \frac{\sigma}{C}}{\ln(t+1)} - 1 \right]^m \quad (3.4-1)$$

where ϵ = % hoop strain; T = temperature (degrees Kelvin); σ = stress (MPa); t = time (in hours); A = constant, 1.89×10^{-3} ; B = constant, 610 K; C = constant, 450 MPa; and m = constant, -2.58. Although not presented here, it should be noted that the differences in the two models would not produce significant differences in the results.

3.4.1.2 Delayed Hydride Cracking

Another failure mode for the cladding is Delayed Hydride Cracking (DHC). This failure mode has been observed in CANDU zirconium pressure tubes. Hydrides form at the tip of a crack and are brittle. With a sufficiently high stress concentration at the crack tip, the crack will grow. The initial crack growth model was taken from Einziger and Kohli (1984). The crack length is given by:

⁷ Found in Interoffice Memorandum. Subject, *Cladding Degradation*; author, J. Kevin McCoy; correspondence number LV.WPD.JKM.3/95.098.

$$W = 22.1 \left[t \exp \left(\frac{-2.291 \times 10^4}{T} \right) \right]^{\frac{1}{2}} \quad (3.4-2)$$

where W is crack depth (m), t is time (years), and T is temperature (K). The crack depth in a given time is the sum of the crack growth during the previous time steps. The stress is corrected for the crack depth assuming cracks form on both the inside and outside of the clad. The stress concentration factor is calculated using the following equation (R.E. Reed-Hill 1973, p. 800)

$$K = \sigma \sqrt{\frac{W\pi}{2}} \quad (3.4-3)$$

where K is the stress concentration factor ($\text{MPa}\cdot\text{m}^{0.5}$), σ is the stress (MPa), and W is the crack depth (m).

3.4.1.3 Helium Production

Both DHC and strain pin failures are driven by the cladding stress which is driven by the internal gas pressure. The gas pressure will slowly increase over time by the production of helium (He) which is produced in nuclear decay as an alpha particle. Manaktala (1993) gives a curve of helium pressure as a function of time. This curve (adjusted for temperature) was used in this analysis. The curve (in log-log space) was fit by two linear equations, one for below 9,000 years and one for above that time. The He partial pressure is added to the fission gas pressure at each time step and a new stress is calculated. However, results indicate that incorporation of the He gas produced does not affect the pin failure rates because the clad is sufficiently cool by the time any significant amount of He is produced.

3.4.1.4 Cladding Unzipping

If both the cladding and WP fail, the inert gas inside the WP and cladding is replaced with the near-field environment, and oxygen is introduced into the spent fuel. In the oxidizing conditions, UO_2 phase in the spent fuel matrix can oxidize to U_3O_8 phase, which accompanies substantial increases in the spent fuel matrix volume. The oxidation reaction is a temperature-driven process, and the temperature dependence of the reaction rate can be described with the Arrhenius law (i.e., an exponential temperature-dependence relationship) (Einziger 1994). A small gap (about 0.1 - 0.3 mm) is present between the spent fuel pellet and the clad. The volume increase of the spent fuel matrix produces stress on the clad, and above a threshold level, the stress can tear off the clad, thus resulting in a gross rupture of the clad and complete exposure of the spent fuel. The model developed by Einziger (1994) was used for clad unzipping calculation. The cladding unzips in two phases, an incubation phase and an unzipping phase. In the incubation phase, the oxidized spent fuel phase (U_3O_8) builds up just inside the perforation until tearing starts. Einziger describes this incubation time with the following equation:

$$t_i = 9.8 \times 10^{-21} \exp \left(\frac{47,400}{RT} \right) \quad (3.4-4)$$

where t_i is the incubation time (years) relative to the failure time of WP container, R is the universal gas constant (1.987 cal/mol·K), and T is temperature (K). The time required to unzip the cladding is given by

$$t_{uz} = 8.66 \times 10^{-8} \exp\left(\frac{18,400}{RT}\right) \quad (3.4-5)$$

where t_{uz} is the unzip time (years) relative to the incubation time (t_i). The unzip time is based on the assumption that the initial clad penetration is in the center of the pin and the length of the pin is 386 cm (Westinghouse 17 x 17 assembly).

3.4.1.5 Zircaloy Dry Oxidation

For pins that are in failed WPs, Zircaloy oxidation was modeled using the equations developed by Einziger (1994). The oxidation has two effects, thinning of the clad and as a potential failure mechanism itself. The thinning increases the stress and has a very small effect on strain failure. The second effect is direct clad failure but no pins were observed to fail directly by oxidizing through the clad. This is consistent with earlier analysis that showed that this mechanism is about four orders of magnitude slower than clad unzipping and requires 10,000 years above 250°C to fail the clad by this mechanism⁸.

3.4.2 WP Degradation

The models for the cladding degradation modes incorporated in this study are based on the processes driven by temperature. Creep rupture and delayed hydride cracking are operative at all times until the cladding fails, and the resulting failure is in a form of small cracks or punctures (i.e., the degradation processes stop when the cladding fails, with the release of stresses). Zircaloy oxidation and cladding unzipping, which result in a gross cladding rupture, are operative once the WP fails and the inert environment inside the WP is replaced with the near-field environment. A protection against the gross failure of cladding and gross exposure of spent fuel inside the cladding is provided by the WP. Thus, the incorporation of the WP failure into the cladding degradation analysis is needed to estimate the amount of spent fuel that is exposed to the near-field environment.

3.4.2.1 WP Degradation Simulation

The stochastic WP degradation simulation model that was developed for TSPA-1995 was employed to calculate WP degradation. Details of the simulation model are discussed in the TSPA-1995 report (CRWMS M&O 1995c) and recent papers (Lee et al. 1996a and 1996b). The major assumptions made in the stochastic WP simulation are summarized below.

- A. General humid-air and pitting corrosion of the carbon steel outer barrier initiate at a threshold RH that is uniformly distributed between 65 and 75 percent. This threshold is independently chosen for each WP. This assumption is based on numerous data found in literature (see Haynie et al. 1978; Phipps and Rice 1979; Vernon 1933).

⁸ Found in Interoffice Memorandum. Subject, *Cladding Degradation*; author, J. Kevin McCoy; correspondence number LV.WPD.JKM.3/95.098.

- B. General aqueous and pitting corrosion of the carbon steel outer barrier initiate at a threshold RH which is uniformly distributed between 85 and 95 percent. Visual observations, indicating that steel coupon surfaces become covered with a thin film of water at about 85 percent RH in a controlled environment chamber, have been reported (Haynie et al. 1978).
- C. For each WP, complete and positive correlation of the humid-air corrosion initiation threshold and the transition threshold from humid-air corrosion to aqueous corrosion is assumed. That is, if humid-air corrosion initiates at 65 percent RH, aqueous corrosion initiates at 85 percent RH.
- D. Corrosion-allowance outer barrier material (carbon steel) is subjected to general and pitting corrosion both in humid-air and aqueous conditions. The uncertainties in the humid-air and aqueous general corrosion models were utilized to account for pit to pit variability and WP to WP variability. In the postclosure repository, about 10,000 WPs will be spread over the repository area, and a local corrosion environment in one part of the repository may be different from that in another part. This variability of the local corrosion environment is referred to as WP to WP variability. Also, since a waste container has a relatively large surface area (37.26 m^2), the general corrosion rate on one part of the WP may be different from that on another part of the WP. This variability in corrosion rate on a WP is referred to as pit to pit variability. Because information on the degree of the variability among WPs and among pits is not available currently, the variabilities are accounted for in TSPA-1995 (CRWMS M&O 1995c) by equally splitting the uncertainties in the humid-air and aqueous general corrosion models into the variability among WPs and the variability among pits.
- E. Corrosion resistant inner barrier material (Alloy 825) is subjected to aqueous pitting corrosion only (not to general corrosion). The time-independent pit growth rate distributions were utilized to represent pit to pit variability and WP to WP variability. The same reasoning given in item D. is applied also to account for the variability among WPs and among pits.
- F. When pits reach the inner barrier through the outer barrier, aqueous conditions are assumed. This assumption is based on the observations that the capillary condensation of moisture by gel-like porous corrosion products of the outer barrier covering the inner barrier surface (Vernon 1933), and the hygroscopic nature of many corrosion products (Fyfe 1994; Haynie et al. 1978), would provide an aqueous corrosion condition at the surface of the inner barrier.
- G. Pits form uniformly over the entire waste container surface. It is known that pits are most stable when growing in the direction of gravity because the dense, concentrated solution within a pit is necessary for its continuing activity (Fontana 1986, pp. 64-69). Elongation of pits growing in the direction of gravity has been observed (Ruijini et al. 1989). However, there is an uncertainty regarding crevice corrosion at the bottom of the waste container contacting the invert. Additionally, over the containment and isolation periods, rock may fall on the waste container or backfill may be introduced. In these cases, there may be crevice corrosion occurring at the contact points between the rocks and waste

container surface. Because of the uncertainty of the possibility of crevice corrosion at the side and bottom of waste containers, we assumed that pits form uniformly over the entire waste container surface.

- H. All pits have a uniform area of 1 mm^2 which corresponds to a pit radius of 0.56 mm. This may be large for the pits forming in Alloy 825, which tend to be much narrower (Szklańska-Smiałowska 1986, pp. 127-141) but will provide a conservative assumption.
- I. The waste container surface has a pit density of 10 pits/cm² (Marsh and Taylor 1988; Marsh et al. 1988; Strutt et al. 1985), and the same pit density is assumed for the inner barrier.
- J. Taking the pit density (10 pits/cm²), the uniform pit area (1 mm^2), and the nominal surface area (37.26 m^2) of the waste container for a typical large WP, the total number of pits that can form on the waste container is about 4 million. This corresponds to about 10 percent of the total surface area.
- K. All of the pits on a WP start to grow at the same time that the threshold humidity discussed in items A. and B. is reached. That is, pit initiation is not explicitly considered in TSPA-1995.
- L. The WP is assumed to maintain its structural integrity over the simulation period; that is, potential impact of the pitting of a WP on the mechanical stability is not considered. Also, potential effect of rock falling on the WP and damage caused by that are not considered.
- M. This analysis did not consider cathodic protection which could potentially reduce releases.
- N. Microbial enhanced corrosion was not considered.

3.4.2.2 Base Case

The base case in this study is the case with high thermal loading of 20.5 kgU/m^2 (83 MTU/acre), no backfill, and a high infiltration rate of 0.3 mm/yr. The 10,000-year and 100,000-year temperature and RH histories at the WP surface for the base case are shown in Figures 3.4-1a and 3.4-1c, respectively. The 10,000-year temperature and RH histories were calculated using a drift-scale thermo-hydrologic model (CRWMS M&O 1995c), and those from 10,000 years to 100,000 years (shown in Figure 3.4-1b) were approximated by extrapolating the 10,000-year data, assuming it reduces to an ambient temperature at 100,000 years. The WP surface temperature reaches a maximum of approximately 170°C , it reduces to 100°C at 2,000 years, and to about 50°C at 10,000 years (Figure 3.4-1a). As shown in Figure 3.4-1c, the RH increases as the temperature decreases, reaching about 88 percent at 2,000 years and 92 percent at 2,500 years before it essentially levels off with a subsequent slow increase toward an ambient RH (about 98 percent).

Figure 3.4-1a. 10,000-year temperature history of the WP surface for the case of 20.5 kg U/m² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)

Figure 3.4-1b. 100,000-year temperature history of the WP surface for the case of 20.5 kg U/m² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)

Figure 3.4-1c. 10,000-year relative humidity history of the WP surface for the case of 20.5 kg U/m² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)

The cumulative fraction of WPs that fail as a function of time is given in Figure 3.4-2. WP failure is defined as having at least one pit penetration through the container wall. As shown in the figure, WPs begin to fail at about 2,200 years, and the number of WPs that fail increases rapidly before it levels off at about 6,000 years with about 90 percent cumulative fraction of WPs that fail. The cumulative fraction reaches about 95 percent at 100,000 years. Pitting histories of 25 representative WPs are shown in Figure 3.4-3.

Shown in Figure 3.4-4 is the abstraction of WP failures and pitting histories for the RIP implementation.

3.4.2.3 Repository Edge Effect

This section describes approximation of the temperature and relative humidity of the WP surface in the repository edge regions which include about one-sixth of the WP inventory. The simulation results for the WP degradation in the repository edge are discussed.

Temperature and Relative Humidity Approximation. It is generally agreed that for a given thermal loading of SNF, WPs placed at the edge of the repository would experience different near-field environments than those placed in the interior. It is expected that for the case with the reference repository thermal loading of 20.5 kgU/m², WPs at the repository edge would be exposed to the near-field conditions with lower temperatures and higher humidities than those in the interior. A recent study result, although preliminary, conducted as part of TSPA-1995, indicated that the temperature and relative humidity conditions at the WP surface in the edge regions of the repository, with

Figure 3.4-2. Cumulative fraction of WPs that failed for the case of 20.5 kg U/m² (83 MTU/acre) thermal loading, no backfill, and high infiltration rate (0.3 mm/yr)

Figure 3.4-3. Representative pitting histories for 25 WPs for the case of 20.5 kg U/m² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)

Figure 3.4-4. Abstractions for the RIP implementation for the case of 20.5 kg U/m² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)

20.5 kgU/m² thermal loading, are likely to be more representative of interior WPs in a 14.3 kgU/m² (58 MTU/acre) thermal loading (CRWMS M&O 1995c, p. 4-12).

Accordingly, in this study, the temperature and RH histories at the WP surface in the repository edge regions were assumed to be those produced by a loading of 14.3 kgU/m² (58 MTU/acre). The temperature and RH histories were approximated using those available for two thermal loadings of 6.2 and 20.5 kgU/m² (25 and 83 MTU/acre) and by linearly interpolating the values for the two thermal loadings to predict the response for a 14.3 kgU/m² thermal loading. It is assumed that the amount of error introduced with this approximation is acceptable. Approximation (or linear interpolation) of the 10,000-year temperature histories at the WP surface in the repository edge region for the 20.5 kgU/m² thermal loading, is shown in Figure 3.4-5, along with those for WPs in the repository interior for the 6.2 and 20.5 kgU/m² thermal loadings. The WP surface temperature in the repository edge decreases to 100°C at about 400 years, compared to about 2,000 years for the WPs in the interior. At that time, RH at the WP surface is about 74 percent (see discussion with Figure 3.4-6). The temperature histories for 6.2 and 20.5 kgU/m² from 10,000 years to 100,000 years were extrapolated assuming the WP surface temperature cools down to the ambient temperature, and the temperature history for the repository edge effect (i.e., 14.3 kgU/m² thermal loading) was approximated as for the 10,000-year history (see Figure 3.4-5). The RH history approximation at the WP surface in the repository edge region is shown in Figure 3.4-6, along with those for WPs in the repository interior for the 6.2 and 20.5 kgU/m² thermal loadings. The 10,000-year RH history for the two thermal loading cases (6.2 and 20.5 kgU/m²) are calculated results from TSPA-1995. Because the WP surface RH reaches the ambient value (about 98 percent RH) at 10,000 years, the same value was used beyond 10,000 years.

Figure 3.4-5. Approximation of the WP surface temperature in the repository edge for the case of 20.5 kg U/m² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)

Figure 3.4-6. Approximation of the WP surface relative humidity in the repository edge for the case of 20.5 kg U/m² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)

WP Degradation Simulation. Figure 3.4-7 shows cumulative fraction (as a function of time) of WPs that fail in the repository edge conditions for the base case, 20.5 kgU/m² thermal loading, along with that of WPs in the repository interior. WPs in the repository edge begin to fail at about 900 years, about 1,000 years earlier than the WPs in the interior. However, the failure rate of the WPs in the edge are slower than those in the interior. The cumulative fraction of WPs that fail in the edge at 10,000 years is about 75 percent, compared to about 95 percent for the WPs in the interior, and that of WPs in the edge at 100,000 years is about 81 percent, compared to about 96 percent of WPs in the interior.

The earlier initiation of WP failure in the repository edge than in the interior can be mostly attributed to the more humid and "warm" near-field condition in the edge. As previously shown in Figures 3.4-5 and 3.4-6, the WP surface temperature in the edge reduces to 100°C at about 400 years, and the RH at that time is about 74 percent at which point the carbon steel outer barrier undergoes humid-air corrosion. For WPs in the interior, the surface temperature reduces to 100°C at about 2,000 years and the RH at that time is above 85 percent, which is in the threshold humidity range for aqueous corrosion (see the WP degradation simulation assumptions in Subsection 3.4.2.1). The aqueous corrosion rate of carbon steel is higher than the humid-air corrosion rate. Thus, the lower WP failure rate at the edge over that in the interior is mostly due to a long duration (about 1,000 years after the initiation of humid-air corrosion starting at about 400 years) of humid-air corrosion of the carbon steel outer barrier in the edge, and resulting low pit penetration rates in the outer barrier. Thus, when pits reach the inner barrier, temperature is well below 100°C for the WPs at the edge which results in a slower inner barrier pitting rate than would be the case for the WPs in the interior. Pitting histories for 25 representative WPs are given in Figure 3.4-8. Abstractions for WP failure and pitting histories for RIP implementation are shown in Figure 3.4-9.

3.4.3 Probabilistic Cladding Failure Calculation

This section describes the probabilistic cladding degradation model that was developed by incorporating the individual cladding degradation models discussed in the section above. The probabilistic model incorporates the spacial (within the WP) and temporal distribution of temperature and the WP failure distribution. The model calculation results for the cladding degradation in the WPs in the repository interior (base case) and for the cladding in the WPs in the repository edge, are presented. The calculation results are implemented into a total system performance model to assess the contribution of cladding performance to the repository performance. This is discussed in Subsection 3.4.5.

3.4.3.1 Probabilistic Cladding Degradation Model

A Monte Carlo model was developed to estimate the fraction of spent fuel that is exposed to the near-field environments. The model analyzes the performance of a single pin as a function of time and calculates the time that the pin becomes perforated, and the time that the perforated clad unzips. The pin properties, initial conditions, and performance correlations are assumed to be described using log normal distributions. This analysis is repeated thousands of times and the statistics are collected. A log normal distribution was deemed appropriate to use since most, if not all, reactor probabilistic risk assessments use a log normal distribution for failure rates of components and initiating event frequencies when calculating uncertainties in sequences.

Figure 3.4-7. Comparison of cumulative fraction of WPs that failed in the repository edge with the fraction in the repository interior for the case of 20.5 kg U/m² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)

Figure 3.4-8. Representative pitting histories for 25 WPs in the repository edge for the case of 20.5 kg U/m² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)

Figure 3.4-9. Abstractions for the RIP implementation for the WPs in the repository edge for the case of 20.5 kg U/m² (83 MTU/acre) thermal loading, no backfill and high infiltration rate (0.3 mm/yr)

The SAMPLE computer code (NRC 1975) is used to sample the input parameters and keep track of the statistics. This code was developed and listed in the WASH-1400 study (NRC 1975), the first reactor Probabilistic Risk Assessment in the U.S. The user supplies a subroutine to the code which models the specific event (in this case, a model for the behavior of a single clad fuel pin) that is to be sampled.

The base case analysis is for the cladding in a WP containing 21 PWR spent fuel assemblies placed in the potential repository with a thermal loading of 20.5 kgU/m² (83 MTU/acre), no backfill, and high infiltration rate. Additional cases address the effect of other WPs or repository designs with an elevated clad temperature. The following paragraphs describe the various components of the analysis.

3.4.3.2 Incorporation of Cladding Temperature Distribution

Radial distribution across the WP and temporal distribution of clad temperatures were taken from a detailed analysis conducted by the Waste Package Development Department⁹. These temperatures are for a 10-year-old spent fuel. This fuel is hotter than an average fuel to be disposed in the repository and therefore is conservative in terms of the clad temperature distribution. Figure 3.4-10 shows the temperature history for the center pin for the base case. Bahney¹⁰ calculated the

⁹ Found in Interoffice Memorandum. Subject, *Thermal Calculations in Support of the Thermal Loading Study*; Author, Robert. H. Bahney III; LV.WP.RHB.12/95-392, Las Vegas, Nevada.

¹⁰ Ibid

Figure 3.4-10. The temperature history of the center pin in a WP for the base case of 20.5 kg U/m² thermal loading, no backfill and high infiltration rate (0.3 mm/yr)

temperatures for the first 1,000 years. The temperatures after that time were estimated using a time dependent heat source and preserving the thermal emissivity (radiant cooling from the WP to drift wall). The clad temperature peaks at 0.8 years and then slowly decreases. Figure 3.4-11 gives the radial temperature distribution across the WP at 0.8 years.

Bahney's temperature calculations shown in Figure 3.4-10 are peak pin temperatures (95 percent quantile). To provide a very conservative estimate of pin failure these values were used in the analysis discussed below as an artificial average temperature. In the Monte Carlo analysis, the temperature of an individual pin is sampled by assuming that the initial center pin temperature is log normally distributed about this average temperature. The error factor (EF) is the ratio of the median to 95 percent quantile. For this analysis an error factor of 1.4 was used. For the base case, the center pin could be as hot as 386°C (95 percent quantile) in the very conservative calculations. This temperature exceeds the CDA Document (CRWMS M&O 1996f) requirement for the cladding thermal goal, which specifies that no clad temperature will exceed 350°C (CRWMS M&O 1995a).

After sampling the center pin temperature in the WP, the radial position and temperature of the pin to be analyzed is sampled using the curve shape given in Figure 3.4-11. It is important to note that the population of pins in any radial zone increases as the square of the radius and significantly more pins are located in the cooler outer zones than the hotter inner zones.

Shown in Figure 3.4-12 is the distribution of peak cladding temperatures at two different initial center pin temperatures (i.e., 276°C and 325°C). The current probabilistic cladding temperature distribution calculations show that with the initial center pin temperature of 276°C, about 10 percent of the pins exceed the cladding thermal goal temperature (350°C) and, about 10 percent have their peak temperature below 200°C. With 50°C higher initial center pin temperature (i.e., 325°C), about

Figure 3.4-11. Radial distribution of pin temperature across WP at 0.8 years. Radial Index 1 is the center and 13 is the outer-most edge of the WP

Figure 3.4-12. Distribution of peak cladding temperatures with the initial center pin temperature of 276 or 325°C

30 percent of the pins exceed the cladding thermal goal, providing a condition that may cause potentially significant damages to the cladding durability (see discussion below which addresses this issue).

3.4.3.3 Cladding Creep Rupture Failure Calculation

Clad Strain Calculation. Clad strain is calculated with Peehs' model (equation 3.4-1). The median pin stress at room temperature (σ) is specified by the user. For this analysis, the average stress of 32 MPa for a Westinghouse 17 x 17 assembly (Pescatore and Cowgill 1994) was used. An EF of 2.0 was used to include the maximum values given by Pescatore. A log normal distribution was assumed. The stress at any time is calculated using the ideal gas law and the current temperature. In addition, the stress is reduced by including additional free volume inside the clad from the strain. This effect was incorporated in the earlier analysis by Rosen and O'Connell (1995). This volume adjustment appears to reduce the stress by less than 10 percent in this analysis.

The probabilistic model used in this analysis assumes that the expected values of strain are log normal distributed with the median value from Peehs' correlation and an EF of 3.0. The 95 percent quantile strain is three times larger than the median Peehs' correlation. An error factor of 3 is commonly used in nuclear Probabilistic Risk Assessments for component reliabilities (NRC 1983).

Creep Rupture Failure Limit. At a conservative strain of 1 percent, the cladding is assumed to fail by developing a perforation, relieving the internal pressure and stress. Pescatore and Cowgill (1994) collected the stress-rupture data for irradiated Zircalloys and the median value is 1 percent. If a single high value of 11 percent strain is dropped, the mean value is also 1 percent. Thus, the 1 percent strain failure criteria is assumed to be a median value for the failure strain and an EF of 2.0 was used. The smaller error factor was selected to ensure that 95 percent quantile for failure was 2 percent cladding strain, or higher strains without failure were unlikely.

Figure 3.4-13 gives the percent of pins that are expected to fail in a WP of various initial center pin temperatures using the Peehs correlation. The shape of this curve is partially determined by the error factors. Figure 3.4-14 gives the failure fractions if the error factors are halved. The smaller error factors produce a distribution with a higher slope, closer to a step function. Figure 3.4-15 compares pin failure fractions using the Peehs and Chin models in this statistical analysis. Over most initial temperatures, Chin's model would predict a slightly higher clad perforation fraction but the two models are in reasonable agreement.

In addition to clad failure from stress, it is also conservatively assumed that 1 percent (EF = 2) of the pins are initially failed when placed in the WP. Although it was suggested that much less than 0.1 percent of all fuel that will be accepted will be failed (Rothman 1984), the conservative value for pre-failed cladding was used because additional pins might fail during interim dry storage and because about 0.7 percent of the fuel has stainless steel cladding that might fail earlier than the Zircaloy cladding.

Figure 3.4-13. Estimated pin failures at different initial center pin temperatures using the Peehs model

Figure 3.4-14. The effect of reduced EFs on the pin failure estimation using the Peehs model

Figure 3.4-15. Comparison of the cladding failure estimations at different initial center cladding temperatures using the Peehs model and Chin model

3.4.3.4 Delayed Hydride Cracking

Failure by DHC is calculated with equations 3.4-2 and 3.4-3. The stress concentration factor at the crack tip calculated with equation 3.4-3 is compared with a critical stress concentration factor of $10 \text{ MPa}\cdot\text{m}^{0.5}$ (Pescatore et al. 1989) and if it is exceeded, the crack is expected to grow quickly and the pin is assumed to fail by DHC. In the studies to date, less than 0.1 percent of the pins fail by this mechanism and these are in the higher temperature cases. Although the time period being considered is longer than considered in earlier studies, these results are consistent with the analysis and discussions of DHC presented by Rothman (1984) and Pescatore et al. (1989).

F. H. Huang (1995) summarizes the hydride data and shows that the critical stress concentration is almost independent of hydrogen concentration for ranges of 50 to 320 ppm. He also shows that most data shows critical stress concentrations above $20 \text{ MPa}\cdot\text{m}^{0.5}$ so the use of $10 \text{ MPa}\cdot\text{m}^{0.5}$ is quite conservative.

Hydride reorientation was not considered in this analysis. During irradiation, the hydride precipitation is in the circumferential orientation. In one dry storage test, reorientation to the radial direction was observed (Einziger and Kohli 1984). This occurred in a pin that had very high stresses (145 MPa at 323°C). Reorientation was not observed in pins with lower stresses (13 to 26 MPa).

3.4.3.5 Cladding Unzipping

Fraction of unzipped (or grossly ruptured) clad in a failed WP is estimated in the probabilistic model utilizing equations 3.4-4 and 3.4-5. As with other aspects of this analysis, the unzipping times calculated with equation 3.4-5 are assumed to represent median times which are log normal distributed with an EF of 3.0. Table 3.4-1 gives the incubation times and unzip times at various temperatures.

Table 3.4-1. Clad Unzipping Times for Various Temperatures

Temperature (°C)	Incubation Time (Years)	Unzipping Time (Years)
25	5.7E+14	2.7E+6
50	1.2E+12	2.4E+5
100	5.8E+7	5,200
150	3.0E+4	280
200	78	28
250	0.63	4.2
300	0.011	0.9
350	4.2E-4	0.25

Assuming that all the pins are perforated at the time of the WP failure, Figure 3.4-16 gives the fraction of pins that are expected to completely unzip for various WP breach (or oxygen ingress) times. Two different initial center pin temperatures were modeled. The results show that if oxygen ingress can be prevented for over 1,000 years, only a small fraction of the failed (or perforated) pins are expected to unzip.

Figure 3.4-16. Fraction of unzipped cladding as a function of WP failure times at two initial center pin temperatures

3.4.3.6 Incorporation of WP Failure Distribution

The clad failures from creep rupture and DHC generally produce small clad perforations and expose very small areas of the spent fuel inside the failed clad to the near-field environment. If and when the WP is breached, oxygen is introduced, and the UO_2 phase in the spent fuel, if temperature is high enough, can undergo oxidation to U_3O_8 phase with the resultant volume expansion. Under this oxidation process, the fuel pins can have their clad torn open (unzipped). Thus, the timing of the WP failure (or temperature at the time of WP failure) is important in determining the amount of spent fuel exposed.

A WP failure distribution was based on TSPA-1995 (CRWMS M&O 1995b) with minor modifications. The WP failure distribution included in this analysis is for the case with a thermal loading of 20.5 kgU/m^2 (83 MTU/acre), no backfill, and high infiltration rate (0.3 mm/yr). In this case, WPs had a median breach time of 3,600 years and a range from 2,200 to 1 million years (representing no failure for some WPs).

For this analysis, WP failure at time zero was given a probability of 1×10^{-3} . This fraction was to conservatively represent operator errors in loading and handling WPs. The remaining WPs were assumed to fail with a log normal distribution with a median of 3,600 years, based on the TSPA-1995 results (CRWMS M&O 1995c) and an EF of 3.0. The EF was selected to give a failure fraction of 2.5 percent for the WP in 1,000 years. The design goal for the WP is to have less than 1 percent failure in 1,000 years. The distribution used in this analysis was selected to be conservative and to have a slightly larger fraction in that time. This will provide conservatism for cladding failure predictions since earlier WP failures will subject the cladding to higher temperatures and thus slightly higher fractions of cladding will unzip (see below).

Two cases have been analyzed. The base case used an initial (time = 0) median temperature of 276°C for the pin in the center of the WP. This lower temperature case represents the best estimate temperatures¹¹ and peaks at 291°C . The second and higher temperature case (center pin initial, median temperature of 325°C) could represent a different WP or repository design. In this case, the center pin temperature peaks at 344°C (median value). To assess the effect of the WP failure initiation time, additional cases were analyzed where no WP failures occurred before 2,200 years, the time of the first WP failure in TSPA-1995. In this case the failure distribution is the same just shifted to the right. The results are summarized in Table 3.4-2. In the analyses, the WP failure distribution and pin temperatures were considered independent variables. The fraction of clad unzipped for the base case is 0.5 percent, and it is reduced to 0.4 percent for the case with no waste package failure before 2,200 years. The earlier WP failure initiation does not contribute significantly to the unzipping.

¹¹ Found in Interoffice Memorandum. Subject, *Thermal Analysis to Support Thermal Loading System*; author, Robert H. Bahney, III; correspondence number LV.WP. RHB. 06/96-137.

Table 3.4-2. Effect of WP Failure Distribution on Clad Unzipping

Initial Center Pin Temperature (°C)	Percent Pins Unzipped	
	WP Failure (Base Case)	WP Failure (no WP failure before 2,200 yrs)
276	0.50	0.40
325	3.90	3.20

Also shown in Table 3.4-2 are the results for the case with the higher initial center pin temperature (325°C). This case may represent a hotter near-field environment that can be driven from a higher repository thermal loading, and/or use of materials with a lower thermal conductivity than the base case. The hotter condition may provide a drier environment in the proximity of the WPs, delay the onset of corrosion, and potentially delay WP failure initiation. In the analysis, there was no correction made for delay of corrosion. With the hotter cladding temperature, the fraction of clad unzipped increased from 0.5 percent to 3.9 percent. Again, the unzipped fraction is not affected much (reduced to 3.2 percent) with no WP failure before 2,200 years.

3.4.3.7 Cladding Model Results for Base Case for RIP Implementation

One of the objectives of this study is to assess the contribution of cladding performance to the waste isolation in the potential repository. The RIP was used for the TSPA. In the RIP simulation, WPs are binned into six groups according to their failure distribution in time (CRWMS M&O 1995c) (also see Figure 3.4-4). The probabilistic cladding degradation model developed for this study was used to calculate the fraction of unzipped clad in each WP group.

The base case in this study is the case with a high thermal loading of 20.5 kgU/m² (83 MTU/acre), no backfill, and high infiltration rate, and for the WPs in the repository interior. For each WP group, a separate median WP failure time and EF were developed. The results are shown in Table 3.4-3. The WP failure times vary from 2,400 years to 7,260 years. For each group, the fraction of pins that unzipped was calculated. The unzipped fraction ranges from 0.62 percent to 0.17 percent.

Table 3.4-3. Cladding Degradation Model Results for RIP Implementation for WP Groups in the Repository Interior for the Case of 83 MTU/acre, No Backfill, and High Infiltration

WP Group	Median WP Failure Time (Years)	Cladding Pins Unzipped (%)
1	2,400	0.62
2	2,890	0.56
3	3,300	0.52
4	3,760	0.44
5	4,290	0.38
6	7,260	0.17

3.4.3.8 Cladding Model Results for Repository Edge Effect for RIP Implementation

As in the case for the degradation calculation for the claddings in the WPs in the repository interior, the WPs were binned into six groups based on their failure times as shown in Figure 3.4-9. The results given in Table 3.4-4 show a lower cladding unzipping fraction than for the base case (i.e., WPs in the repository interior). The WPs at the edge of the repository operate at a lower temperature; this produces two conflicting effects with respect to cladding integrity. The lower temperatures produce earlier WP failures because of earlier contact with water. This would cause an early exposure of perforated fuel pins to oxygen and permits more cladding unzipping. The positive effect of the lower temperatures is lower strains and slower clad unzipping rates that decrease the amount of exposed fuel. Current clad modeling suggests that the positive effects of lower temperatures on clad degradation can somewhat offset the negative effects on the source term in terms of exposed fuel for the WPs at the repository edge. It should be noted, however, that microbial enhanced corrosion was not considered in this analysis and this could enhance releases in the edges if it proves to be important.

A concern has been raised that the more humid environment might also affect the corrosion of zircaloy. Of course zircaloy cladding was designed to operate in water. Rothman 1984, summarizes the experiments performed on zircaloy. He reports that the zircaloy oxidation rate is strongly dependent on temperature but the rate was constant for experiments performed in water, steam, or air (at the same temperature). Experimenters also report that the oxidation rate appears to be constant for aerated, de-aerated and de-ionized water experiments (at the same temperature). The oxidation rate appears to be independent of pH for a range of 1 to 12. In separate publication, C. Hansson (1984), reports no corrosion rate increase in cement pore solutions of a pH of 12.0 to 13.8. This information indicates that the corrosion should be relatively insensitive to the conditions in the edge of the repository and corrosion in general of zircaloy is so slow that it was not a factor in this analysis.

Table 3.4-4. Cladding Degradation Model Results for RIP Implementation for WP Groups in the Repository Edge for the Case of 83 MTU/acre, No Backfill, and High Infiltration

WP Group	Median WP Failure Time (Years)	Cladding Pins Unzipped (%)
1	1,560	0.25
2	2,040	0.25
3	2,660	0.25
4	3,140	0.21
5	4,180	0.17
6	8,300	0.06

3.4.3.9 Cladding Model Results for Higher Initial Cladding Temperature

One of the objectives of this task is to examine the thermal goal for the cladding temperature of 350°C. As discussed previously (see Figure 3.4-12), with the initial center cladding temperature of 276°C (base case), about 10 percent of the claddings exceed the cladding thermal goal temperature (350°C), and with 50°C higher initial center pin temperature (i.e., 325°C), about 30 percent of the claddings exceed the cladding thermal goal. This higher fraction of the claddings exceeding the thermal goal temperature would cause a greater number of claddings to fail and increase the fraction of the failed claddings that undergo a gross rupture. The impacts of the higher initial center clad temperature on the repository performance (or the cladding performance contribution to the repository performance) were studied (see Subsection 3.4.4.6). For the RIP implementation, the fraction of unzipped (or grossly ruptured) claddings for each WP group was calculated. A number of different near-field condition scenarios and different WP failure distributions may be associated with the higher cladding temperature. However, since any modeling results for the near-field conditions and WP failure distributions for such scenarios were not available, the same WP failure distribution as in the base case (Subsection 3.4.3.7) was used in the cladding degradation calculation. The calculated cladding unzipped fractions for each WP group are given in Table 3.4-5. Compared to the base case (Table 3.3-3), about 10-times increase in the unzipped cladding fraction is estimated.

Table 3.4-5. Cladding Degradation Model Results for RIP Implementation for WP Groups in the Repository Interior with Higher Initial Center Cladding Temperature (325°C) for the Case of 83 MTU/acre, No Backfill, and High Infiltration

WP Group	Median WP Failure Time (Years)	Cladding Pins Unzipped (%)
1	2,400	4.83
2	2,890	4.50
3	3,300	4.25
4	3,760	3.65
5	4,290	3.02
6	7,260	1.21

3.4.3.10 Summary of Probabilistic Cladding Degradation Model Results

A Monte Carlo model was developed to estimate the fraction of spent fuel that is exposed to the near-field environment as a function of time. The model analyzes the behavior of a fixed number of pins by following their behavior as a function of time. The modeling approach, major assumptions, and parameters for the model are listed below.

- A. The pin properties and initial conditions are assumed to be described using log normal distributions with an uncertainty.
- B. The stress on cladding is modified from temperature, He-gas production, clad oxidation, and fuel cladding dimensional (strain) changes.

- C. The Zircaloy stress/strain relationship used is from Peehs et al. (1986).
- D. Clad puncture is conservatively assumed to occur at 1 percent strain.
- E. Delayed hydride cracking is included.
- F. WP failure distribution is incorporated.
- G. Pre-existing (or premature failure) for both cladding and WPs occurs with a specified frequency.
- H. Clad tearing (or unzipping) model used is from Einziger (1994).

The base case for the cladding analysis is for a WP containing 21 PWR assemblies (assuming Westinghouse 17 x 17 class) at a thermal loading of 20.5 kgU/m², no backfill, and high infiltration rate (0.3 mm/yr). The base case represents the most probable or best estimate of the sequence of events. Table 3.4-6 summarizes the input parameters.

Table 3.4-6. Input Summary for Clad Degradation Analysis

Variable	Source or Median* Value	Error Factor
Sample size	5,200	NA
Initial center pin temperature	276°C (base)	1.4
Clad hoop stress (room temp.)	32 MPa	2.0
Initial clad failure (Time = 0)	1%	2.0
Strain	(Peehs 1986)	3.0
Strain failure limit	1%	2.0
Crack velocity	(Einziger 1984)	2.0
Critical stress intensity factor	10 MPa m ^{0.5}	1.67
Initial zircaloy oxide thickness	1.2E-3 cm	1.5
Zircaloy oxidation rate	(Einziger 1994)	2.0
Clad zip times	(Einziger 1994)	3.0
WP failure due to defects	0.1% at 0 yrs	1.4

* Variables assumed log normal distributed, Error Factor = 95% quantile divided by the median

The cladding analysis results of the base case (initial center pin temperature = 276°C) and a case with a higher cladding temperature (initial center pin temperature = 325°C) are summarized in Table 3.4-7. The same WP failure distribution is assumed for the two cases. The higher cladding temperature case might reflect the effects of different repository designs such as a higher thermal loading. In any of the two cases, most of the clad failures (in the form of puncture) come in a very early emplacement period (i.e., median failure time less than 2 years). With an increase in the cladding temperature by 50°C, the fraction of clads that puncture increases from 6 percent to 19

percent, and the unzipping fraction from 0.5 percent to 3.9 percent. These analyses based on the current cladding models indicate a sensitive dependence of cladding performance to temperature.

These calculations are intentionally conservative. The early (or premature) clad and WP failure fractions are high. A higher fraction of WP (than specified in the CDA Document (CRWMS M&O 1996f)) are assumed to fail in the first 1,000 years. The clad temperatures are based on 10-year-old fuel, younger than the expected average fuel. These and other conservative assumptions biases the results toward higher clad failure fractions than might be expected.

Spent fuel fractions with a gross exposure (i.e., fractions of pins unzipped) of less than 5 percent are currently predicted.

Table 3.4-7. Summary of Cladding Degradation Analysis Results

	Base Case (Init. Center Pin Temp = 276°C)		Case with Higher Clad Temp (Init. Center Pin Temp = 325°C)	
	Clad Failed (%)	Median Time (Years)	Clad Failed (%)	Median Time (Years)
Punctured Clad	6	1.5	19	0.8
WP Failure	2.5 50.0	(before 990 yrs) 3,563	2.5 50.0	(before 990 yrs) 3,563
DHC Failure	0.00	---	< 0.1	---
Unzipped Clad	0.5	3,020	3.9	3,700
Partially Unzipped Clad	0.00	---	0.00	---

Caveat in the Probabilistic Cladding Degradation Analysis. As discussed in the previous sections, the probabilistic cladding degradation analyses based on the current cladding degradation models indicate that relatively small fractions of clad undergo unzipping failures that result in a gross exposure of the spent fuel inside the failed claddings. There are several cautions that need to be considered in using the current analysis results. The cladding degradation models (e.g., creep rupture, delayed hydride cracking, zircaloy dry oxidation and cladding unzipping) used in the probabilistic analyses were developed for an interim dry storage of spent fuel, and the driving force of cladding degradation in the models is temperature. In other words, the cladding degradation models are for short-term (tens or hundreds of years) cladding behaviors and the inherent uncertainties in extrapolating to long-term (thousands or tens of thousands years) predictions of cladding degradation behaviors produce potentially significant uncertainties. For example, measurements of cladding failures are currently on the order of ten years yet the predicted median times for cladding unzipping range from 3,000 to 3,700 years.

Zircaloy (clad) is a highly durable material (Rothman 1984). However, zircaloy clad is relatively thin with an average thickness of only about 0.6 mm (or 600 μm), and up to 10 percent of the original thickness (depending on the burnups, reactor types, locations on a rod, etc.) is consumed during the service in the reactor operations (Guenther et al. 1991). Claddings have already been exposed to very severe conditions (high temperature, high pressure, high neutron flux, etc.) during

the reactor operations. After discharge from the reactor, claddings are likely to be constantly under stress during interim storage. In the permanent disposal conditions in the potential repository, claddings that have both failed and not failed are also likely to be constantly under stress for extended periods of time from various sources; such as elevated temperature, neutron flux, localized corrosion, and static loads resulting from a collapse of the structural components (e.g., basket materials) inside WP.

To better quantify the cladding (long-term) performance during the permanent disposal in the potential repository, the current cladding degradation models should be extended and/or modified to include long-term degradation effects indicated above. However, lack of long-term data makes the development of new reliable, representative models and/or improvement of the existing models difficult.

3.4.4 RIP Simulation

This section describes the results of a series of RIP simulations which incorporate the cladding performance as calculated in Subsection 3.4.3. Implementation of the cladding failure estimation into RIP is discussed, the descriptions for the cases evaluated with RIP are given, and the RIP simulation results are analyzed in detail.

The RIP simulation results to be discussed in this section are predicted radionuclide release and radiation dose at the accessible-environment boundary, 5 km from the repository footprint boundary. Inherent in the nature of any such prediction is its uncertain or stochastic nature. This statistical behavior is captured by plots of the complementary cumulative distribution function (CCDF) of a particular performance measure over the time period of interest (either 10,000 or 1,000,000 years). Note that $CCDF = 1 - \text{cumulative distribution function (CDF)}$, where CDF is the cumulative distribution function. The expected value of a statistical distribution is one of the most important parameters used to characterize the behavior of the distribution. Thus, besides showing CCDFs that represent the entire range of the various parameter distributions, expected-value time histories ("breakthrough curves") are also shown for the radionuclides that contribute significantly to the release rates or doses at the accessible environment. In the following subsections, the RIP simulation results will be discussed using the time-history curves and CCDFs.

3.4.4.1 RIP Implementation

The cladding failure analyses given in Subsection 3.4.3 are based on the temperature history (Figure 3.4-10) for the case with 20.5 kg U/m² (83 MTU/acre) thermal loading, ten-year old SNF, and no backfill. The probabilistic cladding failure analyses given in Table 3.4-3 provide a fraction of cladding that unzips for each of the WP groups in the interior of the repository. The cladding failure results for the WP groups in the repository edge region are given in Table 3.4-4, and the model results for 50°C higher initial center clad temperature are given in Table 3.4-5. Implementation of the cladding failure analyses into RIP are summarized as follows:

- A. The failure time and subsequent pitting degradation of each WP group were implemented into RIP as the primary container failure module.

- B. The fraction of cladding unzipped in each WP group was implemented into RIP as the secondary container failure module.
- C. The surface area of the spent fuel waste matrix in the unzipped cladding was increased by 100 times to account for the expansion of the spent fuel from the oxidation of UO_2 phase to U_3O_8 phase.
- D. The spent fuel waste in intact cladding in each WP group was not available for release over the entire simulation period (oxidation of cladding was extremely slow and creep rupture only produced small holes).

3.4.4.2 RIP Simulation Cases

All the RIP simulation cases discussed in this section are for a thermal loading of 20.5 kg U/m² (83 MTU/acre), no backfill, and a high infiltration rate (0.3 mm/yr). A total of five different cases were simulated with RIP to investigate the contribution of cladding performance to the repository performance. The cases studied are listed below:

- Case I: Base case, this is the nominal case without cladding performance credit
- Case II: Base case with cladding model
- Case III: Repository edge effect
- Case IV: Repository edge effects with cladding model
- Case V: Base case with cladding model with 50°C higher initial cladding temperature.

Case V was included to study the impacts of increasing peak cladding temperatures on the repository performance. Various combinations of the RIP simulation results for the five cases are discussed in the following sections.

The RIP simulation results to be discussed in the following sections are for two time periods, 10,000-year simulation and 1,000,000-year simulation. The 10,000-year simulation results will be discussed in a more quantitative manner than the 1,000,000-year simulation results. In the discussion of the repository performance in terms of radionuclide release, three types of radionuclide releases are included, the total release; ⁹⁹Tc release; and ²³⁷Np release. ⁹⁹Tc (half life of 2.12×10^5 years) is a representative radionuclide of those with a high solubility and mobility, and its release dominates the 10,000-year total release rate at the accessible environment. ²³⁷Np (half life of 2.14×10^6 years) is a solubility-limited radionuclide and one of the radionuclides that dominates long-term release and radiation dose rates at the accessible environment. The accessible environment is defined as the boundary 5 km away from the repository footprint. More detailed descriptions for the repository and accessible environment are found in the TSPA-1995 report (CRWMS M&O 1995c).

3.4.4.3 Release Rate History at Accessible Environment

The 10,000-year total release rate histories at the accessible environment for different cases using the expected values of all stochastic simulation parameters, are shown in Figure 3.4-17a. Also shown in Figure 3.4-17a, the repository with edge effect case has the earliest release initiation, and it is about 1,200 years earlier than the base case. This early release initiation is expected from the

Figure 3.4-17a. 10,000-year total release rate history at the accessible environment using expected values

WP failure distribution shown in Figure 3.4-7. The base case release behavior, lagging behind by about 1,200 years, generally follows that of the repository with edge effect case. This case shows the highest peak release rate at about 0.01 Ci/yr at 10,000 years. The peak release rate for the base case which also occurs at 10,000 years is about 0.006 Ci/yr. Although the base has a higher cumulative WP failure distribution (Figure 3.4-7) and greater WP pit penetration profiles (Figures 3.4-3 and 3.4-8) than the repository with edge effect case, these effects are not clearly seen in the 10,000-year accessible environment release behaviors. These differences in the WP failures may not be large enough to affect the accessible environment release behaviors. In addition, dispersion and dilution of radionuclides during the transport in the geosphere (unsaturated and saturated zones) may have obscured the effects from the different WP failure behaviors for the two cases. The peak release rates for the two cases with cladding models (Repository with cladding model and Repository with cladding and edge effect) at 10,000 years are generally two orders of magnitude lower than the cases without cladding model. The 10,000-year ^{99}Tc release rate histories at the accessible environment for the cases are shown in Figure 3.4-17b. Comparison of Figures 3.4-17a and 3.4-17b indicates the ^{99}Tc release rate dominates the total release rate. Shown in Figure 3.4-17c is the 10,000-year ^{237}Np release rate histories at the accessible environment for these cases. The step-functional release rate changes of ^{237}Np reflect its solubility-limited release behaviors from the source term and the WP failure distributions (WPs grouped according to zones). The release rates for the base case and the repository with cladding model case overlap, indicating that the release rates of ^{237}Np (solubility-limited radionuclide) from the limited sources with the cladding model case are comparable to those for the base case for which no cladding performance is taken into account.

Figure 3.4-17b. 10,000-year ^{99}Tc release rate history at the accessible environment using expected values

Figure 3.4-17c. 10,000-year ^{237}Np release rate history at the accessible environment using expected values

The total release rate histories at the accessible environment as a function of time out to 1,000,000-years using the expected values of simulation parameters, are shown in Figure 3.4-18a. Unlike in the 10,000-year releases, the repository edge effect does not show any noticeable differences in the predicted release behaviors. The peak total release rates for the cases without cladding performance (about 6 Ci/yr) occur at about 50,000 years. With the cladding model, the peak release rates are reduced by almost two orders of magnitude. Figure 3.4-18b shows the ^{99}Tc release rate histories at the accessible environment. The ^{99}Tc release dominates the total release rate for up to about 300,000 years; after then, about 60 to 70 percent of the total release rates are contributed by the ^{237}Np release (Figure 3.4-18c).

The predicted release rates at the accessible environment indicate that with the cladding performance calculated with the current cladding degradation models, the peak release rates for both the 10,000-year and 1,000,000-year repository performance are reduced by more than an order of magnitude and possibly as much as two orders of magnitude compared to the peak release rates for the cases without cladding performance. For the 10,000-year repository performance, the repository edge effect initiates radionuclide release earlier than the case without the edge effect; however, there is no noticeable differences in the 1,000,000-year repository performance.

Figure 3.4-18a. 1,000,000-year total release rate history at the accessible environment using expected values for the stochastic simulation parameters

Figure 3.4-18b. 1,000,000-year ^{99}Tc release rate history at the accessible environment using expected values for the stochastic simulation parameters

Figure 3.4-18c. 1,000,000-year ^{237}Np release rate history at the accessible environment using expected values for the stochastic simulation parameters

3.4.4.4 Cumulative Release at the Accessible Environment

One of the performance measures for the potential repository is to calculate the total (i.e., the sum of all radionuclides) cumulative release at the accessible environment. The calculated cumulative release is normalized to the Table 1 values in 40 CFR 191, *Environmental Radiation Protection Standards for Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes*, and measured against the standards (note: the current standards are under revision). The 100-realization CCDFs for the 10,000-year normalized cumulative release at the accessible environment are shown in Figure 3.4-19. The cases with the repository edge effect show generally higher normalized cumulative release than the corresponding cases without the edge effect; however, as in the release rate histories discussed in Subsection 3.4.4.3, the repository edge effect is insignificant. With the cladding model, the normalized cumulative release at 10,000 years is reduced by about two orders of magnitude. The 100-realization CCDFs for the 1,000,000-year normalized cumulative release at the accessible environment (Figure 3.4-20) show similar performance (Base case vs. Repository with cladding model case) with about two orders of magnitude reduction in releases to the accessible environment.

Figure 3.4-19. CCDF of the 10,000-year total normalized cumulative release to the accessible environment

Figure 3.4-20. CCDF of the 1,000,000-year total normalized cumulative release to the accessible environment

3.4.4.5 Dose at the Accessible Environment

Another performance measure for the potential repository is the radiation dose (in rem/yr) to a person (the "maximally exposed individual") at the accessible environment (5 km boundary) using the tuff aquifer for his or her drinking water (2 liters/day) (CRWMS M&O 1995c). One method for the performance measure is the total (i.e., the sum of all radionuclides) peak dose to the maximally exposed individual. The expected value of a statistical distribution is one of the most important parameters used to characterize the behavior of the distribution. Thus, besides showing CCDFs that represent the entire range of the various parameter distributions, expected-value time histories (or breakthrough curves) for the total dose exposure (rem/yr) at the accessible environment are also shown. The dose histories are calculated with a single realization that uses the expected values for all stochastic parameters.

Shown in Figure 3.4-21 is the 10,000-year dose histories at the accessible environment. For all the cases the peak dose occurs at 10,000 years. The base case and the repository edge effect case give about the same peak dose at about 0.1 mrem/yr at 10,000 years. The cases with the cladding model result in about two orders of magnitude lower dose than the cases without the cladding performance. Figure 3.4-22 shows the 1,000,000-year dose histories. In the cases without cladding performance, small peak doses at about 30 mrem/yr occur at about 50,000 years. After the peak at about 50,000 years, the doses increase steadily with time, reaching the peak doses (about 70 mrem/yr) at 1,000,000 years. For the cases with the cladding performance, the doses reach the maximum values (about 3 mrem/yr and about an order of magnitude lower than the base case) at about 300,000 years, then decrease with time to about 1 mrem/yr at 1,000,000 years.

Figure 3.4-21. 10,000-year total dose history at the accessible environment using expected values of the stochastic simulation parameters

Figure 3.4-22. 1,000,000-year total dose history at the accessible environment using expected values of the stochastic simulation parameters

Figure 3.4-23 shows 100-realization CCDFs of predicted total peak dose at the accessible environment during the first 10,000 years. The repository edge effect gives insignificant changes in the total peak dose for all the cases. The cladding performance (base case and repository with edge effect case) reduces the total peak dose by two orders of magnitude compared to the cases without cladding performance. The 50th percentile of the total peak dose for the cases without cladding performance is in a range of 0.03 to 0.06 mrem/yr, and the 90th percentile for the same cases is about 2 mrem/yr. The 50th percentile total peak dose for the cases with the cladding performance is about 4×10^{-4} mrem/yr, and the 90th percentile is about 0.02 mrem/yr. For the 10,000-year performance, the cladding performance reduces the total peak dose by two orders of magnitude compared to the cases without cladding performance.

Figure 3.4-24 shows 100-realization CCDFs of the predicted 1,000,000-year total peak dose at the accessible environment. The total peak doses for the cases with the cladding performance are generally lower by an order of magnitude than the cases without cladding performance. The 50th percentile total peak doses for the cases without cladding performance are in a range of 70 to 100 mrem/yr, and the 90th percentile total peak doses for the same cases are in the range of 200 to 300 mrem/yr. For the cases with the cladding performance, the 50th percentile total peak doses are about 5 mrem/yr, and the 90th percentile total peak doses are about 30 mrem/yr. For the 1,000,000-year performance, taking credit for the cladding performance reduces the total peak dose by one to one-and-one-half orders of magnitude compared to the cases without cladding performance.

Figure 3.4-23. CCDF of the 10,000-year total peak dose at the accessible environment

Figure 3.4-24. CCDF of the 1,000,000-year total peak dose at the accessible environment

3.4.4.6 Effects of Temperature on Cladding Performance

The objective of this task was to examine the 350°C cladding thermal goal to determine if it is a valid criterion. The cases described above had a median initial center cladding temperature of 276°C at emplacement, which then increased slightly during the first year or two with a subsequent gradual decrease. Only a small percentage (about 10 percent) exceeds 350°C (see Figure 3.4-12). To evaluate the effect that increased temperature has on performance of the cladding, the median temperature of the cladding was increased 50 degrees to 325°C. For this case, about 30 percent exceed the 350°C temperature limit. Using the median WP failure time of 2,200 years, the estimated fraction of unzipped clads increased from 0.5 percent for the base case to 3.90 percent for the higher initial clad temperature (Table 3.4-2).

By implementing the estimated fraction of unzipped cladding for each WP group (Table 3.4-5), a series of RIP simulations were conducted to study the impacts of the higher initial center clad temperature on the cladding contribution to the repository performance. Figure 3.4-25 shows the simulation results for the higher temperature cladding case for the 10,000-year total release rate history at the accessible environment using expected values for stochastic simulation parameters. The results are compared with those of the base case and the reference clad temperature case (i.e., 276°C initial center cladding temperature, labeled as "Repository with cladding model"). As shown in Figure 3.4-25, the total release behavior for the higher clad temperature case for the first 10,000 years is comparable to the base case, and the peak release rate which occurs at 10,000 years is about the same as the base case and about two orders of magnitude higher than the reference clad temperature case. The 1,000,000-year total release rate history at the accessible environment for the higher clad temperature case is compared with the base case and the reference clad temperature case

Figure 3.4-25. 10,000-year total release rate histories at the accessible environment using expected values for stochastic simulation parameters to compare the effects of 50°C higher initial cladding temperature

in Figure 3.4-26. The peak release rates for all three cases occur at about the same time (about 50,000 years). The peak release rate for the higher clad temperature case is about three times higher than the reference clad temperature case, and is about an order of magnitude lower than the base case. The release rate at 1,000,000 years for the higher clad temperature case is about an order of magnitude higher than the reference clad temperature case and about an order of magnitude lower than the base case.

It is indicated that with about 4 percent unzipping (and accompanying 100 times spent fuel surface area increase) from the higher initial center clad temperature by 50°C, the total release behavior at the accessible environment for the first 10,000 years is comparable to the base case in which no credit for cladding performance is taken. For the 1,000,000-year repository performance, the higher clad temperature increases the peak release rate by a factor of three compared to the reference clad temperature case, but reduces the peak release rate by an order of magnitude compared to the base case.

The 10,000-year total dose history at the accessible environment for the higher clad temperature case using expected values for stochastic simulation parameters is shown in Figure 3.4-27, and compared with the base case and the reference clad temperature case. The peak total doses for all three cases occur at 10,000 years; the peak dose for the higher clad temperature case is about the same as the base case and about two orders of magnitude higher than the reference clad temperature case. For the total dose histories at the accessible environment for 1,000,000 years (Figure 3.4-28), the total

Figure 3.4-26. 1,000,000-year total release rate histories at the accessible environment using expected values for stochastic simulation parameters to compare the effects of 50°C higher initial cladding temperature

Figure 3.4-27. 10,000-year total dose histories at the accessible environment using expected values for stochastic simulation parameters to compare the effects of 50°C higher initial cladding temperature

Figure 3.4-28. 1,000,000-year total dose histories at the accessible environment using expected values for stochastic simulation parameters to compare the effects of 50°C higher initial cladding temperature

peak dose for the higher clad temperature case is about an order of magnitude lower than the base case and about an order of magnitude higher than the reference clad temperature case.

The 100-realization CCDF of the 10,000-year total peak dose for the higher clad temperature case is compared with the base case and the reference clad temperature case in Figure 3.4-29. The 50th percentile total peak dose for the higher clad temperature case is about an order of magnitude higher than the reference clad temperature case and about an order of magnitude lower than the base case. Similar predictions for the 90th percentile total peak dose are given for the three cases. The 100-realization CCDFs of the 1,000,000-year total peak dose for the three cases are shown in Figure 3.4-30. In the 1,000,000-year predictions, the 50th percentile total peak dose for the higher clad temperature is lower by a factor of three than the base case, and higher by a factor of 5 than the reference clad temperature case. The 90th percentile total peak dose for the higher clad temperature case is about the same as the base case, and about an order of magnitude higher than the reference clad temperature case.

These analyses indicate that in terms of the repository performance measure of the total peak dose at the accessible environment, an increase of the initial center clad temperature by 50°C (i.e., higher cladding unzipping fractions) would worsen the repository performance for the first 10,000 years by an order of magnitude compared to the reference clad temperature case, but would still improve the repository performance by an order of magnitude compared to the base case. The effects of the higher clad temperature become less for the 1,000,000-year repository performance; the repository performance with the higher clad temperature is worse, by about a factor of five, than the reference clad temperature case, but the performance is better, by about a factor of three, than the base case.

Figure 3.4-29. CCDFs of the 10,000-year total peak doses at the accessible environment to compare the effects of 50°C higher initial cladding temperature

Figure 3.4-30. CCDFs of the 1,000,000-year total peak doses at the accessible environment to compare the effects of 50°C higher initial cladding temperature

3.4.4.7 The Effect of Changing Standards

The calculations of cladding performance in the preceding pages were all done by estimating releases at the accessible environment which was a distance of 5 km from the potential repository. Some very recent planning guidance (DOE 1996c) has been issued that suggests a possible change to the location of what is considered as the accessible environment. In addition, the planning guidance suggested an interim postclosure standard of an exposure limit of 15 mrem/yr from all radionuclides at about 30 km down-gradient from Yucca Mountain. This subsection evaluates the impact that such a change might have on the recommendations made with respect to cladding.

Calculations were done similar to the previous set of calculations in which the total peak dose at 30 km is estimated. The total peak dose base case at the 5 km accessible environment is compared to a new case at 30 km, the case with cladding at the 5 km accessible environment, and the case with cladding at 30 km. The 10,000 year peak dose for these four cases is plotted in Figure 3.4-31 and the 1,000,000 year peak dose is plotted in Figure 3.4-32.

Figure 3.4-31. CCDFs of the 10,000-year total peak dose comparing the cases for a standard at 30 km

Figure 3.4-32. CCDFs of the 1,000,000-year total peak dose comparing the cases for a standard at 30 km

These figures show that placing the accessible environment at 30 km reduces the doses by almost two orders of magnitude over what would occur at the 5 km boundary. This, of course, is due to the increased dispersion/diffusion and travel time to travel the additional 20 km. The total peak doses predicted to be observed at 30 km are comparable with what would be observed at the 5 km accessible environment boundary when cladding is considered. Considering cladding produces doses which are about one to two orders of magnitude less at 30 km than the case without cladding and almost four orders of magnitude less than the base case at 5 km.

All cases, even the base case, should meet the 15 mrem/year standard at 10,000 years. At 1,000,000 years the new case (no cladding) at 30 km exceeds 15 mrem/year at the 99th percentile although is somewhat less than this at the 50th percentile. Including performance for cladding reduces the total dose at 30 km almost an order of magnitude below the 15 mrem/year at the 99th percentile. Thus, cladding appears to provide a substantial barrier which can limit the releases at both 10,000 and 1,000,000 years and the proposed change in standard would not alter the conclusion to consider cladding performance that was reached above.

3.4.5 Summary

Incorporating the individual cladding degradation models available in the literature, a probabilistic cladding degradation analysis tool was developed. The probabilistic model incorporates the cladding temperature distributions within the WP and as a function of time. The cladding degradation (cladding oxidation and unzipping) in an oxidizing condition is calculated by incorporating the WP failure distribution. The current probabilistic analyses indicate that under the current design specifications and the expected near-field thermal environments, only about 6 percent of cladding fails in a form of small punctures and a much smaller fraction (about 0.5 percent) of cladding was predicted to undergo a gross rupture (or unzipping).

However, the cladding degradation models (e.g., creep rupture, delayed hydride cracking, zircaloy dry oxidation and cladding unzipping) used in the probabilistic analyses were developed for an interim dry storage of spent fuel, and the only driving force of cladding degradation in the models is temperature. In other words, the cladding degradation models are for short-term (tens or hundreds of years) cladding behaviors and lack in predicting long-term (thousands or tens of thousands years) cladding degradation behaviors. Thus, confirmation of the cladding degradation models for the long-term cladding behaviors would be required for licensing, and suitable care should be exercised in using the current analysis results. Such confirmation would require testing to establish the material degradation. In some cases cladding degradation could be examined as part of performance confirmation. Examination of claddings which have currently been in storage for 10 to 20 years would be appropriate but in addition some laboratory testing would be likely.

In order to claim a credit for cladding performance with a higher level of confidence in future repository performance evaluations and eventually for the licensing, the current individual cladding degradation models (i.e., creep rupture, delayed hydride cracking, zircaloy dry oxidation, and cladding unzipping) should be re-evaluated, especially for their long-term effects on cladding degradation. Additional cladding degradation processes, not considered in the current study, should be included, such as stress corrosion cracking (induced primarily by iodine in the interior side of the clad, and induced by the near-field factors such as salt formation on the clad surface), long-term localized corrosion in radiolysis-induced acidic conditions, and long-term degradation under static loads that may be caused by a collapse of the internal structure (e.g., basket material). One major obstacle to improving the current models and possibly developing new model(s) is a lack of long-term performance data. Development of testing data for such purposes is both lengthy and costly, and may not be practical in view of the time limitation for the licensing. Most practical approach for an immediate use would utilize the data available in the literature, and combine and synthesize the data with theoretical models that have been developed for other programs. Analysis of cladding that has remained in storage for extended periods may also provide useful information, but the initial state of the cladding should be known. In order to achieve the objective, a comprehensive compilation of the cladding degradation data currently available in the literature should be considered as a priority effort.

The RIP simulation results indicate that with the cladding performance that was estimated with the current probabilistic analyses, the repository performance is greatly improved (one to two orders of magnitude in releases to the accessible environment). The 10,000-year total peak release rate at the accessible environment is reduced by two orders of magnitude compared to the case without

cladding performance; for the 1,000,000-year performance, the total peak release rate is reduced by one to possibly two orders of magnitude. Similar results are reported for the total peak dose at the accessible environment. With the cladding performance, the 10,000-year total peak dose is reduced by two orders of magnitude compared to the case without cladding performance, and the reduction in the total peak dose is an order of magnitude for the 1,000,000-year repository performance.

As described above, cladding performance was shown to be sensitive to temperature. The number of clads that fail increases as the temperature increases. It was predicted that with about 4 percent unzipping (and the accompanying 100 times spent fuel surface area increase), which was estimated for a higher clad temperature (i.e., an initial center clad temperature of 325°C), the total release behavior at the accessible environment for the first 10,000 years is comparable to the base case in which no credit for cladding performance is taken, and the total peak release rate is about two orders of magnitude higher than the reference clad temperature case (i.e., an initial center clad temperature of 276°C). For the 1,000,000-year repository performance, the higher clad temperature increases the peak release rate by a factor of three compared to the reference clad temperature case, but still reduces the peak release rate by an order of magnitude compared to the base case.

These analyses indicated that in terms of the repository performance measure of the total peak dose at the accessible environment, an increase of the initial center clad temperature by 50°C (i.e., higher cladding unzipping fractions) would worsen the repository performance for the first 10,000 years by an order of magnitude compared to the reference clad temperature case, but would still improve the repository performance by an order of magnitude compared to the base case. The effects of the higher clad temperature become less for the 1,000,000-year repository performance; the repository performance with the higher clad temperature is worse by a factor of five than the reference clad temperature case, but the performance is better by a factor of three than the base case.

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4. EDGE LOADING EVALUATIONS

A number of analytic calculations, for example Ryder (1993) and Buscheck, Nitao, and Saterlie (1994), have shown that the edge of the repository will cool and rewet substantially faster than the center and thus performance at a high thermal load may be degraded at the edges. Calculations were done in the 1995 Thermal Loading Study (CRWMS M&O 1996b), which showed that edge cooling could be alleviated to some extent by loading the edges of the repository with either hotter fuel or loading it to a higher density. The duration of boiling and time to rewet increased significantly when fuel was emplaced at a higher density at the edges. However, the analyses also showed that this increased fuel density resulted in significantly higher temperatures at the edges than in the center of the repository, and several thermal goals were violated. Thermal goals may be traded for performance if in fact an increase in performance is achieved. This year's effort included performance evaluations to establish whether an improvement in performance is, in fact, achieved by increasing the density at the edges of the repository. Additionally, the operations issues were addressed. For example, violation of the drift wall 200°C thermal criteria (as discussed earlier) may require more extensive tunnel support be used to ensure that other performance measures, such as ability to retrieve, are preserved.

The calculations were done using inputs which are non qualified, although many of those inputs are contained in the *Reference Information Base*. The V-TOUGH code is a non-qualified code which has not been validated as yet. Thus, the recommendations in this section should not be used for procurement activities without further verification.

4.1 THERMOHYDROLOGIC CALCULATIONS OF NON-UNIFORM AMLs

Calculations were done for non-uniform AMLs using the V-TOUGH thermohydrologic model. Most of this work is reported in the 1995 Thermal Study (CRWMS M&O 1996b). The discussion of the calculations to include input and output are provided in the Lawrence Livermore National Laboratory *Near Field and Altered Zone Environment Report* (Wilder et al. 1996). Temperature, duration of boiling, relative humidity changes, and liquid saturation changes as a function of time and location in the potential repository were calculated for cases in which the AML in the outer edge (in this case outer 25 percent) of the repository is increased somewhat to offset the cooling experienced by the edge. The waste stream used was based on a YFF(10) selection criteria, which had an average age of SNF of about 22.5 years. The calculations were run with a nominal binary gas-phase diffusion where the gas-phase tortuosity factor was $t_{eff}=0.2$ and the infiltration rate was zero. Using a nonzero infiltration rate will decrease the time that the repository remains above boiling since the infiltration is assumed to be distributed over the entire repository area it should not change the conclusions reached in this section (CRWMS M&O 1995c).

The methodology used to develop a non-uniform AML is described in more detail in the cited reference (CRWMS M&O 1996b). However, it basically used a constant value of AML for the inner 75 percent of the potential repository and a linear increase over the outer 25 percent. The average AML for a region was based on trying to match a local duration of boiling time to the average duration of boiling. For example, one case that was run was to increase the AML in the outer edge of an ACD like design. Thus, the inner 75 percent of the repository has a uniform AML of 20.7 kgU/m² (83.4 MTU/acre) while the outer 25 percent had a linearly increasing AML to the edge

with an average AML in the region of 34.0 kgU/m^2 (137.4 MTU/acre). The results of those calculations and others showed that the duration of boiling could be increased well beyond 1,000 years with an increase in AML at the edges. The base case, a uniform AML everywhere, had the outer edge (about 10 percent) of the repository below boiling at about 1,000 years. The nonuniform AML produced an increase of about a factor of two in the duration of boiling. What needed to be shown was whether or not the edge cooling could produce a degradation in releases to the accessible environment and this will be addressed below.

The calculations also showed that due to the high concentration of fuel at the repository edge the temperatures in the drifts in these edge regions were significantly higher than 200°C during the first 100 years. Thus, thermomechanical issues need to be addressed since these temperatures violate the drift wall thermal criteria. The thermomechanical issues, primarily tunnel support, will be addressed in the next subsection.

4.2 THERMOMECHANICAL EVALUATIONS

Subsection 3.3 provides the analysis of the thermomechanical evaluations that were done in support of this effort. The results of the evaluations indicated that without tunnel support there was significant potential for rock failure at temperatures above 200°C . When tunnel supports such as steel sets and concrete liners are considered in the thermomechanical evaluations, the conclusions are similar, although in this case the concern is more the failure of tunnel support and subsequent potential for rock failure. These differences between emplacement drifts in which the temperature is below and above 200°C are illustrated by comparing the predictions shown in Figures 3.3-3 and 3.3-4 for unsupported drifts, comparing Figures 3.3.7 and 3.3.8 for steel set supports, and comparing Figures 3.3-9 and 3.3-10 for concrete liners. While the thermomechanical calculations were fairly conservative, and there may be methods to add joints to the steel sets or increase the thickness of the concrete liner, it appeared that it would take significant effort, and possibly increase the cost, to support an emplacement drift where temperature exceeded 200°C . Thus, the predictions found no reason to eliminate the 200°C thermal criteria, and in fact reinforced the choice of that criteria.

4.3 TOTAL SYSTEM PERFORMANCE ASSESSMENTS

In Subsection 3.3, simulations were run for the evaluation of cladding performance in which a base case (one in which releases to the accessible environment were predicted assuming uniform heating throughout the repository disk) was compared with a more realistic case which considered edge cooling. Predictions of CCDF for releases to the accessible environment were done for a 10,000 year period and a 1,000,000 year period.

All the simulation cases discussed in Subsection 3.3 were for a thermal loading of 20.5 kg U/m^2 (83 MTU/acre), no backfill, and a high infiltration rate (0.3 mm/yr). A total of five different cases were simulated to investigate the contribution of cladding performance to the repository performance. The cases studied are listed below.

- Case I: Base case, this is the nominal case without cladding performance credit
- Case II: Base case with cladding model
- Case III: Repository edge effect

- Case IV: Repository edge effects with cladding model
Case V: Base case with cladding model with 50°C higher initial cladding temperature.

However, of primary interest in the evaluation of edge loading are the comparisons of Case I and Case III. The base case, as indicated above, considers the heat produced by the SNF as being uniform over a disk which approximates the entire area of the potential repository. This case essentially treats all WPs as if they were located in the center of the repository. Case III however, takes a more realistic approach in which the WPs at the edge of the repository experience faster cooling. In this case one-sixth of the inventory of WPs is assumed to be distributed in this outer zone which is somewhat consistent with thermohydrologic predictions of Buscheck as reported in the 1995 Thermal Study (CRWMS M&O 1996b). The predicted WP failure distributions with time are shown for the base case and the case with edge cooling in Figure 3.3-7. An examination of this figure shows that the edge cooling tends to result in earlier WP failures although in later years the WPs in the edges actually have a somewhat lower fraction of failures due to the lower temperatures upon return of the water.

The way in which the temperature and RH histories at the WP surface in the repository edge regions were estimated, was by assuming the environment in the edge could be represented by one similar to that produced by a thermal loading of 14.3 kgU/m² (58 MTU/acre) (CRWMS M&O 1995c). Because the drift-scale temperature and RH histories for the 14.3 kgU/m² thermal loading were not available, the temperature and RH histories were approximated using the temperature and RH histories available for two thermal loadings of 6.2 and 20.5 kgU/m² (25 and 83 MTU/acre), and by linearly interpolating the values for the two thermal loadings.

The results of the CCDF calculations show that the lower temperatures in the repository edge result in some earlier releases of radionuclides. This is demonstrated in Figure 3.4-17a, which shows that for the expected-value total releases to the accessible environment, the edge cooling case results in releases appearing at the accessible environment between about 5,000 to 6,000 years. The base case delays releases by about 1,000 years from the edge cooling case consistent with the delay in WP failures by a similar time. These releases are still small, however. By 10,000 years the total releases between the base case and the case which considers edge cooling are very similar.

To illustrate the results that edge cooling does not appear to significantly impact performance, the figures showing the 10,000 and 1,000,000 year total peak dose are reproduced in this section from Subsection 3.4. Figure 4-1 shows the total peak dose at 10,000 years for the base case, the repository with edge loading, the repository with a cladding model (base case plus cladding), and the repository with cladding and edge loading. As indicated in Figure 4-1, there is negligible difference between the CCDFs for the base case and the case which includes edge cooling. Similarly, Figure 4-2 shows the total peak dose at 1,000,000 years for the same cases. This figure also shows that there is little difference between the CCDFs for the base case or the one with edge cooling. Thus, the TSPA calculations do not support a need to increase the thermal loading at the edge of the repository.

Costs were not specifically evaluated in this section. Since there appeared to be a technical reason for not considering edge loading it did not seem practical to evaluate costs.

Figure 4-1. CCDF of the 10,000-year Total Peak Dose at the Accessible Environment

Figure 4-2. CCDF of the 1,000,000-year Total Peak Dose at the Accessible Environment

4.4 SUMMARY

The edges of the repository have been shown to cool faster than the center of the repository and to also rewet faster for the cases of high thermal loading. This effort investigated whether any performance degradation might occur as a result of the edge cooling. Suggestions have been made that higher loading of WPs at the edges of the repository might be a solution to mitigate the edge cooling. However, previous calculations (CRWMS M&O 1996b) found that edge loading sufficient to increase the duration of boiling significantly at the edges would produce temperatures above 200°C, which could have consequences on tunnel stability. These issues are addressed in this section.

TSPA calculations were performed to assess the possible impact on performance. The results of these calculations showed that, although somewhat earlier releases could be anticipated, the total peak doses at 10,000 and 1,000,000 years showed negligible differences between the idealized case with no edge cooling and the more realistic case with edge cooling. The early releases were very small and thus should not impact our ability to meet release standards. This conclusion could be impacted if microbially induced corrosion is found to be more significant under these conditions than for a higher thermal load.

On the other hand, the thermomechanical calculations indicated potential rock stability problems and tunnel support problems at temperatures above 200°C. Tunnel support failure is a possibility, although measures could possibly be taken to either develop expansion joints for the steel sets or increase the thickness of the concrete liner. In either case, this would pose a greater challenge and the cost would increase.

In summary, there appears to be no compelling reason to advocate edge loading at this time and in fact it appears as if there would be a potential cost impact and risk associated with doing edge loading. Specifically thermal criteria would be violated with edge loading

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5. WASTE STREAM VARIABILITY

5.1 INTRODUCTION

We know (CRWMS M&O 1996b) that a significant degree of variability of WP heats will exist in the waste stream that arrives at the potential repository for disposal. This variable waste stream can produce large variations in the heat output of individual WPs. Most of the calculations to date have used an average waste stream which results in only providing indications as to how a uniform heating would perform. Recent calculations with variable heat output WPs have indicated that this fuel variability could impact performance. This section will discuss whether or not waste stream variability could result in performance issues, what steps could be taken to mitigate this waste stream variability, and will provide recommendations for design.

The question that must be addressed is do WP heat variations result in degradation in performance. Last year's thermal study (CRWMS M&O 1996b) found that temperature variations of the rock could exceed 100°C in distances of only 10 m or so. This was found to result in drift wall temperatures exceeding 200°C in some locations, which could cause rock stability and tunnel support problems as shown in Section 3 of this report.

The current design approach is to use heat to mobilize water and "dry" out the repository. The DHLW and some of the BWR packages are cooler than the other WPs and will result in cooler spots where they are emplaced. Evaluations were done to evaluate whether or not mobilized water could be driven from the hotter areas to these cooler ones. Some calculations were done in support of this study and the Engineered Barrier System Performance Requirements Study which showed the effect that variations in temperature would have on relative humidity. The environment in a drift with a relatively cool DHLW (Hanford), a moderate heat output BWR package, and a hot (10 year old SNF) PWR package was calculated. Figure 5.1-1 shows the temporal variations in relative humidity around the various packages. The results show that the DHLW package has a relative humidity of essentially 100 percent a few years after emplacement and the humidity never gets low enough that corrosion wouldn't occur on those WPs. While this results in some of the DHLW failing earlier, as shown in Figure 5.1-2, the WP failure distributions are not affected much and the resulting performance predictions do not show much change.

Current WP failure models primarily use relative humidity and temperature to predict failure. Corrosion models which consider dripping on the WPs are needed if these cooler areas develop higher liquid fluxes then WP release predictions might be different than current predictions since heat driven percolation can easily exceed natural infiltration. Evaluations are needed to determine whether or not the cooler WPs can be placed in close proximity to the hotter ones in such a way that a "thermal umbrella" could form to keep those packages dry.

Calculations were done with a three-dimensional model to evaluate whether or not a mixture of WPs with different heat outputs and heat decays could move moisture from hotter packages to cooler ones in the emplacement drifts. The calculations were done for the ACD Report (CRWMS M&O 1996a) design with an AML of 20.6 kgU/m² (83.4 MTU/acre). The results found, as shown in Figure 5.1-3, indicate that substantial flux (well in excess of the assumed percolation flux of 0.3 mm/yr) can occur

Figure 5.1-1. Relative Humidity Calculations for Several Different WPs for the ACD Design

Figure 5.1-2. Predictions of Functions of Failed Packages for Several Different WPs for the ACD Design

Liquid-phase seepage flux at upper drift wall at various WP locations for AML = 83.4 MTU/acre, the ACD rev 00 design, LML = 0.46 MTU/m, drift spacing = 22.5 m, sand invert, drift diameter = 5.5 m, WP emissivity = 0.8, and percolation flux = 0.3 mm/yr.

Figure 5.1-3. Moisture Flux on the Drift Wall at the DHLW Locations for the ACD Design for a) 400 Years and b) 100,000 Years

over the cooler packages in the early years. Thus, fluxes of 65, 16, 7.5, and 5 mm/yr were predicted at 10, 100, 200, and 300 years after emplacement. At later times these fluxes approach zero and ultimately return to ambient. The hotter packages do not experience any appreciable fluxes above ambient at any times. Although, as indicated above, the WP corrosion predictions (which are only sensitive to relative humidity and temperature) do not indicate substantial WP degradation, there could be a potential problem with high fluxes if it is later found that drips on the WP could produce more rapid degradation. The source of these calculations and those described in the previous two figures to include descriptions of inputs and outputs is contained in the Lawrence Livermore National Laboratory *Near Field and Altered Zone Environment Report* (Wilder et al. 1996).

It appeared to be prudent to attempt to mitigate the effects of variations in WP heat output due to the fact that thermomechanical criteria might be exceeded and/or high levels of moisture flux may occur in the cooler regions of the potential repository. This study looked at several different methods to mitigate this heat variability and these are discussed below.

In this study analyses were done to determine whether or not simply changing WP spacing could mitigate the effects of waste stream variability. Possibly moving the packages closer together could result in heating up the cooler packages and lowering the temperature of the hotter ones. Reducing packages spacing is also attractive from the standpoint of reducing the amount of emplacement drifts needed and thus the excavation costs. Ventilation was considered as another method to mitigate the heat effects during the preclosure period. Much of the heat variability occurs during the first hundred years after emplacement. Some level of natural ventilation is likely as well. Ventilation algorithms were coupled with a thermohydrologic model to calculate the effects of heat conduction and the latent heat of vaporization. Finally, thermal management on the surface by aging the fuel and

blending of assemblies was examined. Most of the assemblies arriving at the potential repository are likely to be bare assemblies packaged in a dual-purpose container (DPC). This allows some flexibility to select SNF assemblies to tailor a WP to a desired heat output (e.g., blending). Additionally, legislation is pending which may establish an interim storage facility (ISF) which would provide some aging of the fuel and would provide a "pool" of assemblies to select from in the event that blending is considered a workable option.

5.2 THERMAL MANAGEMENT WITH WP SPACING

One of the easiest methods of altering the near-field thermal performance is to adjust the WP spacing in the emplacement drifts. As discussed in the previous section, predictions have shown that the hotter packages can drive moisture to the cooler packages, particularly if those packages are separated some distance. The SNF decay heat produces significant thermohydrologic and thermomechanical effects at the drift scale, which includes the emplacement drifts and the rock pillars separating the emplacement drifts throughout the repository area. There has been considerable discussion about the pros and cons of various thermal loading strategies, with much of the debate focused on the AML. However, the details of the way the WPs are configured within the repository (e.g., in a square configuration versus a line-load configuration that utilizes tight axial WP spacing and wide drift spacing) may play as great or greater role in driving near-field thermohydrologic behavior than the overall AML of the repository itself. High temperatures in a local area or significant thermal gradients in a local area can impose problems on tunnel stability and on tunnel supports as discussed in Section 3.3. One of the primary objectives of this section is to establish functional relationships (i.e., the parametric sensitivity) between repository system parameters and near-field thermal behavior, and thereby help develop a quantitative framework upon which thermohydrologic management principals may be incorporated into the design of the repository system. The advantages and disadvantages of using WP spacing to tailor the thermal behavior will be discussed and evaluated.

The ACD Report (CRWMS M&O 1996a) used essentially a square spacing with a drift separation of 22.5 m and a WP spacing of about 19 m. Both SNF packages and DHLW packages were interspersed in the potential repository. These packages can have widely different heat outputs from less than a few kilowatts to more than 15 kilowatts. In the ACD case, locally hot and "cool" spots can form. The effects of this spacing on the thermal performance and the effect of changing this spacing were evaluated in this section.

Discussion of Models Used, Inputs, and Assumptions. The primary model used in the analysis was a three-dimensional conduction and radiation model (using ANSYS Version 5.1 [ANSYS 1995]) that calculated the drift wall and WP temperatures for the various scenarios. The calculations were done for WPs with various heat outputs. The calculations evaluated a thermal load of 20.6 kgU/m² and considered WP spacings (see below) of as much as about 19 m to as little as 0.1 m. The drift diameter considered was 5.0 m. Further details can be found in a memorandum from Bahney (1996).

Four WP heat outputs were considered and these are emplaced in a repeating pattern. One of the WPs was a large BWR (44 assemblies) package which had average fuel characteristics as defined

in the CDA Document¹² (CRWMS M&O 1996f), and thus a heat output at emplacement of about 7.2 kW. Another WP was a below average PWR (21 assemblies) package which had, at emplacement, a heat output of about 2.0 kW. The third type of WP was a DHLW package of four assemblies which had an emplacement heat output of about 2.8 kW. The fourth package was a design basis package (21 PWR assemblies) which had a heat output of about 17.8 kW.

To define the thermal loading scenarios, the following assumptions were used:

- A. Thermal loading is determined (consistently) as a function of thermal mass loading in kgU/unit area; and the reference thermal loading is 20.6 kgU/m².
- B. WPs are horizontally emplaced, centered in a 5.0 m diameter circular drift with a concrete invert, with no backfill, and no ventilation heat removal.
- C. Only large uncanistered SNF WPs and large DHLW WPs (21 PWR, 44 BWR, and 4 DHLW) were considered.
- D. Since the DHLW heat decays quickly, and by definition DHLWs contain negligible amounts of heavy metals, the DHLW packages are assigned a uranium mass of zero (that is they generate heat, but do not factor into the mass loading calculation).
- E. Given assumption C. (and the information in the ACD Report (CRWMS M&O 1996a), about 27 percent of the WPs may be DHLW packages. Therefore, one DHLW package will be included in the emplacement drift for every three spent fuel WPs (i.e. assumed to be 25 percent); and the multiple WP model will consider a total of four WPs.

Some thermohydrologic calculations were also done in support of this effort. These model calculations were done using both the V-TOUGH and NUFT codes (Nitao 1989; Nitao 1993), both two- and three-dimensional drift-scale models. The models include all major hydrostratigraphic units in the UZ, which are assumed to be horizontal and of uniform thickness; the initial and boundary conditions were the same as those used in past studies (Buscheck and Nitao 1993; Buscheck and Nitao 1994). For most of the calculations $k_b = 280$ millidarcy was assumed and an initial vertical liquid saturation profile based on a 0.3 mm/yr percolation flux (saturation at the repository horizon was 99 percent) was used. The initial vertical temperature and pressure distribution are consistent with the nominal geothermal flux and pneumatostatic conditions. For all of the calculations, the atmospheric RH is assumed to be 100 percent, so the model allows no loss of moisture by vapor diffusion to the atmosphere. Because actual (desert) RH is much lower than 100 percent, the model under represents this loss. This neglected loss may be large for high AMLs, which can steepen the temperature gradient near the ground surface by a factor of 50 relative to ambient conditions. The effect of this assumption is offset (to some degree) by the assumption of zero percolation flux made in some of the calculations. All of the drift-scale and hybrid models used in this study assumed that the water table is fixed at a constant temperature, liquid saturation, and pressure.

¹² Found in Interoffice Memorandum. Subject, *CDA Follow-on Data*; authors M. Rose and J. King; correspondence number, VA.SA.JK.OY96-003.

Drift-scale thermal-hydrological behavior is represented by a two-dimensional model that incorporates the geometric details of the WPs and emplacement drifts in a cross-section transverse to the drift axes. Heat transfer in the drift occurs as thermal radiation, heat convection, and conduction. Drifts are assumed to be rectangular; however, as long as the cross-sectional areas of the WP and drift are the same as in the actual circular geometry, the model is found to accurately model heat and mass flow within the drift. Because the two- and three-dimensional drift-scale models effectively assume an infinite repository area, they are applicable to the region not affected by cooling at the repository edge (for the first 1000 years).

Evaluating the effect of a mixture of WPs with different heating histories requires a three-dimensional, multiple WP model. The three-dimensional model is used to compare two repository designs, the ACD, which is called the ACD Report Rev. 00 design (CRWMS M&O 1996a); and the line-load design, which places WPs at close spacing. The focus is to examine differences between the two designs with respect to temperature T and RH experienced by WPs and within the drifts and the near field itself. These quantities strongly affect WP integrity and the integrity of repository components, such as steel sets that may be required for drift stability.

A mixture of WP types is examined from those containing very hot SNF to virtually cold DHLW. The three-dimensional, multiple-WP model includes six major WP types (see Appendix D), resulting in a WP inventory that is representative of that assumed for the ACD Report Rev. 00 design, including four SNF WP types:

- "very hot" 10-yr-old "design basis fuel" PWR WPs (comprising 10 percent of the WPs in the model)
- "relatively cool" 40-yr-old PWR WPs (10 percent of the WPs)
- nominal 26-yr-old PWR WPs (20 percent of the WPs)
- nominal 26-yr-old BWR WPs (20 percent of the WPs), and two types of DHLW, including those from the Hanford site (10 percent of the WPs) and those from the Savannah River site (20 percent of the WPs).

Note that the ACD Report Rev. 00 design assumes that 27 percent of the WPs are DHLW WPs, while for the three-dimensional, multiple-WP hydrothermal model, 30 percent of the WPs are assumed to be DHLW WPs. It should also be noted that no consideration was given as to the difficulty of the logistics needed to try to have an appropriate mix of WPs available for emplacement.

The drift diameter is assumed to be 5.5 m. Heat transfer within the drift occurs as thermal radiation, heat convection, and conduction. Thermal radiation occurs between all surfaces, including thermal radiation from WP to WP.

There are two different ways that WPs can be arranged in the repository at Yucca Mountain. The ACD Report Rev. 00 design utilizes a "square" geometry with the spacing between drift centerline being roughly the same as the axial center-to-center spacing between SNF WPs. The ACD Report Rev. 00 has a lineal mass loading (LML) of 0.46 MTU/m and drift spacing of 22.5 m. The line-load

design places WPs nearly end-to-end, a 0.1-m gap between WPs was assumed, resulting in LML = 1.11 MTU/m, and drift spacing of 53.8 m to keep the AMLs the same as the ACD reference. The drift spacing in the line-load design is 2.4 times greater than in the ACD. Additionally, a line-load design with a 1.0-m gap between WPs resulting in LML = 0.94 MTU/m and drift spacing = 46.1 m was considered since Subsurface Design indicated that it would be very difficult to place the WPs closer than 1 m. These cases were analyzed at an AML of 20.6 kgU/m² (83.4 MTU/acre) although additional AMLs were considered.

Influence of Repository Design on Thermal Behavior. The influence of axial WP spacing and drift spacing on the thermal behavior of the potential repository was examined in this study. The large axial WP spacing (as much as 19 m) in the ACD design may thermally isolate the WPs from one another, causing the heat flux that is delivered to the drift surfaces to vary substantially along the drift axis. This results in substantial variations in WP and rock temperatures and RHs along the axis of the drift. The ACD has an LML = 0.46 MTU/m of emplacement drift. The line-load design places WPs nearly end-to-end with an LML of about 1.33 MTU/m for the four WPs; to keep the AMLs the same (20.6 kgU/m²) in the two designs, the drift spacing in the line-load design is 2.9 times greater than in the ACD. We also consider a second line-load case with a 1.0-m gap between WPs, resulting in LML = 1.12 MTU/m. Another case with a fixed 12 m spacing was also considered which had an LML of 0.74 MTU/m. Figure 5.2-1 shows the layout of WPs for these various cases.

Calculations of the ACD base case were done and temperature predictions for the WP and for the emplacement drift wall as a function of time are presented in Figures 5.2-2 and 5.2-3 respectively. As shown in Figure 5.2-2, the WP temperatures are well below the 350°C cladding criteria except for the design basis fuel package. This package slightly exceeds the criteria but uses a very conservative estimate for predicting temperatures. Such a hot package may require some aging prior to emplacement underground. Figure 5.2-3 shows that the drift wall temperatures are well behaved and do not get any higher than about 170°C. The temperature variation of the drift wall between the hottest and coolest package in the ACD case is about 28°C.

As the WPs are moved together the packages and drift wall get hotter. Figures 5.2-4 and 5.2-5 show the predicted WP and emplacement drift wall temperatures, respectively, as a function of time for the case in which the WPs are separated by one meter. Figure 5.2-4 shows that the WP temperature of the design basis package is significantly hotter with internal temperatures reaching almost 400°C, clearly in violation of the cladding criteria. Figure 5.2-5 shows that the emplacement drift wall temperatures are significantly hotter. Wall temperatures over all four of the packages exceed the 200°C wall temperature criteria. The temperature variation of the drift wall between the hottest and coolest package in this case is about 25°C. This is somewhat less than the variation in the ACD case but not substantially less.

The case for a 0.1 m spacing between WPs, although not shown here, is somewhat hotter than the 1 m spacing case. The variation between the hotter and cooler packages is somewhat less, about 22°C, but still not a significant reduction in variation.

Case 1: Nominal ACD Spacings, Drift Spacing = 22.5 m

Case 2: Fixed 12.0 m c/c SNF WP Spacing, Drift Spacing = 36.096 m

Case 3: Fixed 1.0 m End/End WP Spacings, Drift Spacing = 54.864 m

Case 4: Fixed 0.1 m End/End WP Spacings, Drift Spacing = 64.698 m

Figure 5.2-1. WP Types and Spacings for the Cases Considered

Multiple WPs Peak Temperatures

Figure 5.2-2(a). Multiple WP Peak Temperatures for the ACD Spacing Case

Multiple WPs Surface Temperatures

Figure 5.2-2(b). Multiple WP Surface Temperatures for the ACD Spacing Case

Figure 5.2-3. Multiple Drift Wall Temperatures for ACD Spacing Case

Figure 5.2-4. Multiple WP Peak Temperatures for the 1-meter Spacing Case

Figure 5.2-5. Multiple Drift Wall Temperatures for the 1-meter Spacing Case

Some thermohydrologic calculations were done, as indicated above, using the NUFT code and varying the spacings over the range discussed above. The results of those calculations are not presented in this section but can be summarized briefly. The thermohydrologic predictions tend to support the predictions done with ANSYS (ANSYS 1995). As the packages are moved closer together the temperatures increase and the temperature differences between packages decrease. However, the thermohydrologic predictions do not show temperatures as high as ANSYS and they indicate somewhat more benefit for reducing temperature variations. It is not anticipated that the presence of moisture would affect the calculations much (ANSYS is heat conduction and radiation only) in the early years since the rock should dry out rapidly and heat conduction should be the dominant mechanism of heat transport in the near field for the first few hundred years. Another thermohydrologic model coupled with ventilation analyses (the base case was no ventilation), is in reasonable agreement with ANSYS and shows the higher temperatures (see Section 5.3). Although not fully addressed here, the thermohydrologic model predicts more hydrologically homogenous conditions exist for the higher line loads, especially upon cool down.

Costs. Changing the spacing of the WPs can affect the costs of excavation. Cost savings can be realized if the WP spacing is decreased since less tunnel needs to be excavated even if the drift spacing has to be increased. This does not decrease the total area requirements since that is based primarily on AM and waste quantity. The length of emplacement drift needed for the ACD design is 179 km which, at a drilling cost of \$7,468/m of drift (1995 dollars), amounts to excavation costs of \$1.34B. At the highest line loading (0.1 m gap between packages), if achievable, the length of emplacement drift required is 89.8 km at a cost of \$0.67B. This is a cost savings of about \$0.67B or about 6 percent of the MGDS costs. More detailed cost analysis for a variety of options is provided in Section 6.

Costs associated with establishing the logistics of insuring that the appropriate mix of hot and cooler packages was beyond the scope of this study and was not examined. Based on the current waste receipt schedule (CRWMS M&O 1995b, Key #3), a line loading concept would not be achievable since the DHLW will not be received at the repository until the sixth year of emplacement. Significant schedule constraints would be incurred if the Program had to wait six years to start emplacement. Even if those scheduling problems were worked out it is still not clear that sufficient packages of the appropriate heat output would be available for disposal when needed. A storage facility at the surface would be essential. Some additional information on surface storage is contained in a subsequent subsection of this report. However, further details on the logistics of WP scheduling or costs associated with that was beyond the scope of this study.

Summary. Calculations were done to multiple heat WPs to evaluate the effect of varying the WP spacing on near-field temperatures and temperature variations. The results appear to indicate that close spaced WP spacing will result in thermal criteria (cladding and drift wall) being violated. Additionally, while the temperature variations between packages decrease somewhat, there does not appear to be a dramatic decrease in variability. The higher line loading can reduce excavation costs but it appears that the current waste receipt schedule would not support such a concept at this time. Thus at this time there does not appear to be sufficient evidence to warrant changing the design to close spacing. It should be noted that analyses with the NUFT code have shown greater potential benefits than did work performed using the ANSYS code. Further evaluations are recommended to resolve the reasons for the inconsistent results obtained using the two codes.

5.3 THERMAL MANAGEMENT WITH VENTILATION

Ventilation as a thermal management tool has the potential to provide enhanced flexibility in design, increased safety of operations, and/or mitigation of risk for a potential repository such as the risk posed by high heat load at emplacement or emplacing WPs with variable heat output. This section describes the evaluations done using a ventilation code to determine whether or not smoothing of the heating of the drift walls and packages could be accommodated through ventilation. However, there could be a cost associated with ventilation and this is also examined as well. Additionally, if credit is to be taken for ventilation, even natural ventilation it must operate throughout the entire preclosure period and could add operational complexity. Monitoring would be needed in all drifts to ensure it is functioning.

Realistic calculations of the psychrometric environment in a potential repository require an understanding of the amount of heat and moisture that are removed from the emplacement drifts and the near-field rock by ventilation. To achieve this, a coupled simulation procedure was developed in 1995 using the Lawrence Livermore National Laboratory NUFT code for the hydrothermal calculations in the near field (Nitao 1995) and the Mackay Thermal Enhancement and Climate Simulation model (Danko 1992; Danko and Mousset-Jones 1992; Danko and Mousset-Jones 1993; and Danko 1994) for the heat and mass transport calculations in the air. The coupled codes, using projected site properties, produce three-dimensional calculations of the hydrothermal behavior of the near-field rock-air interface, and the dilution of water vapor in the drift air flow and subsequent transport out of the system.

Calculations of the amount of heat (sensible and latent heat of vaporization) and moisture removed by ventilation were done in this evaluation. For many of these calculations, it was only necessary to use WPs that had an average heat output (no WP variability). However, a number of calculations were also done in which six WPs, each with a different heat output, were modeled. An overview of the results of these calculations is discussed below and the detailed results are provided in Appendix D.

The coupled codes, as first developed in this effort, were not designed to calculate multiple heat output WPs. The code was only modified at the end of the effort to calculate different heat output packages. Thus, most of the calculations used in this section have WPs which have all the same heat output. Only a few calculations were done with this enhanced capability. Thus, while the calculations will clearly demonstrate the benefits of ventilation, only qualitative results will be possible in determining the ability of ventilation to mitigate the effects of waste stream variability.

Ventilation Calculations. Essentially three cases were run with ventilation and compared with the base case in which no ventilation was used. For these cases an ACD like case was considered which had large, 21 PWR sized packages which used a weighted average for BWR and PWR fuel equivalent to about 7.4 MTU per package (based on earlier line load calculations and OFF SNF was assumed) so that with a WP spacing of 16 m and a drift spacing of 22.5 m the thermal loading was 20.6 kgU/m^2 (83 MTU/acre). The diameter of the emplacement drift was 5 m. Various air flow rates from essentially no air flow (the base case) to a forced flow of $10 \text{ m}^3/\text{s}$ were considered. Inlet air temperature was 26°C with a relative humidity of 30 percent. Further details can be found in papers by Danko et al. (1995 and 1996). The three cases were a ventilation rate of 10, 1, and $0.1 \text{ m}^3/\text{s}$. These cases range from a relatively high flow that would require forced ventilation to a very low flow that could easily be achieved with natural ventilation. The ACD Report (CRWMS M&O 1996a) found that the average leakage was expected to be between 0.1 to $0.6 \text{ m}^3/\text{s}$. In most cases calculations were made for a drift length of 1152 m but predicted temperatures for the first 600 m of drift will be used to be consistent with the current ACD concept which considers only 600 m long emplacement drift segments and the costing analysis done in this effort.

The details of the calculations and plots of such parameters as air temperature, wall temperature, partial vapor pressure, heat flux, and moisture flux are contained in Appendix D. Figure 5.3-1 shows a plot of predicted drift wall temperature as a function of tunnel length and time after emplacement for the $10 \text{ m}^3/\text{s}$ ventilation case. Looking at the maximum temperature profile, which in a 600 m long drift would occur at the end of the drift, we see that the temperature peaks at about 45°C at 10 to 20 years after emplacement and then cools to about 33°C at around 100 years. Significantly cooler temperatures exist at distances closer to the entrance of the emplacement drift. These are average temperature values since in fact variations around this will occur as one goes from a location on the wall that is above a WP to one that is between WPs. These variations are approximately plus and minus 2 to 4 degrees depending on time. Air temperatures are somewhat cooler. Although not shown here, one should recall that without any ventilation peak wall temperatures can reach 160 and 170°C for an average PWR WP.

A sensible heat transfer ventilation model was run for the various cases by Subsurface Design in an effort to evaluate what was needed to support such ventilation rates and perform the cost analyses.

High Air Flow – FUNTIONALIZED NUFT

Figure 5.3-1. Drift Wall Temperatures for the High Flow (10m³/s) Ventilation Case

These results are in Appendix E. For comparison sake, the drift wall temperatures are plotted as a function of time and distance along the drift and are shown in Figure 5.3-2. These predictions show that the temperatures peak about 51°C and then cool to about 38°C at 100 years. These temperatures are in good agreement with the coupled model. The slightly lower temperatures predicted with the coupled model may be due to the additional heat being removed through the latent heat of vaporization.

A modest air flow case of 1 m³/s, which is probably close to what would occur by natural ventilation, was run next. The wall temperatures are plotted in Figure 5.3-3. At a drift length of 600 m the temperatures the coupled code predicts average peak temperatures of about 120°C which then cool to about 90°C. These temperatures are substantially cooler than the case with no ventilation.

A low air flow case of 0.1 m³/s, which simulates a low flow natural ventilation case, was conducted. The wall temperatures are plotted in Figure 5.3-4. At a drift length of 600 m the temperatures the coupled code predicts average peak temperatures of about 150 to 160°C which then cool to about 120 to 130°C. These peak temperatures are similar to the temperatures with no ventilation but at later times even this low ventilation rate provides some cooling of the wall temperatures.

Calculations were also made of the amount of moisture which was removed from the rock by the ventilation. The integrated predictions of average moisture flux per meter of drift are shown in Figures 5.3-5 through 5.3-7 for the 10, 1, and 0.1 m³/s cases respectively. An examination of the figures indicates an interesting trend in that the lower ventilation rates actually produce a higher flux of moisture. This result indicates that the heat is the real driver at eliminating moisture from the rocks. The results show that for a 600 m drift, about 3 to 9 x 10⁶ kg of water are removed in 100 years. This can be compared with the how much water can be replaced over the area of the drift during one hundred years. Assuming an infiltration rate of 0.3 mm/yr, this would amount to about 9 x 10⁴ kg of water. Thus, about a factor of 100 times more moisture is removed by ventilation at the low flow rate, about a factor of 30 more at the high flow rate, than can be replaced by natural infiltration. However, in the long term this will be replaced.

At the close of the effort, a capability was developed to do multiple WPs, each with a different heat. The WP heats and spacings are described in more detail in Appendix D. In summary, six different heat output packages were used. Two of these packages were very low heat output (the lowest about 1.6 kW) DHLW, there was an average PWR heat package, a small (12 PWR) package, an average BWR package, and a very hot PWR package which had a heat output at emplacement of about 18 kW. This latter package is possible if an uncontrolled waste stream is allowed. ACD spacing was used for the packages and the DHLW were emplaced between the packages with a much shorter spacing allocated to them. The calculated drift wall temperature for the base case with no ventilation is provided in Figure 5.3-8. The temperature variability is immediately evident. Although some heating of the cooler packages occurs, these packages produce considerably cooler drift wall temperatures of between 100 and 150°C. On the other hand, the hottest package produces drift wall temperatures that peak at almost 250°C and are above 200°C for the entire 100 year preclosure period. These conditions would clearly violate the 200°C emplacement drift wall criterion. The reader should note that these temperatures seem to be somewhat higher than those predicted by ANSYS (ANSYS 1995) (see Section 5.2) and should be verified. However, the calculations are valid to examine trends and the effects of ventilation.

Figure 5.3-2. Drift Wall Temperatures Using a Conduction Only Module for a High Flow ($10 \text{ m}^3/\text{s}$) Ventilation Case

Medium Air Flow - FUNCTIONALIZED NUFT

Figure 5.3-3. Drift Wall Temperatures for the Moderate Flow ($1\text{m}^3/\text{s}$) Ventilation Case

Low Air Flow - FUNCTIONALIZED NUFT

Figure 5.3-4. Drift Wall Temperatures for the Low Flow (0.1m³/s) Ventilation Case

Figure 5.3-5. Integrated Moisture Flux for the High Flow (10m³/s) Ventilation Case

Figure 5.3-6. Integrated Moisture Flux for the Moderate Flow (1m³/s) Ventilation Case

Figure 5.3-7. Integrated Moisture Flux for the Low Flow (0.1m³/s) Ventilation Case

ACD - No Cooling Enhancement, No Ventilation

Figure 5.3-8. Drift Wall Temperatures for Multiple Heat Packages with No Ventilation

A case was run for this multiple heat WP simulation in which a low level flow of $0.1 \text{ m}^3/\text{s}$ was simulated. This flow rate would be equivalent to a low level natural ventilation. The results, shown in Figure 5.3-9, indicate that this low level flow provided substantial smoothing of the heat. The drift wall temperatures above the very hot package are now in the range of 160 to 180°C . The drift wall temperatures over the other packages are all close to 150°C . Thus, just a small amount of natural ventilation could be instrumental in removing temperature peaks from very hot packages and distributing the heat to cooler ones. Of course, no safety measures (shielding, handling, transportation limits, etc.) associated with moving such a hot package as the 18 kW package were examined in this effort. It may be necessary for other reasons to restrict the waste stream.

A case with high air flow ventilation ($10 \text{ m}^3/\text{s}$) was run for the multiple heat WP simulation. The results of these calculations are shown in Figure 5.3-10 for the drift wall. These results show that substantial smoothing is achieved. The drift wall temperatures can be kept below about 40 to 50°C for most of the emplacement period at this ventilation rate. Only in the first few years after emplacement are higher temperatures experienced over the hottest packages and these do not exceed about 65°C .

There are some operational concerns associated with any decision to take performance credit for ventilation, that need to be discussed. Specifically, if one relies on ventilation, including natural ventilation, then efforts are needed to ensure that ventilation operates as planned throughout the preclosure period. Monitoring of the ventilation system or the emplacement drifts to ensure appropriate conditions are met will be required. Redundant systems will also be needed. In the case of natural ventilation it might be necessary to install an active ventilation system as a backup to ensure that the appropriate flow occurs. These issues will need to be addressed in the process of making a decision to employ ventilation.

Alternative Thermal Management Techniques. Some discussion is needed for alternative thermal management techniques which can provide passive or active modification of the temperature fields in the drift. Several calculations were done in which alternate thermal management techniques were examined to evaluate their ability to smooth the temperature fields produced when variable heat output WPs. The six heat output WPs discussed above were used as the source term for the calculations. In addition to the base case and the case with natural ventilation, three other cases were considered. Specifically, a case in which ventilation between two drifts is looped (e.g. air between the two drifts is recirculated with no addition of fresh air). For this case a high flow condition of $10 \text{ m}^3/\text{s}$ was established for 30 years and then a low flow of $0.1 \text{ m}^3/\text{s}$ was maintained thereafter. In a second case, an axial heat pipe (thermal resistance of $0.00133 \text{ W}/^\circ\text{C}/\text{m}$) was placed in contact with the WPs. The axial heat pipe was a copper tube of 0.5 m diameter filled with water and an outer concrete (or shotcrete) coating that is 0.2 m thick. In a final case thermal rock bolts (thermal resistance of $0.0133 \text{ W}/^\circ\text{C}/\text{m}$) were placed in the wall on a $1.5 \times 1.5 \text{ m}$ pattern. Additional details can be found in Appendix D or in Danko (1994, pp 890-898).

ACD - Natural Ventilation ($0.1 \text{ m}^3/\text{s}$), No Cooling Enhancement

Figure 5.3-9. Drift Wall Temperatures for Multiple Heat Packages with Low Flow ($0.1 \text{ m}^3/\text{s}$) Ventilation

Figure 5.3-10. Drift Wall Temperatures for Multiple Heat Packages with High Flow ($10 \text{ m}^3/\text{s}$) Ventilation

Figure 5.3-11 shows the drift wall temperature for the looped ventilation case. Even though the air only recirculated, the temperature is reduced significantly for the hotter package from the base case (see Figure 5.3-8) with no ventilation and no cooling enhancement. Temperatures are reduced initially, when the air flow is large, to no more than about 150°C and then when the flow is low, the temperatures increase but do not exceed about 180°C over the hottest WP. Over the other packages the temperatures are increased somewhat over the cooler packages, keeping them within the thermal umbrella.

In the case of the axial heat pipes, Figure 5.3-12 shows that these heat pipes are also fairly effective at reducing the heat of the hottest package and increasing the heat of the cooler packages. In this case the drift wall temperature at the location of the hottest package is decreased although its peak approaches 200°C. The variation in WP heats (not shown here) is fairly smooth although the largest package is still somewhat hotter than the others.

In the last case examined, thermal rock bolts can also effectively distribute the heat, although in this case the heat is distributed into the rock. Figure 5.3-13 shows that the temperature of the drift wall over the hottest package is reduced significantly. The temperatures are smoothed over the base case although there does not appear to be as much smoothing as in the other cases considered above.

Cost Analysis. A cost analysis was done to determine how much it would cost to implement ventilation systems which could provide the air flows examined in this effort. The detailed cost breakdowns for each case are shown in Appendix E. Additional cases of 2, 5, and 0.6 m³/s were run and costed. Costs for the ventilation that would be needed to develop the emplacement areas have been done for ACD and are reproduced in Appendix E and this was defined as the base case; no ventilation of the emplacement drifts. The cost of the base case was found to be about \$14 M. Costs to support the various ventilation cases were identified and the differences in costs between these and the base case were calculated.

The analysis found that no additional cost was needed for ventilation rates that were less than about 1 m³/s. The additional costs above the base case were due to the fact that additional intake shafts, intake mains, and exhaust mains were needed as the ventilation increased. Table 5.3-1 provides the differences between the base case and the respective ventilation case. An examination of the table clearly shows that the highest flow rate will require a fairly substantial investment due to the fact that a significant number of additional shafts and main drifts are needed to carry the air flow. Natural ventilation cases will not cost any additional amount of money although there may still be a need for filters to meet National Environmental Protection Act requirements. Only modest costs are needed to support a 1 m³/s ventilation case. The costs for a 2, 5, or 10 m³/s ventilation system would amount to about 2, 8, or 25 percent of the MGDS costs (\$11B; see Section 6).

Figure 5.3-11. Drift Wall Temperatures for Multiple Heat Packages for Looped Ventilation of $10 \text{ m}^3/\text{s}$ for 30 Years and $0.1 \text{ m}^3/\text{s}$ Thereafter

ACD - axial heat pipe cooling enhancement, no ventilation

Figure 5.3-12. Drift Wall Temperatures for Multiple Heat Packages for Axial Heat Pipes on the WPs

ACD - Thermal Rock Bolt Cooling Enhancement, No Ventilation

Figure 5.3-13. Drift Wall Temperatures for Multiple Heat Packages for Thermal Rock Bolts

Table 5.3-1. Differential numbers of shafts and costs of ventilation between various cases and the base case with no ventilation

Ventilation Rate (m ³ /s)	Number of Intake Shafts	Number of Intake Mains	Number of Exhaust Mains	Cost Differences (\$M)
0.1	0	0	0	0
0.6	0	0	0	0
1	1	0	0	39
2	1	1	1	212
5	2	1	1	857
10	7	2	2	2763

5.4 THERMAL MANAGEMENT THROUGH SURFACE ACTIVITIES

In the preceding sections we examined subsurface thermal management methods to moderate WP variability. This section will examine what thermal management methods can be used on the surface to establish WPs for emplacement which do not have as much variability as the base case which assumes that as the SNF is received in a dual purpose container it is just repackaged in a disposal WP and sent underground for emplacement. The elimination of the MPC concept allows a certain amount of flexibility in being able to select assemblies (blending) to configure a WP to achieve some target heat load. Additionally, lag storage at the surface would allow aging of the SNF and would provide a "pool" of SNF to facilitate blending. This section will explore these different issues to determine the advantages and disadvantages.

Assumptions. A number of assumptions were made to conduct this supporting study. These assumptions were made, in part, using the expected conditions that will likely exist for the receipt of waste (EIA 1995; CRWMS M&O 1996f) and anticipated legislation. The assumptions used were the following:

- A. There is no longer an MPC.
- B. Subsurface waste emplacement will begin in 2010.
- C. For the cases which consider an ISF, receipt of waste at the ISF will begin in 2003.
- D. No ISF costs are included. It is assumed that the costs associated with the design, construction, and operation of the ISF are totally separate and out of the scope of this effort since the ISF will be mandated by legislation and will be a cost the program must bear.
- E. The ISF is in reasonable proximity to the repository so long distance and/or long term travel was not considered.
- F. Disposal limits at the MGDS will be about 70,000 MTU, consistent with the CDA Document (CRWMS M&O 1996f) and ACD Report (CRWMS M&O 1996a).

- G. Disposal containers (WPs), except for DHLW or other fuel, will be large containers which could contain either 21 PWR or 44 BWR assemblies. Once sealed no blending will be done.
- H. BWR and PWR assemblies will not be mixed in the same disposal package.
- I. Essentially all SNF will arrive as bare SNF assemblies since the SNF will arrive in either DPCs or as bare fuel.
- J. The MGDS thermal loading is a high thermal loading of 20.5 kgU/m² (83 MTU/acre).
- K. DHLW and other fuel will be emplaced as received.
- L. The thermal output of each assembly is known accurately enough for our purposes or, if necessary, will be measured.

Other more specific assumptions for the cost analysis or the waste stream selection are identified in the respective appendices.

Options Evaluated. A surface facility will provide the necessary thermal management through receipt of SNF at the repository, actions necessary to store the SNF in an ISF, actions to retrieve from the ISF, as appropriate will perform the blending of the assemblies and configuration of the WPs, and preparation of the WPs for disposal. Details of the surface facility operation can be found in Appendix F.

A number of options were selected for evaluation which would provide different amounts of blending and/or storage which could be used to provide some level of thermal management. These options do not necessarily represent current planning; however, they all are considered feasible and could be incorporated into the designs if the benefits and costs associated with them justify their consideration. Several terminologies have been used which need explanation. *Fine Blending* means that individual assemblies are selected based on their thermal characteristics. *Coarse Blending* means that entire canisters, such as DPCs, have been selected. *Lag Storage* is storage of canisters and/or carriages containing canisters in a designated area adjacent to the waste handling building (WHB). *Interim Storage Facility* is a large area located somewhere reasonably near the MGDS which can be used to store canisters for sufficiently long periods of time up to the time of operation of the MGDS. The following options or scenarios were considered:

Case 1. Base Case. This is the base case which represents the ACD Report design (see CRWMS M&O 1996a and Appendix F). This scenario has no ISF and receives the waste as it is delivered from the utilities and processes it through the operations with no effort being made to consider any thermal management issues. Waste receipts begin in 2010 at the same time as MGDS operation begins. This scenario assumes that OFF fuel selection is used.

Case 2. This case is similar to Case 1 except that a lag storage is provided from which waste can be selected for thermal management. The primary impacts of this scenario are the costs associated with constructing, operating, and maintaining the lag storage yard. This scenario

assumes that OFF fuel selection is used. Four sizes of lag storage were considered and these are:

- 600 DPC capacity requiring 5 acres of storage area.
- 1,200 DPC capacity requiring 10 acres of storage area.
- 3,000 DPC capacity requiring 25 acres of storage area.
- 4,200 DPC capacity requiring 53 acres of storage area.

Case 3. This case considers an ISF which begins operation in 2003 and receives and stores waste until the start of the MGDS. MGDS operation starts in 2010 and emplaces waste as it is received. The waste stored in the ISF remains there until the end of emplacement when this waste is withdrawn and emplaced. This scenario assumes that OFF fuel selection is used.

Case 4. This case assumes an ISF begins operation in 2003 and the repository begins operating in 2010. All waste shipped to the ISF arrives in DPCs. Waste shipped directly to the repository arrives as DPCs or bare fuel assemblies in transportation casks. Bare fuel assemblies are placed in WPs and sent underground for emplacement. This scenario assumes that OFF fuel selection is used. Two subcases were considered.

- The repository operation does coarse blending by selecting DPCs from the ISF based on their thermal load. There is no fine blending.
- This case is the same as Case A except some fine blending of up to 5 DPCs (105 PWRs or 220 BWRs) is allowed in the WHB at the same time. 5 DPC storage in the surface facility would be available for each shipment underground.

Case 5. This case has an ISF and is similar to Case 4A except that after 2010 the bare fuel assemblies being received will be placed in DPCs and sent to the ISF. These DPCs will later be returned to the WHB as they are selected for disposal. Coarse blending is used in this case. This scenario assumes that OFF fuel selection is used.

Case 6. This case allows for fine blending in the WHB. An ISF is available starting in 2003 which acts as a "pool" from which the assemblies are selected for disposal which starts in 2010. This scenario assumes that OFF fuel selection is used.

Case 7. This is the same as the base case except YFF waste stream selection is used.

Case 8. This is the same as Case 4A except that YFF waste stream selection is used.

Case 9. This is the same as Case 3 except that YFF waste stream selection is used.

Case 10. This is the same as Case 6 except that YFF waste stream selection is used.

WP Heat Variability Evaluations. Estimates of the WP heat variations were made for the various scenarios. These calculations were done using predictions of assembly heats, SNF age, enrichment, and numbers of packages arriving at the potential repository on an annual basis. The assumptions used and the detailed tables of DPC package characteristics and numbers are given in Appendix G.

Figures 5.4-1 and 5.4-2 show the WP heat output and the plus and minus one-standard deviation heat outputs for each year of fuel received at the repository for the PWR and BWR packages respectively. These figures show that substantial variability exists in the package heat outputs. The tabulated values of heat output are shown in Appendix G. The results indicate that the average WP heat output of PWR fuel is about 9 or 10 kW for OFF fuel except during the first few years of emplacement. The variability is quite large with some packages, particularly in the later years, being over 14 to 15 kW and some of the cooler packages being less than 5 kW. The BWR fuel has an average WP heat of about 8 kW except in the early and later years and has a one-standard deviation of about 2 to 3 kW. The case run with YFF fuel (Case 7), see Figure 5.4-3 for the PWR characteristics (see Appendix G for the BWR), has WPs with heat outputs in the 11 to 12 kW range but the variations have a number of packages above 18 kW and a number less than 4 kW.

Case 3 which has an ISF that stores the first seven years of SNF (receipts from 2003 to 2010) until the end of the emplacement period has little advantage over Case 1. The WP variability for the majority of the emplacement years is no different than Case 1. The last few years of emplacement when the packages in the ISF are withdrawn are considerably cooler.

The largest capability to modify the waste stream occurs with Case 6 which allows fine blending of the assemblies. In this case DPCs are stored in the ISF which starts operation in 2003. In 2010 when disposal commences assemblies are withdrawn from the ISF in an attempt to make a WP of a specific heat output. In this case the target heat output per package was chosen to be about 10 kW. This value was chosen because it is near the average PWR heat output. This same target heat was chosen for the BWR for consistency, but, as one will see from the following figures, it was probably an inappropriate choice because it was too high. Figure 5.4-4 for the blended PWR SNF shows that the heat variations are considerably reduced. In this case the one-standard deviations are a few tenths of a kilowatt. In the case of the BWR SNF the variations are even smaller, about a tenth of the PWR deviations (see Figure 5.4-5). In the case of the PWR SNF a 10 kW average WP heat output was readily achieved for most years, except the last few emplacement years when only the coolest SNF remains. Because too high a target SNF package target heat was selected for the BWR packages, it was difficult to maintain a fairly constant heat output over the various emplacement years even though the deviations were small in any given year. A target heat of about 7 or 8 kW would have been a much better choice for the BWR SNF.

Case 4 in which coarse blending (selection of WPs only based on their heat output) was done was also evaluated. Although not shown here (see Appendix G) the calculations indicated that the one-standard deviation on heat of the WPs which could be emplaced in any given year was reduced significantly over that of the no blending case. The averages were almost as small as the fine blending case.

Figure 5.4-1. Average and One-Standard Deviation WP Heat Outputs for Case 1 OFF; PWR Fuel

Figure 5.4-2. Average and One-Standard Deviation WP Heat Outputs for Case 1 OFF; BWR Fuel

Figure 5.4-3. Average and One-Standard Deviation WP Heat Outputs for Case 1 YFF; PWR Fuel

Figure 5.4-4. Fine Blending of WP Heats for Case 6 OFF; PWR Fuel

Figure 5.4-5. Fine Blending of WP Heats for Case 6 OFF; BWR Fuel

Concepts of Operation and Cost Impacts Study. Concepts of operation for the surface facility to be able to handle the waste stream and perform the thermal management for the various options was developed in this study. Operations considered were the cask receiving and preparation, canistered waste transfer, disposal container welding and transfer, uncanistered waste transfer, canister filler addition, cask preparation and shipping, and WP underground transfer. More details of these operations are provided in Appendix F. These operations and the differences in these operations as a function of case were used to establish the costs of the different options and compare these costs against the base case (Case 1).

The description of the various cases is provided above. These cases and the operations associated with the cases are described in Appendix F but a top level conceptual outline of the process needed to perform the thermal management operations for some of the cases is depicted in Figure 5.4-6.

The costs for the various operations on a case by case basis were developed. Detailed cost analyses are shown in Appendix F. The costs estimated for the base case surface operations was \$3.34 B. The increase in cost for the various options is provided below in Table 5.4-1.

Table 5.4-1. Cost Differences for Surface Thermal Management Options

Case Description	Total Cost (\$M)
Case 2; 5 acre lag storage	44
Case 2; 10 acre lag storage	48
Case 2; 25 acre lag storage	63
Case 2; 35 acre lag storage	72
Case 3	0
Case 4A	19
Case 4B	24
Case 5	19
Case 6	45
Case 7	0
Case 8	19
Case 9	0
Case 10	45

These cost differences with the base case are shown in Figure 5.4-7. Each cost bar on the figure shows the amount of costs that can be attributed to the various activities such as engineering, caretaker, etc. As the figure shows the case with lag storage has the largest cost differences. Case 6 and 10 with fine blending are the next most expensive with costs of \$45 M but this is only a little over a 1 percent increase in the costs for the surface facility and easily within the current uncertainty in cost factors that currently exists. Thus cost does not appear to be a big driver in the selection of one of these options.

THERMAL LOADING STUDY CASES

Case 1 - No ISF

Case 2 - No ISF

Features:
 Optional Canister Selection from 1 - 7 Years of Waste Receipts
 Store in Transport Casks or on Concrete Pad

Case 3 - ISF

Features:
 Optional Canister Selection from 1 - 7 Years Waste Receipts
 ISF Stores on Concrete Pad
 7 Years of Storage Available for selection

thrmop01

Figure 5.4-6. Pictorial Concept of Surface-Storage Interactions for the Various Study Cases

THERMAL LOADING STUDY CASES

Cases 4 & 5

ISF With Bare Fuel in Storage

Without Bare Fuel in Lag Storage

Features:

Case 4 has no Fine blending

Case 5 has Fine Blending Options

THRMOP02

Figure 5.4-6. Pictorial Concept of Surface-Storage Interactions for the Various Study Cases
(continued)

Figure 5.4-7. Surface Repository Cost Variations from the Base Case

5.5 SUMMARY

A significant amount of variability will exist in the waste stream arriving at the potential repository for disposal. This waste stream variability means that the different WPs will have different heat outputs, from as little as about 1 kW to over 20 kW at emplacement. The study determined that potential degradation in performance could occur as a result of this variability. Specifically, thermomechanical problems such as tunnel stability/tunnel support problems may develop over the hotter packages if 200°C is exceeded and large expansion variations in the axial direction due to temperature differences in 10 to 20 m of 50 to 100°C could result which could cause problems. Additionally, it was shown that hotter packages could push moisture to cooler packages during the first few hundred years which could result in faster corrosion of those cooler packages. However, it should be noted that the current performance predictions made, which rely on temperature and relative humidity, do not indicate any significant degradation in releases to the accessible environment due to the cooler packages. However, the TSPA analyses does not consider moving moisture from hotter to cooler packages. It is recommended that such analyses be included in

subsequent TSPAs. Based on the potential thermomechanical and hydrologic issues, such thermal management techniques as varying WP spacing (line loading), ventilation, and surface aging and WP selection were examined.

The analysis of the line-loading concept indicated that some smoothing of the heat distributions could be achieved. However, the close spacing of the WPs appears to result in significantly increased temperatures which violate such thermal criteria as the 200°C wall temperature or the cladding criteria and the 350°C cladding criteria. This should be considered work in progress and should be investigated further when additional assurance can be developed in the calculations. The analysis did show that some cost savings (about \$670M) could be achieved by going from the ACD case to a close (0.1 m gap) spacing. However, problems in the logistics of providing an appropriate waste stream with sufficient numbers of DHLW, cooler WPs, average WPs, and hotter ones were found to be significant. At the present time the waste receipt schedule would not support implementation of the high line loading concept. Some adjustment would be needed in the waste receipt schedule and a surface storage facility would be needed. The costs of such a surface storage facility could offset the cost advantages of less excavation. The logistics of supporting the line loading concept and the costs associated with that were not considered in this study.

The study was instrumental in developing a coupled ventilation-thermohydrologic calculation capability in 1995. The code was used to evaluate the effect of using ventilation to reduce preclosure temperatures and to mitigate the effects of waste stream variability. Ventilation cases from a very low flow of 0.1 m³/s consistent with a low natural ventilation condition to a high flow of 10 m³/s simulating a forced ventilation condition were evaluated. The results show that ventilation would reduce temperatures in the repository significantly. For the case of 20.6 kgU/m² (83 MTU/acre), ventilation of even a low air flow of 0.1 m³/s would drop temperatures after 10 to 20 years to about 120 to 130°C compared to the no ventilation case of about 150 to 170°C. A 1 m³/s could reduce the temperatures in the drift to below boiling after the first 10 to 20 years and a high flow ventilation case would reduce temperatures for this same period to less than 40°C. These same ventilation calculations showed that anywhere from a factor of 30 to 100 times the amount of natural infiltration received in 100 years can be taken out of the host rock by ventilation. Interestingly, the lower air flow ventilation rates were more effective at removing the moisture because of the fact that temperature is the primary driver for moisture mobilization.

Ventilation in a drift with multiple heat output packages was also considered. Even a low flow ventilation was effective in reducing the temperature in the drift and smoothing the heats of the packages. Even the temperatures around a very high heat package were reduced to acceptable levels and the temperatures around the cooler WPs were increased. Substantial cooling was achieved with a high flow ventilation.

Costs of ventilation were evaluated. The results of these analysis found that natural ventilation (less than about 1 m³/s) would have essentially no cost impacts to the Program. To provide for 1 m³/s ventilation would have relatively minimal cost impact (about 0.3 percent of MGDS costs) while a high flow rate would add a significant increase in cost (about 25 percent of MGDS costs). In addition to costs, the high flow case would need to add an additional 7 shafts and there is a concern in increasing the number of holes that would be put in the mountain. The number of inlets to the repository should be kept to a minimum.

In addition to ventilation effects, the effects of alternative management techniques such as looped ventilation, axial heat pipes, and thermal rock bolts were addressed. The looped ventilation recirculates air between two drifts and allows no fresh air to enter. This has the effect of smoothing the temperature distributions but appears to have little other advantage. Axial heat pipes and thermal rock bolts were also found to be able to smooth the temperature profiles and distribute heat. The thermal rock bolts appeared to be more effective at reducing the temperature of the drift walls than did the axial heat pipe method. These deserve further investigation.

WP aging and/or selection of WP heats for emplacement was evaluated in the study. These thermal management methods can be applied on the surface prior to disposal and were found to be effective at reducing waste stream variability. The elimination of the MPC concept allows a certain amount of flexibility in being able to select assemblies (blending) to configure a WP to meet some heat limit. Additionally, it is anticipated (based on pending legislation) that some form of ISF will be available. Thus, the study examined a variety of cases from the base case that exists now of emplacing whatever is received in the order it is received to selection of assemblies (fine blending) from a "pool" of assemblies stored in an ISF.

Significant variability of heat outputs of the WPs was found for the base case which emplaced WPs as received. One-standard deviation heats for OFF PWR fuel were almost 3 to 4 kW while the standard deviation for YFF PWR fuel is almost 6 kW. This means that while the average heat output at emplacement of a large WP is about 10 kW, some packages could have as little as below 4 kW and some above 18 kW heat output. Using storage and blending to reduce these variations was determined to be very effective. A likely scenario for an ISF operation is to start receiving waste about 7 years prior to the start of waste emplacement. This provides a substantial "pool" of WPs or assemblies to select from for configuration of the waste stream that will be emplaced. Coarse blending which only allowed selection of WPs to meet some target heat provided a substantial reduction in the standard deviation of WP heats on an annual basis. Fine blending, which provided for selection of individual assemblies to meet a target WP heat, provided the most reduction in heat variability with on-standard deviations for PWR fuel on the order of a few hundred watts and for the BWR fuel the deviation is a few tens of watts. These should provide ample opportunity to smooth the heat load in an emplacement drift.

Costs for surface facility operations to perform the blending and WP selections necessary to modify the waste stream for emplacement were evaluated. The costs for an ISF were not included in this analyses since it was assumed that, if created by legislation, this would be a fixed cost to the Program. However, any operations to select packages or assemblies from storage was included. The results were encouraging that this type of effort would not result in a significant impact on the MGDS. Specifically, the cost increase to achieve fine blending to the assembly level was about \$45M or approximately 0.4 percent of MGDS costs.

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6. ALTERNATE THERMAL LOADS

A License Application will require, per 10 CFR 60.21(c)(1)(ii)(D), that "the analyses shall also include a comparative evaluation of alternatives to the major design features that are important to waste isolation, with particular attention to the alternatives that would provide longer radionuclide containment and isolation." Evaluation of alternative thermal loads will be required in this process. The Program is focusing design on a high thermal loading but will, according to the thermal strategy (CRWMS M&O 1995a), "maintain prudent levels of flexibility by including alternative areal mass loadings." Based on these reasons, this study will examine and make recommendations as to what alternative thermal loadings should be considered for the evaluation process. To do this, the study will examine the costs of ensuring a viable option (sufficient detail of design and technical backup) is available. For the most part, in the short term, flexibility can be maintained easily, possibly through some additional figures or sketches. However, at some time, additional (in addition to what is being gathered for the high thermal load) information may be required, and at some point, if a decision has still not been made, constraints may have to be applied to the rate or method used for emplacement. This study will identify some representative alternatives for consideration and will indicate the impacts (to cost and schedule) of maintaining these.

The current design for the ACD is a loading of about 20.5 kgU/m² (83 MTU/acre). Based on preliminary, unverified analytic predictions this thermal load meets the current 10,000 year remanded standard for releases to the accessible environment. However, the Project might want to change thermal loading at some time prior to License Application for a number of reasons. Results of thermal tests and future, verified analyses could indicate that the performance standards, once repromulgated, may not be met at the ACD thermal load. Another reason for changing thermal loading is that possibly improved performance (increased margin of safety and/or confidence) could be achieved for either lower costs or a negligible cost increase. High thermal loads produce coupled (thermal-hydrologic-mechanical-chemical) behavior at large distances from the potential repository (boiling conditions can exist up to the PTn layer). If, based on the results of thermal tests, it is determined that information from near-field tests cannot be adequately extrapolated to larger scales, a decision might be made to reduce the thermal loading so that the coupling is confined to the near field. Also, a lower thermal loading may allow the Project to place more reliance on ambient measurements made in such natural barriers as the PTn or CHn. Thus, maintaining adequate flexibility through alternate thermal loads, at least through design options, can provide a prudent means of risk reduction. There does not appear to be a reason at this time to go to a higher thermal loading as discussed below.

6.1 ALTERNATE THERMAL LOADS FOR INVESTIGATION

The 1993 Thermal Loading Study examined a range of alternative thermal loads and concluded (CRWMS M&O 1994a) that a maximum thermal loading of 24.7 kgU/m² (100 MTU/acre) should not be exceeded. Nothing since that time has provided a convincing argument for exceeding that bound. In fact the results of the evaluations of thermal criteria (200°C drift wall temperature and the 115°C TSw2/3 interface with the suggested revision to 90°C at the top of the zeolite layer) in this study would continue to limit the thermal loading to less than or equal this value.

The 1993 Thermal Study did not put any restrictions on the lower limit of thermal loading to consider. However, the analysis did not consider any thermal loads less than about 6.0 kgU/m² (24 MTU/acre), primarily due to the fact that at the time this would allow emplacement of the statutory maximum (70,000 MTU) at Yucca Mountain in what was then postulated to be the amount of acceptable area. It was believed that approximately 1.2 x 10⁷ m² (2900 acres) might be available, considering expansion areas, for emplacement of waste. This was based primarily on some conceptual designs drawn (CRWMS M&O 1994b) updating the area identified in the SCP which had been about 1.1 x 10⁷ m² (2630 acres). Recently, subsurface ESF have provided information to indicate that possible expansion to the north may be feasible. The consideration of using additional area and the cost associated with this additional area will be addressed in this section.

An evaluation was done in this study as to the feasibility of carrying options for alternate thermal loads. Most of the examples discussed in other sections of this report were calculations performed with high thermal loads (ACD or higher). However, that was done to try to assess the impact of heat on various natural and engineered barriers. This section will look at thermal loads of 6.2, 8.9, 14.1, and 20.5 kgU/m² (25, 36, 57, and 83 MTU/acre). At this point, a reason to go to a higher thermal loading might be to emplace more than 70,000 MTU into the existing area. However, there appears to be additional area available (see below). Higher thermal loads may result in violating thermal criteria. Additionally, higher thermal loads would use less area than the primary area but would provide negligible cost savings since characterization costs would be unchanged. Thus, thermal loads above the ACD design were not considered. Based on the following evaluations, additional discussion will be provided as to why higher thermal loads were not chosen.

6.2 ESTIMATES OF USABLE EMPLACEMENT AREA

This subsection explores the issue as to how much potential area may be available for emplacement of spent nuclear fuel at Yucca Mountain. Site information acquired from the ESF and site geologic modeling activities have been used to estimate the maximum amount of potential emplacement area available to a repository at Yucca Mountain.

This subsection uses a certain set of assumptions. These assumptions are listed below.

- A. The study considers the statutory maximum of 70,000 MTU of nuclear waste consisting of 63,000 MTU of spent nuclear fuel and 7,000 MTU of DHLW.
- B. ACD WP schedule and dimensions.
- C. Length of mains was estimated using the drift spacing times four main drifts (ACD Layout). (e.g. every emplacement drift requires 4x22.5m=90m of main drifting)
- D. The three lower AML cases were also assumed to require additional main drifting to access the non-contiguous emplacement areas (lower block, and Optional Areas A, B, & C). Six thousand meters were added to the 14.1 kgU/m² (57 MTU/acre) case, 12,000 m to the 8.9 kgU/m² (36 MTU/acre) case, and 18,000 m to the 6.2 kgU/m² (25 MTU/acre) case.

- E. Thermal buffer width was varied with AML. 20.5 kgU/m²: 35 m, 14.1 kgU/m²: 30 m, 8.9 kgU/m²: 25 m, 6.2 kgU/m²: 20 m.

A previous M&O report (1994b) showed potential expanded repository layouts based on limited site information. This work showed four adjacent "optional" emplacement blocks in addition to the primary area's upper and lower blocks. One optional area was located north of the primary area while the other three were shown west of the primary area.

Work currently in progress in repository design is aimed at re-defining the northern limits of the primary area. This activity was prompted by excavation of the ESF tunnel through the area traversed by the Drill Hole Wash Fault. This fault was thought, based on surface mapping and drill information, to be a significant feature. For this reason, it had been used as the northern boundary of the primary area since the development of the Site Characterization Plan Conceptual Design Report in 1987. Tunneling through the area during 1995 showed the structure to be less prominent than originally thought, and its use as a bounding feature is being reconsidered.

There is limited drilling information north of the Drill Hole Wash Fault area. A single hole, G-2, located approximately 2,400 m north of the northern edge of the emplacement area shown in the ACD Report (CRWMS M&O 1996a), provides data for the repository design three-dimensional stratigraphic model. Preliminary results from the model show that, based on these data, the potential exists to expand the current repository layout concept approximately 1,000 m to the north of the ACD northern limit while staying within the TSw2 and under at least 200 m of cover. A potential disadvantage of such an expansion (at least beyond about 500 m) is that the minimum vertical distance from the repository to the water table would be approximately 100 m, as opposed to 200 m in the ACD layout. Using the same logic and information, the lower block area can also be extended northward. The Sever Wash Fault has been used as the new northern bounding feature in this expansion. A concern could be raised over emplacing a high thermal load in this additional area because it has been shown (CRWMS M&O 1996b) that closer proximity to the water table will result in much earlier rewetting of the repository due to the heat drawing water from the water table. However, this should be less of a concern for using this area for emplacing a lower thermal load.

Figure 6.2-1 shows the northward expansion, and the other three non-contiguous "optional areas." The northward expansion encompasses what was called "Optional Area A" (CRWMS M&O 1996b), while the other three optional areas are shown as they were in the 1996 work, but have been re-designated "A," "B," and "C."

The total emplacement area potentially available is given in Table 6.2-1. The areas labeled primary area and lower block include the potential expansion to the north. The area shown is assumed usable for emplacement, i.e.; thermal buffers, mains, etc. are accounted for elsewhere. Thus, there is more area associated with those blocks and optional areas but it was not included in this table. There is, however, no allowance made for faulting or other poor ground conditions resulting in loss of emplacement area.

Figure 6.2-1. Estimate of Maximum Available Emplacement Area

Table 6.2-1. Maximum Emplacement Area Available

Area	Usable* Emplacement Area (10 ⁶ m ²)	Usable *,** Emplacement Area (Acres)
Primary Area - Upper Block***	4.65	1,150
Lower Block Expansion Area***	2.16	535
Optional Area "A"	1.76	435
Optional Area "B"	1.46	360
Optional Area "C"	2.16	535
Total	12.20	3,015

* No allowance made for potential loss of area due to faulting or other ground conditions

** Thermal buffer areas and access drift areas not included in totals

***Include potential expansion to the north beyond the ACD Primary Area

It is important to understand that the areas shown in Figure 6.2-1 which lie outside the current "Primary Area" as defined in *Definition of the Potential Repository Block* (CRWMS M&O 1995h) are speculative. The areas shown are based on minimal geologic information, and significantly more site data would be required before the utility of these areas could be considered proven. There is, however, some evidence from limited borehole core samples which showed that some of the expansion areas had mineral distributions, thicknesses, and abundances which were similar to the range of these parameters observed in the Primary Area. Thus, it was concluded (CRWMS M&O 1996b) that at least some of the expansion areas may be similar in performance to the Primary Area for emplacement of waste. At least there is no evidence at this time which would indicate that these areas are not useable.

Areas Used by Various AMLs

The four AMLs considered in the area evaluation were 6.2, 8.9, 14.1, and 20.5 kgU/m². The usable emplacement area required for each option, based on emplacing 70,000 MTU at the given thermal loading, is shown in Table 6.2-2.

Table 6.2-2. Usable Area Needed For Emplacement

Areal Mass Load (kgU/m ²)	Areal Mass Load (MTU/acre)	Usable Area Required (10 ⁶ m ²)	Usable Area Required (Acres)
20.5	83	3.41	843
14.1	57	4.97	1,228
8.9	36	7.87	1,944
6.2	25	11.33	2,800

The total amount of area needed is larger than the usable area requirement because it includes the area needed for mains and thermal buffers in addition to that needed for emplacement. Table 6.2-3 shows the estimated total area needed for each of the four AML options. The purpose of this table is for costing purposes for characterization since one should recall that buffer and access areas needed have already been removed from the usable area table (Table 6.2-1).

Table 6.2-3. Total Area Needed

Areal Mass Load (kgU/m ²)	Areal Mass Load (MTU/acre)	Total Area Required (10 ⁶ m ²)	Total Area Required (Acres)
20.5	83	4.21	1,041
14.1	57	6.00	1,484
8.9	36	9.30	2,298
6.2	25	13.10	3,238

Comparing Tables 6.2-1 and 6.2-2, one can see that, for emplacement of 70,000 MTU, the 20.5 kgU/m² (83 MTU/acre) option would fit entirely within the upper block of the primary area, with approximately 1.21×10^6 m² (300 acres) to spare. Emplacement at 14.1 kgU/m² (57 MTU/acre) would require use of the entire upper block as well as a portion of the lower block. The use of a mass loading of 8.9 kgU/m² (36 MTU/acre) would require all of the upper and lower blocks (as depicted on Figure 6.2-1) as well as a portion of Optional Area "A." The 6.2 kgU/m² (25 MTU/acre) option would use all of the upper and lower blocks, all of Optional Areas "A" and "B," and about two-thirds of Optional Area "C."

Drifting Required for Two Different WP Emplacement Arrangements

Each of the four AMLs was evaluated for drifting requirements under two different WP emplacement arrangements. One arrangement kept the WP spacing within the drifts at the same value shown in the ACD Report. The drift spacing was adjusted to reach each of the four AMLs evaluated. The second arrangement was a "line-load" concept in which WPs were assumed to be emplaced 1 m apart. Again, the emplacement drift spacing was adjusted to reach each of the four AMLs. The width of the thermal buffers was assumed to vary for each of the AML cases. The ACD value of 35 m was used for the 20.5 kgU/m² (83 MTU/acre) case. The buffer width was reduced 5 m for each subsequent case. That is, the 14.1 kgU/m² (57 MTU/acre) case assumed a thermal buffer of 30 m. The 8.9 kgU/m² (36 MTU/acre) case was done based on a 25-m thermal buffer width, and the 6.2 kgU/m² (25 MTU/acre) case assumed a 20-m thermal buffer. This accounts for the fact that the total length of emplacement drift changes for each case even though the WP spacing within the drifts is constant across all options. Table 6.2-4 shows the resulting required lengths of emplacement drifting and main drifting for the ACD WP spacing, and Table 6.2-5 shows the same information for the "line-load" concept.

Table 6.2-4. Required Length of Drifting ACD WP Spacing

Areal Mass Load (kgU/m ²)	Emplacement Drift Required (Meters)	Main Drifting Required (Meters)
20.5	179,000	15,660
14.1	174,200	28,173
8.9	170,100	46,254
6.2	167,000	66,406

Table 6.2-5. Required Length of Drifting Line-Load WP Spacing

Areal Mass Load (kgU/m ²)	Emplacement Drift Required (Meters)	Main Drifting Required (Meters)
20.5	89,788	15,405
14.1	87,817	27,883
8.9	85,930	46,208
6.2	84,123	66,048

6.3 COST ANALYSIS

A cost analysis was done for the various thermal load cases to estimate the difference between the base case of 20.5 kgU/m² (83 MTU/acre) and another thermal load. Consideration was given to characterizing the additional area needed and these estimates were obtained based on discussions with site characterization personnel. Management costs, and the cost of drifting and developing the additional emplacement areas, were included.

Assumptions. The cost analysis conducted for this study considers the statutory maximum of 70,000 MTU of nuclear waste consisting of 63,000 MTU of spent nuclear fuel, and 7,000 MTU of DHLW as defined in the base case documented in the 1996 ACD Report (CRWMS M&O 1996a). The cost is presented in constant FY 1995 dollars. All cost presented in this document intended to provide differentiation between thermal load study options, is a Rough Order of Magnitude in nature and should not be taken as a substitute for a detailed cost estimate based on a point design required to facilitate options implementation. Specific assumptions follow:

Development and Evaluation. Development and Evaluation costs in this study contain only costs associated with suitability determination analyses for the repository area. Reference data pertaining to the repository primary area.

- A. Historical Costs for the period FY 1983 through FY 1989 are all attributed to suitability determination.
- B. Historical Costs for the period FY 1990 through FY 1995 and all future costs were allocated as shown in Table 6.3-1. The historical costs through FY 1995 are shown in Table 6.3-2.

Table 6.3-1. Historical Costs Allocation Table

WBS #	WBS Title	Percent of WBS Actuals/Projections
1.2.1	Systems Engineering	50
1.2.3	Site Investigation	100
1.2.6	Exploratory Study Facility	100
1.2.7	Test Facilities	100
1.2.9	Project Management	30
1.2.11	Quality Assurance	30
1.2.12	Information Management	30
1.2.15	Support Services	30
Other WBS element are assumed not to affect site suitability.		

- C. Future years cost: Period FY 1997 through FY 2002 data from *Civilian Radioactive Waste Management Program Plan* (Program Plan), Revision 1 Draft (DOE 1996B), as available in planing at the third level WBS element and are presented in Table 6.3-3.
- D. Future years cost: Period FY 2003 through FY 2010 estimates from the 1995 Total Systems Life Cycle Costs Analysis. Future years' costs are provided in Table 6.3-4. Design and evaluation (D&E) cost summary is presented in Table 6.3-5.

Table 6.3-2. Historical D&E Costs Attributed to Site Suitability Determination
(Million FY 1995 Dollars)

Source: Project Cost & Schedule Baseline, YMP/CM-0015, Rev 5, 6/8/95

WBS#	WBS TITLE	FY1983	FY1984	FY1985	FY1986	FY1987	FY1988	FY1989	FY1990	FY1991	FY1992	FY1993	FY1994	FY1995	TOTALS
1.2.1	Systems Engineering	1.90	5.35	4.65	11.11	9.01	9.07	10.49	10.74	12.13	13.06	3.17	3.23	3.91	97.82
1.2.3	Site Investigation	29.51	30.57	23.07	32.14	33.23	42.12	30.65	39.31	52.65	44.72	40.57	46.01	88.85	533.40
1.2.6	Exploratory Study Facility	5.81	4.05	8.05	11.62	15.29	22.79	21.20	14.25	15.03	8.02	34.58	52.45	103.99	317.16
1.2.7	Test Facilities	4.25	3.54	1.95	1.16	0.52	1.13	1.95	1.29	1.58	1.88	-	-	21.23	40.48
1.2.9	Project Management	-	-	-	-	-	-	-	-	-	-	-	-	-	-
1.2.11	Quality Assurance	-	-	-	-	-	-	-	-	-	-	3.07	2.80	2.85	8.72
1.2.12	Information Management	-	-	-	-	-	-	-	-	-	-	3.37	3.15	4.16	10.68
1.2.15	Support Services	-	-	-	-	-	-	-	-	-	-	1.13	1.14	5.18	7.45
Totals		41.47	43.52	37.74	56.02	58.04	75.10	64.30	65.60	81.39	67.68	85.89	108.78	230.17	1,015.71

Table 6.3-3. Development and Evaluation Costs Attributed to Site Suitability Determination
(Million FY 1995 Dollars)

Source: Program Plan (DOE 1996b) Revision 1 (Draft) inputs, Primavera Project Planner, run # 3971,5/16/96

WBS #	WBS TITLE	FY 1996	FY 1997	FY 1998	FY 1999	FY 2000	FY 2001	FY 2002	TOTALS
12.1	Systems Engineering	2.94	2.77	2.94	2.71	2.94	1.68	0.35	16.33
12.3	Site Investigation	39.19	43.17	28.97	26.85	23.36	19.50	5.04	186.08
12.6	Exploratory Study Facility	59.43	36.31	25.29	22.03	9.24	8.49	4.14	164.93
12.8	Environ. Health & Safety	16.78	18.03	16.95	14.87	13.86	9.84	3.88	94.21
12.9	Project Management	3.15	3.97	3.89	3.74	3.50	3.37	1.35	22.97
12.11	YMP QA Support	3.82	7.13	7.13	7.13	6.34	6.30	2.60	40.45
12.12	Information Management	9.56	4.94	5.73	5.71	4.33	4.20	2.02	36.49
12.15	Support Services	9.40	3.11	2.92	2.79	2.70	2.59	1.04	24.55
Totals		144.27	119.43	93.82	85.83	66.27	55.97	20.42	586.01

Table 6.3-4. Development and Evaluation Costs Attributed to Site Suitability Determination
(Million FY 1995 Dollars)

Source: 1995 Total Systems Life Cycle Cost Analysis, DOE/RW-0479, Dated September 1995

WBS #	WBS TITLE	FY 2003	FY 2004	FY 2005	FY 2006	FY 2007	FY 2008	FY 2009	FY 2010	TOTALS
1.2.1	Systems Engineering	7.82	7.12	6.08	5.21	4.34	3.47	2.69	2.69	39.42
1.2.3	Site Investigation	25.74	25.74	25.74	25.74	25.74	25.74	25.74	25.74	205.92
1.2.6	Exploratory Study Facility	-	-	-	-	-	-	-	-	-
1.2.7	Test Facilities	10.38	8.30	6.75	6.75	6.75	6.75	4.15	4.15	53.98
1.2.9	Project Management	4.98	4.98	4.98	4.98	4.98	4.98	4.98	4.98	39.84
1.2.11	Quality Assurance	7.16	7.55	7.81	8.06	8.52	8.97	9.42	9.57	67.06
1.2.12	Information Management	7.60	7.67	7.69	7.80	8.01	8.16	8.13	8.23	63.29
1.2.15	Support Services	7.48	7.48	7.48	7.48	7.48	7.48	7.48	7.48	59.84
Totals		71.16	68.84	66.53	66.02	65.82	65.55	62.59	62.84	529.35

Table 6.3-5. Development & Evaluation Summary

Cost Reference/Period	Million Dollars (FY 95)
Historical (FY 83 - FY 95)	\$1,015.71
Program Plan Rev. 1 (FY 96 - FY 02)	\$586.01
95 TSLCC Post Program Plan (FY 03 - FY 10)	\$529.35
Totals	2226.07

Primary repository area. The primary repository land area and underground layout (Source: 1996 ACD data) is summarized in Table 6.3-6.

Table 6.3-6. Primary Area ACD Land Usage

Area Designation	Acres
Main Drifts	70
Inspection Drifts	16
Thermal Buffer	133
Emplacement Area	856
Totals	1,075

The ACD source identifies a total of 949 acres as the amount of the primary area available for emplacement. However, as indicated in Subsection 6.3, expansion of the Primary Area to the north may be possible. The area identified in Table 6.3-6 refers to the primary area that was used in the MGDS ACD Report (CRWMS M&O 1996a). Additional emplacement area (optional areas plus expansion of the primary area to the north), if required, is assumed to require site characterization/suitability determination investment.

6.4 WASTE PACKAGES

The waste package design defined in the MGDS ACD Report (CRWMS M&O 1996a) is assumed, based on the latest waste package designs and current corrosion models, to be sufficiently robust and thus will perform similarly in the range of thermal loads investigated in this study. The disposal container for HLW glass that was developed during ACD appears to be the most resistant to corrosion in the Yucca Mountain environment. This container has a cupronickel corrosion allowance barrier. The thickness of the containment barrier on the SNF and defense HLW is driven primarily by rockfall and radiolysis effects requirements and should be more than adequate to handle the potentially more humid environments associated with lower thermal loads. If waste package materials change and/or microbial corrosion is found to be a problem at some thermal loads and not others then this assumption will need to be reevaluated. Thus no waste package procurement cost

deltas, as a function of thermal loads, are assumed. Waste package quantities, associated thermal outputs, and related variables based on the 1996 ACD design base, are summarized in Table 6.4-1.

Table 6.4-1. ACD 1996 - Design Base Summary

	125 Ton Canistered		75 Ton Canistered			Bare Fuel (UCF ²)	DHLW ³ (4 pour glass canisters)
	BWR	PWR	BWR	PWR	B-In-P ¹		
WPs	2,242	4,041	1,505	765	40	185	3,259
Total MTU	15,851	35,682	6,291	3,573	167	1,634	7,007
MTU/W Pkg.	7.07	8.83	4.18	4.67	4.18	8.83	2.15
WP Length (m)	5.68	5.68	5.65	5.65	5.33	5.34	3.68
ACD Waste Package Spacing (m)	15.32	19.12	9.08	10.12	9.08	19.12	5.18

¹ BWR emplaced in PWR WPs

² Uncanistered Fuel

³ Defense High-Level Waste

Thermal Load Options. This cost analysis consists of a comparison between the cost associated with the following thermal load and emplacement area layout options:

1. ACD design spacing Concept. WPs are spaced as specified in the table above.

- 1.1 AML equals 20.5 kgU/m² (83 MTU/acre)
- 1.2 AML equals 14.1 kgU/m² (57 MTU/acre)
- 1.3 AML equals 8.9 kgU/m² (36 MTU/acre)
- 1.4 AML equals 6.2 kgU/m² (25 MTU/acre)

2. Line load spacing concept. WPs are spaced 1 m apart.

- 2.1 AML equals 20.5 kgU/m² (83 MTU/acre)
- 2.2 AML equals 14.1 kgU/m² (57 MTU/acre)
- 2.3 AML equals 8.9 kgU/m² (36 MTU/acre)
- 2.4 AML equals 6.2 kgU/m² (25 MTU/acre)

Area Characterization Cost Factors. The site characterization process at Yucca Mountain was phased as follows.

- Preliminary Site Characterization (FY 1983 - FY 1990), Area characterized ~1,075 acres
- Primary Area Site Characterization (FY 1991 - FY 2002), Area ~1,100 acres
- Primary Area Site Characterization in support of License Application (and License Application update) (FY 2003 - FY 2009), Area ~1,100 acres
- Area characterization cost factors developed for this study are summarized in Table 6.4-2
- The preliminary site investigation phase is assumed to have been completed for all potential expansion areas
- Available site characterization and surface drilling measurements indicate that mineralogy in other areas of Yucca Mountain is similar to that in the primary area and subsurface features may not be as pronounced as originally thought. Thus, site characterization estimates that it will be less expensive to characterize additional areas. It is assumed that the cost required to characterize expansion area will be reduced to 10 percent of the primary area cost per acre. This results in a cost ratio of \$140,000/acre of expansion area for acreage that is within the preliminary site investigation area. The historical characterization costs included costs of an extensive drilling program (WBS 1.2.3), an Exploratory Study Facility (WBS 1.2.6) and various Testing Facilities (WBS 1.2.7). The Site investigation professionals consulted have indicated that based on historical borehole data analysis it was determined that some of the characteristics for any ground structure that have been characterized in the primary area will be valid for similar type ground structure in the additional area and drilling and testing for those characteristics need not be repeated (defined as lessons learned). It was assumed that some uncertainty related to ground structure type will require some borehole drilling and testing (~10%). Likewise for similar type ground structure no additional exploratory tunneling will be required. Those were the technical factors in defining the remaining cost as ~10% of the historical cost.

An assumption used in this evaluation, that deserves additional explanation, is that the planned thermal tests (laboratory, in situ, and natural analog studies) are adequate for any thermal loading (low or high). This has not been established as yet since there is currently an uncertainty as to how long thermal tests will be needed to adequately characterize the coupling (THMC) and the impact on such distant natural barriers as the PTn and the CHn. There is the possibility that high thermal loads that result in boiling conditions hundreds of meters above the potential repository, could require significantly longer testing than would be required with a low thermal loading. Until preliminary information from the thermal tests is analyzed, and the Waste Isolation Strategy defines the important natural barriers, the assumption that the currently planned tests are adequate is all that could be done.

Cost Reference Base. The cost reference case is the MGDS ACD Report dated March 1996, Volume IV (CRWMS M&O 1996a). The base case costs are provided in Table 6.4-2 for characterization and the total ACD base case costs in Table 6.4-3.

Table 6.4-2. Area Characterization Cost Factors

	Total Million Dollars (FY 95)	Total Area Characterized (acres)	Cost Factors (FY 95 Dollars)
Preliminary Site Investigation (FY 1983 - FY 1990)	\$442	~1,075	\$41,100/acre
Primary Area Site Investigation, Pre LA (FY 1991 - FY 2002)	\$1,160	~1,100	\$0.92 Million/acre
Primary Area Site Investigation, Post LA (FY 2003 - FY 2010)	\$529	~1,100	\$0.48 Million/acre
Totals	\$2,226		

Table 6.4-3. Advanced Conceptual Design Cost Summary (Million FY 1995 Dollars)

	Repository Construction	Repository Operations		Repository Closure & Decommissioning	Repository Total
		Emplacement	Caretaker		
Totals	\$2,024	\$7,280	\$1,335	\$449	\$11,088

The total reference ACD repository cost includes estimates of D&E required to support design and design related efforts. That D&E estimate does not reflect any site characterization costs and is omitted here.

The ACD underground layout included 179 km of emplacement drifts and 15.7 km of main drifts, it utilized $4.21 \times 10^6 \text{ m}^2$ (1,041 acres) in the Yucca Mountain Lower and Upper blocks; however, a total of $4.35 \times 10^6 \text{ m}^2$ (1075 acres) were characterized and available. This data was used in the cost delta from ACD analysis presented in the results section.

Cost Results. A repository layout for each of the thermal loading options was generated and used as a basis for computing the total required area, and the total length for emplacement and main drifts, respectively. These computation and the ACD cost factors for underground capital and operation investment over the ACD life cycle were used to generate delta cost estimates. The calculations reveal that as the AML is reduced the total emplacement drift length is reduced since lower AML requires less buffer area and associated stand off excavation. The total main drift length increases as the AML is reduced due to longer drift spacing; however, the net life cycle cost delta (not including D&E costs) does not exceed \$600,000 (FY 1995) in the range of interest for this study. This change to the ACD \$11 billion dollar life cycle cost (excluding D&E) is negligible and within the range of estimating uncertainties. The maximum delta estimated for this study constitutes about a 2.5 percent change to the ACD reference cost which does not contain all the D&E cost, it is

therefore negligible and within the range of estimating uncertainties. The results are shown in Table 6.4-4.

Table 6.4-4. Cost Delta from ACD - Summary

		Drifts Delta from ACD		Delta from ACD Area Required (acres)	Costs (Million FY 95 Dollars)		
Option #	Area Mass Loading (kgU/m²)	Main (km)	Emplacement (km)		Capital & Operating Cost Delta	Site Characterization Cost Delta	Delta Summary
ACD WP spacing concept.							
1.1	20.5	0.0	0.0	0	0.00	N/A	0.00
1.2	14.1	12.5	(4.8)	443	0.21	62.02	62.23
1.3	8.9	30.6	(8.9)	1,257	0.54	175.98	176.52
1.4	6.2	50.7	(12.0)	2,197	0.91	307.58	308.49
Line load WP spacing concept.							
2.1	20.5	0.0	0.0	0	0.00	N/A	0.00
2.2	14.1	12.5	(2.0)	443	0.23	62.02	62.25
2.3	8.9	30.8	(3.9)	1,257	0.58	175.98	176.56
2.4	6.2	50.6	(5.7)	2,197	0.96	307.58	308.54

6.5 DECISIONS POINTS

Carrying alternative designs in a such a Project as Yucca Mountain is certainly a prudent thing to do, even if the regulations did not require evaluation of alternative, however, at some point the Project could possibly begin to incur cost and schedule constraints by carrying alternatives. Carrying alternative thermal loads provides contingencies against such unexpected events as results from thermal tests, which are typically several years in duration, indicating that the spent nuclear fuel cannot be safely emplaced at a high thermal load. Although such an outcome is not anticipated based on currently unverified models it is not beyond the realm of possible outcomes and retaining alternatives would mitigate this from causing a major delay in the Project. The cost and subsurface design information in the preceding sections provides some basis to try to address when decision points are needed in the process of developing a repository.

At the early stages of the repository development, carrying alternatives is relatively easy since it generally involves making a few additional drawings and possibly performing some calculations (design and performance) for a few additional cases. However, as the design matures and the Program gets into the License Application process there are times when decisions are needed to reduce the alternatives as a result of cost and schedule constraints which would be incurred.

The most likely scenarios would be for unexpected outcomes to be found in the thermal tests near the end of those first tests (around 1999). If the results were to indicate higher thermal loads would be needed there would be no impact on the Program other than running some additional calculations, unless more testing is indicated. Additional area would not be needed. If on the other hand, lower

thermal loading is indicated (it is likely to be in the range of 6.2 to 9.9 kgU/m² (25 to 40 MTU/acre)), additional area would be needed. It should be noted that one of the reasons for the selection of the 6.2 to 9.9 kgU/m² loading is because this establishes conditions where the bulk average repository is below boiling. At this point the Project would be less than three years from submitting the License Application and might not have time to characterize the additional area in time to include it in the initial application. However, this should not preclude the Project from applying to construct the repository to accommodate the low thermal load using the area previously characterized (the Primary area). For example, using all of the Primary Area (both upper and lower block) would allow about 61,000 MTU to be emplaced at a thermal load of 8.9 kgU/m² (36 MTU/acre). At the time of License Application plans would need to be provided to show how the additional areas would be characterized. Additionally, discussion would be needed in the License Application as whether or not the characterization of the additional areas would impact waste isolation and if it possibly might how will the Project mitigate this problem. For example plans will exist as to how boreholes are to be sealed to avoid them becoming preferential pathways. Additional boreholes could be handled in the same way. The drifting to the optional areas may be more challenging but similar steps, as will be taken to seal the repository upon closure, are the most likely mitigating options.

The study therefore recommends that the alternative thermal loading 8.9 kgU/m² (36 MTU/acre) be pursued at a relatively low level of effort until sufficient results from thermal testing are available to predict with confidence that the tentatively chosen high thermal loading will support the repository in meeting its performance objectives. These results are expected to be available by the end of 1999. The scope of the effort to maintain the alternative thermal loading can be limited to a low level of design work, an additional performance assessment case, and development of a plan for characterizing additional area if required. These minimal costs are believed to be supportable and prudent in order to prepare for the contingency that the relatively high thermal loading case might be determined to be unacceptable. Management may choose to continue to pursue the alternative thermal loading design even further into the future, balancing the additional cost of maintaining the option and the (hopefully) increasing confidence in the adequacy of high thermal loading against the significant delays should low thermal loading later be found necessary.

A firm decision on thermal loading should be made as soon as practical after sufficient thermal testing results are available, because it would take time to characterize additional potential emplacement areas and to revise the licensing basis to be presented to the NRC in the License Application if the alternative thermal loading must be used. Also, it is very desirable, from a licensing standpoint, to have thermal loading issues resolved prior to License Application submittal to minimize the likelihood of a licensing issue emerging on this subject.

If the need to use a low thermal loading does not become apparent until after the License Application is submitted (perhaps as a result of performance confirmation activities), the need for additional area characterization and amendment to the already-submitted License Application could result in significant delay in receipt of the License to Construct. An even worse situation would occur if emplacement of wastes had already begun when the need to reduce thermal loading became apparent. Retaining design flexibility by, for example, initially emplacing waste in every other drift or at a wider line spacing could minimize both delays and the need to move waste already emplaced, though at potential cost in emplacement rate. Options such as these are discussed in the *Waste Emplacement Management Evaluation Report*.

6.6 SUMMARY

The regulations [10 CFR 60.21(c)(1)(ii)(D)] and Thermal Strategy (CRWMS M&O 1995a) directs that alternatives, in this case alternative thermal loads, be considered. In addition to the design basis thermal loading of 20.5 kgU/m² (83 MTU/acre) which is currently in the MGDS ACD Report (CRWMS M&O 1996a), this study evaluated three other thermal loads which were 6.2, 8.9, and 14.1 kgU/m² (25, 36, and 57 MTU/acre).

Higher thermal loads than 20.5 kgU/m² were not evaluated for the following reasons. First, a 1993 Thermal Study (CRWMS M&O 1994a) recommended that loadings above 24.7 kgU/m² (100 MTU/acre) were too hot. A 24.7 kgU/m² loading was not considered due to the fact that, although not all of the thermal goals were violated, some were violated at this loading. Thus, this thermal loading was considered as too close to the margin of safety to be a prudent choice. Some suggest going to the higher loading (higher than 20.5 kgU/m²) to ensure that if the law is changed all of the countries nuclear waste can be emplaced in the upper block. Yet if the upper block contains the additional area (see Figure 6.2-1 and Table 6.2-1) then 96,000 MTU can, essentially, be emplaced in the upper block. Even if some of the northern expansion cannot be used (without further characterization of the northernmost 500 m) then, at most, about 25 percent of the lower block in the primary area would be used. Finally, there did not appear to be any cost impacts of going to a higher thermal loading (i.e., no additional area beyond the primary area is needed). The cost analysis depends on the assumption of a waste package which can be used for either a high or low thermal loading. If this proposed waste package design is found to be suitable for both high and low thermal loads, then the cost implications associated with pursuing lower thermal loads is small.

Evaluations showed that potential additional area is likely to exist. The Drill Hole Wash Fault has not been found to be a significant feature and thus expansion of the Primary Area northward may be possible. Other optional areas to the west have been proposed, and although very limited, examination of drilling cores indicate that at least some of these areas may be similar to the Primary Area, at least similar stratigraphic features, thicknesses, and mineralogic characteristics (CRWMS M&O 1996b). As much or more area than 1.22×10^7 m² (3015 acres) may exist. Developing and characterizing this additional area for waste emplacement (i.e., going to a thermal load of 6.2 kgU/m² (25 MTU/acre)) would increase the cost of the MGDS by about 2.5 percent which is easily within the uncertainty bands of cost estimation.

Carrying alternative thermal loads, especially lower thermal loads which require the most emplacement area, is a prudent course of action primarily for the following reason. The results of the long duration in-situ thermal tests will not be known for several years, possibly not even until after License Application. If the tests would indicate that a high thermal load would not be licensable (could not be shown with reasonable assurance to meet standards) then having an alternative would allow construction or licensing to continue without delays. Thus thermal loads of 6.2 or 8.9 kgU/m² (25 or 36 MTU/acre) should be considered. In the event that some of the additional area might not all be usable, a thermal load of 8.9 kgU/m² should be selected.

Assessments of impacts showed that little impact would result in retaining alternatives up to about the time a License Application to Construct is submitted. At most some additional drawings, some additional performance and design calculations, and a plan to characterize additional area would be

needed. This would mitigate the possibility that thermal tests might not substantiate the use of a high thermal loading. Should this occur and the decision is made to change thermal loading at License Application to Construct, then there will be an impact on cost (up to 2.5 percent) although as yet there does not appear to be a schedule impact. Significant impact on both schedule and cost could possibly occur if a decision to emplace is delayed until License Application.

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7. CONCLUSIONS

This report documents of the work conducted in a Thermal Loading Study over the period from October 1, 1995 through August 30, 1996. The study conducted continues the system analysis role to provide a structured, detailed analyses that will form the technical basis for ultimately making a decision as to what thermal loading should be established for the potential repository. This effort concentrated primarily on developing design requirements by evaluating thermal goals and thermal management techniques for emplacing spent nuclear fuel.

System analysis is needed on many issues involving thermal loading due to the fact that decisions in one area could impact other areas of the Program. The primary objective of this Thermal Loading Study was to provide recommendations for requirements which will provide sufficient definition to facilitate development of design concepts and support life cycle cost determinations. The study performed a reevaluation of select thermal goals which are currently being used by design to decide if recommendations should be provided for requirements. The thermal goals evaluated were the not-to-exceed temperature of 200°C on the emplacement drift wall, the 350°C fuel cladding temperature limit, and a not-to-exceed temperature limit of 115°C on the TSw2/3 interface. The study evaluated whether or not such action as edge loading is needed and must be accommodated in the design. Recommendations were developed to establish requirements on emplacement which will minimize any potential performance impacts resulting from fuel or WP variability of heat output. Additionally, the study developed recommendations as to what alternative thermal loads should be maintained to minimize Program risk, what is needed to ensure these alternative thermal loads are viable, and what constraints (schedule and cost) on the system would be incurred if a thermal loading decision is not made by a given date.

This effort primarily dealt with activities related to the MGDS for the potential repository at Yucca Mountain, Nevada. The scope of the effort encompassed a wide range of activities and involved and interfaced with a number of different organizations within the Office of Civilian Radioactive Waste Management. The basis of the calculations made were the latest data and analytic models. Some but not all of the models used were qualified under the computer software QA procedures. This effort is quality affecting work but due to the fact that in some cases unqualified data and models were used care should be exercised in using the results of this study and should not be used in procurement activities without verification. Data and assumptions identified in this document represent scoping analyses with the intention of facilitating the design process and shall be treated as unqualified. The following discussion in this section provides the results and conclusions of the study.

The evaluations done in this study do not necessarily indicate a performance of a specific design. Instead, the intent of the study was to provide recommendations which would establish requirements that the design would have to meet. In some cases the calculations were performed using conditions and/or parameters which were outside of the current ACD design. Such calculations were performed to identify changes or effects which would result in significant degradation in performance. Finding such changes or effects will allow the development of requirements criteria which will be supportable. The approach taken in this study was a conservative approach at recommending requirements which tried to maintain a defense in depth approach. This was done in part because a significant amount of uncertainty exists in many of these calculations until analytic codes can be

validated with in-situ thermal measurements. Additionally, not all of the aspects and/or thermal goals could be evaluated and thus the impact of allowing a goal that was not evaluated to be violated could not be assessed. Thus, a prudent, conservative approach to developing the following recommendations was chosen.

Data and assumptions identified in this document are for preliminary design and shall be treated as unqualified. These data and assumptions will require subsequent qualification as the testing efforts proceed. The data and assumptions associated with this analysis are not required to be procedurally controlled as TBV. However, use of any data or conclusions from this analysis for input into documents supporting procurement, fabrication, or construction are required to be controlled as TBV in accordance with the appropriate procedures.

Geochemical Thermal Goal Re-evaluation. Evaluations to examine the geochemical temperature goal of requiring the TSw2/3 interface to remain less than 115°C were conducted in this study. No technical reason could be found for the goal nor for the goal to retain the CHn to less than 115°C. In fact Smyth (1982) had recommended that the zeolitized layer temperature not exceed 85°C. Performance calculations did not show any impact as a result of exceeding this goal and recent measurements and examinations of core samples found that the clinoptilolite concentrations (the primary zeolite for sorbing radionuclides) in the variably zeolitized nonwelded and partially welded ash flow tuffs were below the TSw2/3 interface. Thus, it is recommended that both these criteria be dropped from the requirements and the following criteria (see below) be added.

To determine whether or not another criteria should be established, a process model to calculate the effects of dehydration of zeolites due to elevated temperatures was developed and coupled with a thermohydrologic model calculations of performance (in this case duration of boiling and changes in liquid saturations) were done. The calculations showed that at 20.5 kgU/m² (83 MTU/acre) there was negligible change in the repository temperatures (duration of boiling) and liquid saturations for the case which considered zeolite dehydration over the case where no zeolite dehydration was considered. For the 20.5 kgU/m² case the top of the zeolitized layer did not exceed boiling and only experienced a slight reduction in liquid saturation. A higher thermal load of 28.4 kgU/m² (115 MTU/acre) was also considered. The results of evaluations at this higher thermal load also indicated negligible changes in duration of boiling and liquid saturation predicted for the repository horizon. These calculations do, however, show that the top of the zeolitized layer exceeds boiling and significant dry out of the rock occurs for thousands of years. These calculations assumed a conservative depth of the zeolitized layer starting about 100 m below the repository horizon when the depths of this layer beneath most areas of the repository are deeper than 100 m.

The above analyses did not consider any irreversible mineralogic changes from clinoptilolite to analcime. Clinoptilolite has good sorptive properties for some radionuclides while analcime does not. Understanding the kinetics of conversion of clinoptilolite to analcime is very challenging because of slow reaction rates making it difficult to measure in the laboratory. To obtain any information on this reaction it was necessary to use natural analog studies. Natural analog studies at Yellowstone and Yucca Mountain itself were used for this analysis. It was concluded that the predominately sodium enriched clinoptilolite in the Yucca Mountain water chemistry (J-13 water) is probably stable from transitions to analcime at temperatures up to 90 to 100°C. This is reasonably

consistent with earlier findings by Smyth (1982) which indicated the possible reaction of clinoptilolite to analcime at temperatures above 105°C.

Although the calculations of dehydration of clinoptilolite at the predicted temperatures showed no effect on duration of boiling, natural analog studies indicate it would be prudent to place a criteria on the 'zeolites to prevent irreversible changes which could degrade retardation of some radionuclides. These natural analog studies found that conversion of clinoptilolite to analcime at Yucca Mountain could occur at temperatures above 90 to 100°C. The study recommends that a very conservative limit of 90°C be placed on the zeolitized, nonwelded and partially welded ash flow tuffs to limit mineralogic changes. The depth contours for the top of this zeolitized layer beneath the potential repository are shown in Figure 3.2-1. Zeolites are currently anticipated to be pervasive throughout the area of the potential repository in the CHn unit.

Applying a temperature criteria on the zeolites in the Calico Hills nonwelded unit is in keeping with the multiple barriers, defense in depth concept of the emerging waste isolation strategy. Although the zeolites will not provide much barrier against Tc and I, they should provide sorption for a number of other radionuclides such as Np, Pu, and U at times primarily beyond 10,000 years. Zeolites could also provide protection from releases of such radionuclides as Am, Cs, Sr, and others which could result from potential early failures of WPs.

A 90°C temperature limit should be established at the average depth of the top of the zeolite layer in a given emplacement area since it is impractical to know what the depth of the top of the zeolite layer is everywhere. For the upper block of the primary area this implies that the not-to-exceed temperature criteria should be placed at a depth of 170 m below the potential repository horizon. If other emplacement areas are considered, then the temperature limit should be placed at the average depth of the top of the zeolite layer beneath that portion of the repository. The results of thermal calculations found that the 90°C temperature limit will be reached at 170 m for a thermal load of 22.2 kgU/m² (90 MTU/acre). Thus, there should be no impact on the current ACD design of 20.5 kgU/m² (83 MTU/acre). If at some later time there should be a need to exceed the 90°C temperature in the zeolites, then the kinetics of conversion of clinoptilolite to analcime and the effect that porosity change might have on permeability must be understood and incorporated in the process models. Additionally, this should be reviewed occasionally as further information on zeolite compositions becomes available.

Emplacement Drift Wall Thermal Criteria. Thermomechanical stresses in the rock, if large enough, could result in local rock failure which have the potential to degrade WP long term performance and make retrieval difficult. These issues were recognized early in the Program and a not-to-exceed temperature limit of 200°C was placed 1 m into the rock for a borehole [EBDRD 3.7.G.2; SCP (DOE 1988)] and on the drift wall for horizontal emplacement drifts [CDA EBDRD 3.7.G.2; CRWMS M&O 1993]. This study reevaluated this limit, using the most updated measurements and qualified codes, to determine whether or not it was still valid. This study only addressed the near-field thermomechanical performance and did not evaluate other thermomechanical issues which have been raised such as the impact of thermomechanical effects on barriers such as the PTn. Currently we do not have additional information on this layer nor do we have three-dimensional thermomechanical models that can calculate effects on a mountain scale.

The mechanical codes used in this evaluation have been verified and controlled according to the appropriate computer software QA procedures. The data used as inputs for the codes were obtained either from the *Reference Information Base* or from recent TDIFs and, although controlled, some of the data have not been qualified. Thus, the estimates obtained in this effort are the best and highest quality that could be obtained at the time.

The structural response of the host rock in the emplacement drift was obtained as a function of time using various analytic methods. First, calculations were done to investigate the effects of both temperature and temperature gradient in the rock. Additionally, the sensitivity to uncertainties in the choice of parameters such as coefficient of thermal expansion and Young's Modulus were examined. An argument could be made that since the emplacement drifts are likely to have some form of tunnel support that calculations of thermomechanical response must include those tunnel supports and their interface with the host rock. Thus, a series of calculations were done to examine the thermomechanical effects with such tunnel supports as steel sets and a concrete liner.

The structural response of the host rock in an unsupported emplacement drift was obtained for a number of different thermal conditions using conservative boundary conditions. The results were evaluated using a rock mass strength criteria. The results indicate that for rock wall temperatures of 200°C or less no tensile or compressive (shear) failures are predicted in the modeled domain. However, predictions done at 225°C do indicate the potential for compressive failure to occur. The response of the host rock to various temperature gradients was examined and the results indicated that, while larger thermal gradients could exacerbate the extent of failure should it occur, it is the temperature that appears to be the primary driver.

Thermally-induced displacements and stresses in the rock mass and in ground support elements were calculated for times up to 150 years. The stresses were evaluated by comparing against the Mohr-Coulomb yield criterion. The calculations show that the rock mass behaves essentially elastically even with rock temperatures exceeding 200°C. At temperatures above 225°C the depth into the rock at which potential rock mass yield occurs is significantly larger (about a factor of 2) than for emplacement drifts with average heating conditions (about 150 to 180°C). Significantly larger (about 60 to 80 percent) rock displacements occur for temperatures above 200°C. The calculations of the stresses in the steel sets and concrete liner ground supports predicted that the stresses were larger than the yield criterion in all cases except for the concrete liner in a 20.5 kgU/m² (83 MTU/acre) repository with average heat output WPs. However, these calculations were overly conservative in some respects in that they did not consider any relative sliding or normal displacement which is likely to occur. Jointed steel sets or thicker concrete liners are possible to mitigate failure at the higher temperatures but these are as yet untested and would increase the costs of the tunnel supports.

Sensitivity calculations found that predicted stresses are affected by the choice of the coefficient of thermal expansion, Young's Modulus, and the Poisson Ratio. A higher coefficient of thermal expansion will produce more stress for a given temperature field. Higher thermal expansion can result in predicted rock failure even for rock temperatures of 200°C where failure was not predicted with more nominal expansion coefficients. Similarly, increases in Young's Modulus or Poisson's Ratio can result in predictions of stress failures.

Coefficients of thermal expansion being measured in the laboratory from TSw2 rock samples show significant increases at temperatures above 200°C. This behavior is likely indicative of mineralogic transitions. It is possible that this is due to the α - β cristobalite transition.

The analysis conducted in this study found that potential exists for rock failure when unsupported drift wall temperatures exceed 200°C. When tunnel supports are considered the predictions indicate that the potential depth at which rock mass yield can occur and the extent of rock displacements increases dramatically for temperatures above 200°C. Tunnel supports may be possible but are not currently "off the shelf". At the higher temperatures modifications to the tunnel support or thicker liners will likely be required. The tunnel support response needs to be further evaluated in thermal tests. The most compelling reason for keeping temperatures below 200°C is the changes which result in the coefficient of thermal expansion which results in overstress conditions being produced as the temperature exceeds 200°C. Thus, the analysis appears to support the retention of the not-to-exceed 200°C wall temperature goal. It is recommended, based on the conservative, defense in depth approach taken in this study, that the goal be retained and kept in the requirements documents with this work as supporting analysis.

Cladding Performance. Performance of spent fuel cladding was not considered as a barrier to radionuclide transport in past Total System Performance Assessment modeling. However, the CDA Document (CRWMS M&O 1996f) and the requirements documents [MGDS-RD 3.7.3.3.B.2] limits the fuel cladding temperature to less than 350°C to preserve the cladding as a potential barrier. This study examined the performance of cladding to establish whether or not performance could be attributed to it as a barrier to radionuclide transport. As part of the evaluation, the validity of a temperature criteria was examined. To do this evaluation, it was necessary to develop a cladding degradation analysis model. Such a model was being developed for performance assessment and this study supported that model development effort so that it could be completed early and would support the thermal loading study.

A probabilistic cladding degradation model was developed using cladding degradation algorithms available in the literature. It was determined that the primary cladding failure mechanism for zircaloy cladding which would expose the spent fuel inside and allow radionuclide transport is through gross cladding rupture (unzipping), which results when cladding that has developed pin-hole punctures is exposed to oxidizing conditions (i.e. presence of oxygen) at elevated temperatures. Other cladding degradation mechanisms such as creep rupture, delayed hydride cracking, and dry oxidation were found to not produce appreciable exposure of spent fuel over one million years. However, it should be noted that these predictions were based on the cladding degradation models which were developed from "short-term" degradation measurements and extrapolated to long term with all of the attendant uncertainty associated with such extrapolations. Additionally, no consideration was given to the impacts of rock fall on the WP and cladding which would cause their failure. Of course, rock fall with minimal impacts on the WP may have already occurred or backfill, if emplaced, could alleviate the rock fall impact so it is not clear how important such a failure mechanism would be nor is it clear that all of the waste inside the WP would be subject to mobilization and release.

As a part of the evaluations, estimates of grossly ruptured (or unzipped) cladding were incorporated into the total system performance model (RIP simulation model) to predict releases and radiation doses at the accessible environment. The simulation results indicate that with the cladding performance that was estimated with the current probabilistic analyses, the repository performance is greatly improved (one to two orders of magnitude in releases at the accessible environment) over the base case which does not take any performance for cladding. These analyses assumed only the radionuclides exposed by split cladding could be released from the Engineered Barrier System. The 10,000-year total peak release rate at the accessible environment is reduced by two orders of magnitude compared to the case without cladding performance; for the 1,000,000-year performance, the total peak release rate is reduced by one to possibly two orders of magnitude. Similar results are reported for the total peak dose at the accessible environment: with the cladding performance, the 10,000-year total peak dose is reduced by two orders of magnitude compared to the case without cladding performance (90th percentile about 0.02 mrem/year with cladding performance versus about 2.5 mrem/year without cladding performance), and the reduction in the total peak dose is between one and two orders of magnitude for the 1,000,000-year repository performance (90th percentile about 20 mrem/year with cladding performance versus about 300 mrem/year without cladding performance).

Cooling of the repository at the edges was considered in the calculations as an additional set of cases. The results of these simulations showed that over the 10,000 year period, the edge cooling results in somewhat earlier releases at the accessible environment than the base case which treats all the WPs as if they were at the center of the repository. However, these early releases are insignificant. At 10,000 years the expected value total dose for the case with the edge cooling effect is essentially the same as the base case and similarly at 1,000,000 years negligible differences are seen between the two cases.

Evaluations were conducted to examine the effects of an elevated temperature on cladding performance. The number of clads that fail increases as the clad temperature increases. An eight-fold increase in the number of clads that unzip occurs as the initial center clad temperature increases from an average 276°C at emplacement (about 10 percent of the clads exceed the current thermal goal of 350°C in a log-normal distribution at the hottest temperature after emplacement) to an average 325°C at emplacement (about 30 percent of the clads exceed 350°C). The latter case could simulate a higher thermal loading or higher power output or closely spaced packages. The simulations estimated that, for a higher clad temperature (i.e., an initial center clad temperature of 325°C), the total peak dose at the accessible environment for the first 10,000 years is at least an order of magnitude higher at the 90th percentile level than the reference cladding temperature case (i.e., an initial center clad temperature of 276°C), although the total peak dose is still less than the base case. For the 1,000,000-year repository performance, the higher clad temperature increases the total peak dose by about an order of magnitude (at the 90th percentile) compared to the reference cladding temperature case and the total peak dose is only slightly reduced compared to the base. Thus, allowing the cladding temperatures to increase by 50°C results in a substantial reduction in the repository performance over the nominal cladding case.

This analysis used the TSPA 95 assumptions and inputs. These calculations used very low permeability rock properties which throttles the near-field gas flow and allows higher water vapor pressure in the drift than would be the case for higher permeability rock. Thus, this analysis may be overly conservative with regards to waste package corrosion compared to what would be predicted with the rock properties that have been determined to exist in the TS_w2 rock.

The calculations indicate that significant improvement of the calculated repository performance can be achieved if performance credit is taken for cladding as a potential barrier for spent fuel waste containment. It is recommended, as a result of this study, that credit be taken for cladding in future calculations and in support of Viability Assessment and that performance be allocated based on these calculations. To take credit for cladding for License Application, however, will require that the uncertainties associated with the initial condition of the cladding (as received from the utilities) and the cladding degradation modes and their model be addressed. This is discussed below as some things that need to be done. Calculations performed for a standard at 30 km showed that cladding would still provide a substantial performance benefit and such a change in the standard would not change the conclusions of this study.

The current probabilistic cladding degradation analyses indicated that failure of cladding and its performance is sensitive to temperature. From the current cladding analyses it was difficult to identify a "true" temperature limit below which all assemblies need to be kept. Additionally, the clad temperature has both a spatial and temporal distribution within the WPs. The repository performance simulations did show that as the clad temperatures is increased by 50°C over the nominal case (i.e., the initial center clad temperature of 276°C at emplacement with about 10 percent exceeding the current thermal goal temperature of 350°C) significant reduction in the repository performance would occur. Thus, these evaluations provide information which tends to substantiate the current 350°C temperature goal on cladding. It is recommended that this not-to exceed temperature limit of 350°C on the cladding be retained as a requirement and this study used as the technical justification.

Establishing cladding as a barrier for license application will be a significant challenge because of the uncertainties mentioned in the text. In order to claim a credit for cladding performance with a higher level of confidence which would be supportable for License Application, the current individual cladding degradation models (i.e., creep rupture, delayed hydride cracking, zircaloy dry oxidation, and cladding unzipping) should be re-evaluated, especially for their long-term effects on cladding degradation. Additional cladding degradation processes, not considered in the current study, should be included such as stress corrosion cracking (induced primarily by iodine in the interior side of the clad, and induced by the near-field factors such as salt formation on the clad surface), hydride reorientation, long-term localized corrosion in radiolysis-induced acidic conditions, and long-term degradation under static loads which may be caused by a collapse of the internal structure (e.g., basket material). Also, rock fall on the cladding, once the WPs have undergone substantial degradation, would also result in a failure of the cladding and exposure of the spent fuel inside the failed cladding. However, the probability of occurrence of such rockfalls is unknown and if backfill were used, such rockfalls would be unlikely.

One major obstacle to improving the current cladding degradation models and possibly developing new model(s) is a lack of long-term performance data. Development of testing data for such purposes is both lengthy and costly, and may not be practical in view of the time limitation for the licensing. Most practical approach for an immediate use would utilize the data available in the literature, and combine and synthesize the data with theoretical models that have been developed for other programs. Analysis of cladding that has remained in storage for extended periods may also provide useful information but the initial state of the cladding should be known. In order to achieve the objective, it is recommended that a comprehensive compilation of the cladding degradation data currently available in the literature should be considered as a priority effort.

Ultimately, discussions will be needed with the NRC to determine whether or not a case can be made in License Application to take credit for cladding. If it is felt that the potential repository would be able to meet the standards that are ultimately required without cladding, a valid licensing approach is to still provide the evidence and calculations available which show the potential for cladding as a barrier to release as information to help substantiate reasonable assurance.

Edge Loading Evaluations. The edge of the potential repository will cool and rewet substantially faster than the center of the repository and there has been a concern that for a high thermal loading performance may be degraded. Calculations have shown that edge cooling could be mitigated to some extent by increasing the loading or emplacing hotter fuel at the edges. While the duration of boiling and time to rewet increase significantly at a higher emplaced fuel density, several thermal goals are violated at the higher temperatures and the ability to perform retrieval of the waste should it be required could be adversely impacted. This study evaluated the performance and operational aspects of edge loading to determine whether or not edge loading should be recommended.

Thermohydrologic calculations showed that the duration of boiling in the edges of a potential repository could be increased from less than 1000 years to over 2000 years by increasing the loading in the outer 25 percent from 20.5 kgU/m² (83 MTU/acre) to about 34.0 kgU/m² (137.4 MTU/acre). However, by doing this the temperatures in the emplacement drift (drift wall) are increased well over 200°C in the first 100 years after emplacement. Calculations in Section 3.2 showed that under these conditions there is the potential for rock failure. The calculations also showed that developing tunnel supports which would survive these conditions will be challenging and could result in increased costs.

Total System Performance Assessment simulations were run comparing a base case, which did not consider edge cooling (all of the repository was assumed to behave as it would at the center), with a more realistic case which allowed edge cooling in the outer one sixth of the repository. Predictions of the complementary cumulative distribution functions (CCDF) for releases to the accessible environment showed that edge cooling can result in some earlier releases of radionuclides to the accessible environment but the levels are orders of magnitude below the current remanded standards. For releases at 10,000 years and even at 1,000,000 years the predictions show negligible differences between the base case and the case with edge cooling. However, microbial enhanced corrosion was not considered and if this is later found to play an important role then this issue may have to be reexamined.

Based on the current performance predictions which showed no appreciable performance differences there does not appear to be any compelling reason to consider edge loading. This will avoid the difficulty of dealing with the significantly higher temperatures which would result from an increased loading. Thus, based on this study, it is recommended that at this time edge loading not be considered in the designs of the potential repository.

Waste Stream Variability. The waste stream, as received at the potential repository, was found to have the potential for a significant amount of variability. If packaged and emplaced as received this may result in substantial temperature variations in a 10 to 20 m length of emplacement drift of as much as 50 to 100°C. This temperature difference was found to potentially impact performance from thermomechanical effects and will move moisture from the hotter to the cooler packages, increasing the corrosion of those packages. The amount of thermal variability will need to be reduced although estimates of the reductions needed to affect performance could not be done so no quantitative measure of variability can be recommended. It is recommended that subsequent TSPAs evaluate the impact of moving moisture from hotter to cooler packages.

Methodologies to reduce this heat variability were examined. Varying WP spacing (changing the line load), ventilation of the emplacement drift, and modifying the package heat output through surface aging or selection of WPs or assemblies were evaluated. Costs of these various options were also considered.

Varying the spacing of the WPs offered some promise primarily from a cost saving standpoint. The thermal analysis showed that while the temperature variations decreased somewhat as the WPs were moved closer together, there was not a significant decrease in temperature variations. On the other hand, the temperatures appeared to substantially increase so that both emplacement drift wall temperature goals of 200°C and 350°C cladding goal would be violated. Further evaluation of this should be done once more confidence is developed in model predictions based on thermal tests. Decreasing the spacing between WPs has a cost advantage in that up to about a 6 percent cost savings (~\$700M) for the MGDS (in 1995 dollars) might be possible (although this is still within the uncertainty of the cost analysis). However, it appeared impossible with the present waste stream to provide an appropriate mix of WPs needed to support a line loading concept. Thus, the logistics of this option was a disadvantage and at a minimum would require surface facility storage. Based on this it is not recommended that the design be changed from the ACD concept for Viability Assessment although this should be reexamined for License Application.

It is likely that some natural ventilation will occur in the potential repository and should be planned for. The ACD (CRWMS M&O 1996a) predicts that approximately 0.6 m³/s will likely occur. This study was instrumental in developing a coupled ventilation-thermohydrologic calculation capability which can account for the sensible heat and latent heat of evaporation. The analysis done with this code found that substantial smoothing of the temperature profiles in the emplacement drift could be done with even low flow, natural ventilation. High flow ventilation would produce substantial cooling but the cost is prohibitive (about 25 percent of MGDS costs) and would increase risk by requiring more inlet shafts in the mountain. It is recommended that natural ventilation up to at most 1 m³/s be planned for and considered in the design. This value was chosen since it is easily achievable and should result in a negligible cost impact although some operational impact is likely. However, this is, at best, a solution for only the first 100 years. Such a solution could also add

operational complexity and must be evaluated by Subsurface Design. Thermal rock bolts may also provide some thermal management and these should be investigated further to determine their viability.

Elimination of the MPC concept provides for a certain amount of flexibility in selection of WPs and/or assemblies to configure WPs for a target heat output and thus, reduce WP heat variability. The ability to configure WPs will require an ISF which is likely to be available (based on pending legislation). Significant reduction of heat variability can be achieved by selecting WPs by heat output and even more reduction can be achieved by selecting assemblies (fine blending). The cost of this option, neglecting the cost of the surface facility, is not large (no more than 0.4 percent of the MGDS costs). Thus, it is recommended that selection of WPs or fine blending be considered in the design if an ISF is approved. Even if legislation does not materialize the advantages of a lag storage facility appear significant enough that one should be considered.

To summarize the waste stream variability evaluations, it is recommended that the current ACD design be retained for Viability Assessment. As part of that design, natural ventilation should be considered and planned for in the design. Additionally, configuring WP heat outputs or, at a minimum, selecting WPs by heat output is recommended. It is also recommended that the Design Basis Waste Stream Study planned for next fiscal year should consider evaluations which would determine an optimum target heat for emplacement underground. These issues need to be readdressed for License Application when the thermal tests provide more confidence in our understanding of the near field since potential cost savings and increased performance may exist.

Alternate Thermal Loads. Requirements [10 CFR 60.21(c)(1)(ii)(D)] and the Thermal Strategy (CRWMS M&O 1995a) directs that alternatives, in this case alternative thermal loads, be considered. Analyses with as yet unverified models have indicated that the design focused thermal loading of 20.5 kgU/m² (83 MTU/acre) may meet requirements, at least for a 10,000 year peak dose/cumulative release standard. Thermal tests are being initiated to help confirm many of the issues associated with thermal effects and to provide information to validate analytic models. These tests are several years in duration and final results are not anticipated until a couple of years before License Application for Construction. There is the possibility that the thermal tests may uncover conditions which might not support the design thermal load. Based on this current level of uncertainty, it was deemed prudent to maintain alternative thermal loads at some level to mitigate the risk of relying on a point design by providing contingencies. This study examined a number of alternative thermal loads to determine potential impacts of retaining alternatives and when decisions need to be made to avoid unduly constraining the Project from the standpoint of cost and schedule.

The study examined thermal loads of 6.2, 8.9, and 14.1 kgU/m² (25, 36, and 57 MTU/acre) in addition to the design basis thermal load of 20.5 kgU/m² (83 MTU/acre). Higher thermal loads were not considered due to the fact that at least some thermal goals are violated at the higher loads and that higher thermal loads could be accommodated with no adverse cost or schedule impacts.

Emerging information has indicated that the Primary Area may possibly be expanded to the north since the Drill Hole Wash Fault has been found not to be a significant feature. Analysis of Borehole core samples has shown (CRWMS M&O 1996b), based on similar stratigraphic features, thicknesses, and mineralogic characteristics, that there is a possibility that other optional areas may

be similar to the Primary Area, and thus easy to characterize (compared to what has been required for the Primary Area). This study found that as much or more than about $1.22 \times 10^7 \text{ m}^2$ (3015 acres) of emplacement area may exist. This would allow emplacement of 70,000 MTU at a thermal load that was as low as about 6.2 kgU/m^2 (25 MTU/acre). The cost of characterizing and emplacing the entire 3,015 additional acres is estimated to be no more than about 2.5 percent (about \$300 million) of the MGDS costs.

The cost analysis depends on the assumption of a waste package which can be used for either a high or low thermal loading. If this proposed waste package design is found to be suitable for both high and low thermal loads, then the cost implications associated with pursuing lower thermal loads is small.

It is recommended that, at a minimum, an alternate thermal loading of 8.9 kgU/m^2 (36 MTU/acre) be carried in addition to the design base thermal load. This thermal load would provide below boiling, bulk average conditions in a potential repository which would provide sufficiently different conditions to the high thermal load. The study recommends that this alternative thermal loading be pursued at a relatively low level of effort until sufficient results from thermal testing are available to predict with confidence that the tentatively chosen high thermal loading will support the repository in meeting its performance objectives. These results are expected to be available by the end of 1999. The scope of the effort to maintain the alternative thermal loading can be limited to a low level of design work, an additional performance assessment case, and development of a plan for characterizing additional area if required. These minimal costs are believed to be supportable and prudent in order to prepare for the contingency that the relatively high thermal loading case might be determined to be unacceptable. Management may choose to continue to pursue the alternative thermal loading design even further into the future, balancing the additional cost of maintaining the option and the (hopefully) increasing confidence in the adequacy of high thermal loading against the significant delays should low thermal loading later be found necessary.

A firm decision on thermal loading should be made as soon as practical after sufficient thermal testing results are available, because it would take time to characterize additional potential emplacement areas and to revise the licensing basis to be presented to the Nuclear Regulatory Commission in the License Application if the alternative thermal loading must be used. Also, it is very desirable, from a licensing standpoint, to have thermal loading issues resolved prior to License Application submittal to minimize the likelihood of a licensing issue emerging on this subject.

If the alternative (lower) thermal loading is found to be needed at a time too close to planned License Application submittal to characterize additional area without delaying License Application, the Program may choose to submit the License Application at the lower thermal loading using the previously characterized area. The additional area needed to emplace 70,000 metric tons uranium at the lower thermal loading could then be characterized at a later date, to be followed by an amendment to the License Application.

Summary of Conclusions. This effort concentrated primarily on developing recommendations for design requirements by evaluating thermal goals and thermal management techniques for emplacing spent nuclear fuel. It used the latest available analytic capabilities and the latest measurements from subsurface and laboratory tests. However, due to the fact that in-situ thermal tests are just starting

there exists some uncertainty in our current understanding. As such care must be taken in applying these recommendations.

Because of the limited confidence in some of the predictions, the approach taken in this study to develop recommendations was a conservative approach. The objective of defense in depth being followed in the emerging Waste Isolation Strategy was considered in developing these recommendations. In all cases safety was considered as most important although, certainly the costs of maintaining this safety were evaluated.

The study recommended the 115°C geochemical temperature goal at the TSw2/3 interface be deleted. Instead it is recommended that a not-to-exceed criteria of 90°C at the top of the zeolitized layer (specified in the report) be placed in the requirements. The thermal goals of a not-to-exceed temperature of 200°C on the drift wall and the 350°C cladding temperature should be retained and incorporated in the requirements as criteria. Additionally, it is recommended that consideration be given to taking performance credit for cladding.

In other areas, no appreciable performance differences could be established due to edge cooling. Thus, increasing the loading at the edges is not recommended. It is recommended that WP variability be minimized through the use of natural ventilation and through thermal management of the waste stream at the surface. Other thermal management techniques such as rock bolts should be explored. Finally, it is recommended that, at a minimum, an alternate thermal loading of 8.9 kgU/m² (36 MTU/acre) be carried in addition to the design base thermal load. The cost of carrying such an option to License Application is minimal and if it becomes necessary to change thermal loadings it is not anticipated that the cost impact would be more than about 2.5 percent of the MGDS costs (in 1995 dollars) which is within the uncertainty of current cost estimates.

In closing, thermal loading is a critical issue in the performance of the potential repository that must be understood. Thermal tests are underway to better understand the mountain and the thermal effects on the natural and engineered barriers. Once the results of these thermal tests are available and reasonable assurance in understanding the thermal effects can be demonstrated then a system study is needed to establish recommendations for a thermal loading decision for the potential repository to be used in License Application. Such a study would build on the technical basis provided in this and other studies.

The study recommends that the following requirements be established, retained, and/or changed:

Delete the requirement [CDA EBD RD 3.7.G.3] to limit the TSw3 (basal vitrophyre) maximum temperature to less than 115°C.

Delete the requirement [CDA DCSS 025] to limit the CHn maximum temperature to less than 115°C

Establish a not-to-exceed temperature of 90°C for the zeolitized tuff in the Calico Hills unit. This temperature limit is to be established at the average depth that the top of the zeolitized tuff is beneath a given potential emplacement area (e.g. this temperature limit would be at a depth of 170 m beneath the upper block of the Primary Area). The average depth of the top of the zeolitized layer for other potential areas would need to be established from the Los Alamos Site Scale Geologic Model or measurements.

Retain the not-to-exceed emplacement drift wall temperature of 200°C.

Retain the not-to-exceed cladding temperature of 350°C.

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9. ACRONYMS

ACD	Advanced Conceptual Design
AML	Area Mass Loading
BWR	Boiling Water Reactor
CDF	Cumulative Distribution Function
CCDF	Comprehensive Cumulative Distribution Function
CFR	Code of Federal Regulations
CHn	Calico Hills Nonwelded
CRWMS	Civilian Radioactive Waste Management System
D&E	Design and Evaluation
DHC	Delayed Hydride Cracking
DHLW	Defense High-Level Waste
DOE	U. S. Department of Energy
DPC	Dual-purpose Canister
EBDRD	Engineered Barrier Design Requirements Document
EBS	Engineered Barrier System
ESF	Exploratory Studies Facility
HLW	High-Level Waste
I/S	Illite/Smectite
ISF	Interim Storage Facility
LML	Lineal Mass Loadings
M&O	Management and Operating Contractor
MGDS	Mined Geologic Disposal System
MGDS-RD	Mined Geologic Disposal System Requirements Document
MPC	Multi-purpose Canister
MTU	Metric Tonnes of Uranium
NRC	U. S. Nuclear Regulatory Commission
NRG	North Ramp Geologic
NUFT	Nonisothermal Unsaturated-Saturated Flow and Transport
OFF	Oldest Fuel First
PTn	Paintbrush Tuff layer
PWR	Pressurized Water Reactor

QA	Quality Assurance
RDRD	Repository Design Requirements Document
RH	Relative Humidity
RIP	Repository Integrating Program
RMQ	Rock Mass Quality
SCP	Site Characterization Plan
SNF	Spent Nuclear Fuel
SNL	Sandia National Laboratories
TBV	To Be Verified
TDIF	Technical Data Information Form
TSPA	Total System Performance Assessment
TSw3	Topopah Spring Basal Vitrophyre
WP	Waste Package
YFF	Youngest Fuel First

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