ISSUE RESOLUTION STATUS REPORT

KEY TECHNICAL ISSUE:
CONTAINER LIFE AND SOURCE TERM

Division of Waste Management
Office of Nuclear Material Safety and Safeguards
U.S. Nuclear Regulatory Commission

Revision 3

January 2001

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Office of Nuclear Material Safety and Safeguards
U.S. Nuclear Regulatory Commission

Revision 3

January 2001

UNITED STATES
NUCLEAR REGULATORY COMMISSION
WASHINGTON, D.C. 20555-0001

January 10, 2001

Dr. Stephan J. Brocoum, Assistant Manager
Licensing and Regulatory Compliance
U.S. Department of Energy
Yucca Mountain Site Characterization Office
P.O. Box 30307
North Las Vegas, NV 89036-0307

SUBJECT: ISSUE RESOLUTION STATUS REPORT (KEY TECHNICAL ISSUE: CONTAINER LIFE AND SOURCE TERM, REVISION 3)

Dear Dr. Brocoum:

As you know, the staff of the U.S. Nuclear Regulatory Commission (NRC) has developed a program for early resolution of technical issues at the staff level. The NRC staff documents the status of issue resolution of Key Technical Issues (KTIs) in its Issue Resolution Status Reports (IRSRs). Revision 0 of the IRSR on the Container Life and Source Term (CLST) focused on four subissues related to: (1) container corrosion; (2) materials stability, initial failure, and mechanical failure; (3) spent nuclear fuel (SNF) degradation; and (4) high-level waste (HLW) glass dissolution. Revision 1 of the IRSR included two additional subissues related to criticality within the waste packages (Wps) (5) and alternate Engineered Barrier System (EBS) design features such as drip shields and backfill (6). The U.S. Department of Energy (DOE) completed its Viability Assessment (VA) of a Repository at Yucca Mountain (YM) in December 1998. Revision 2 of the IRSR reflected CLST staff review of the VA, and covered work done by the staff and its contractor, the Center for Nuclear Waste Regulatory Analyses (CNWRA), after the issuance of Revision 1.

The current revision (Revision 3), enclosed, has documented the staff understanding of the status of the subissues after the issuance of Revision 2. Since the VA, DOE has changed the WP design from a corrosion-allowance container to a corrosion-resistant container, with additional drip shield protection. Also DOE has issued Process Model Reports (PMRs) and Analysis Model Reports (AMRs), and has begun to present results of Total System Performance Assessment (TSPA) - Site Recommendation (SR). The staff and CNWRA have evaluated all available PMRs and AMRs, and has begun to review the TSPA-SR results, related to WP and EBS. The staff has revised the IRSR based on the independent analyses of the NRC/CNWRA staffs and on staff reviews of the DOE reports and presentations. In Revision 3, the staff also considered DOE's comments on Revision 2. The staff had technical exchanges with DOE three times during fiscal years 2000 and 2001. Revision 3 also includes the results of these technical exchanges. Another change reflected in Revision 3 is the removal of Review Methods and Acceptance Criteria from Chapter 4 and insertion and use of these acceptance criteria in Chapter 5, to determine the status of various subissues. Thus, major revisions made to Chapter 5 include addition of new materials and removal of some material considered either redundant or unnecessary. To be consistent with Chapter 5, other chapters are modified accordingly. Please note that the status of subissue resolution for the CLST KTI, as defined in the attached IRSR, reflects the results of the technical exchanges mentioned above.

We look forward to having meaningful interactions with your technical staff and making progress in our effort, to resolve all subissues for the CLST KTI at the staff level, consistent with the NRC-DOE agreement on pre-licensing consultations. As you know, such resolutions do not preclude issues being reopened and considered at the time of a potential licensing review by NRC. You also are aware that we welcome dialogue on the CLST KTI with other stakeholders including the U.S. Nuclear Waste Technical Review Board, State of Nevada, and other interested parties. If you have any questions about this letter, please contact Tae Ahn of my staff at (301) 415-5812, or via internet mail service (tma@nrc.gov).

Sincerely,

C. William Reamer, Chief
High-level Waste Branch
Division of Waste Management
Office of Nuclear Material Safety
and Safeguards

Enclosure: Issue Resolution Status Report
(Key Technical Issue: Container Life and Source Term)

cc: See Attached Distribution List

Letter to S. Brocoum from C. W. Reamer dated: 1/10/01

cc:

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Change history of "Issue Resolution Status Report, Key Technical Issue: Container Life and Source Term"

Revision #	Section/Paragraph	Date	Modification
Rev. 0	All	March 1998	None. Initial issue.
Rev. 1	All	November 1998	Wholly revised
Rev. 2	Acknowledgments	September 1999	Revised to include names of authors, reviewers, and QA related information
Rev. 2	1.0/1, 3–6	September 1999	Revised to update NRC strategy for prelicensing, new NRC regulation, and DOE VA information
Rev. 2	2.1/1–3	September 1999	Revised to include new regulation and DOE information on VA design
Rev. 2	2.2/1–3	September 1999	Modified to change format of subissues, Figure 1, and content of Subissue 2.
Rev. 2	3.0/1	September 1999	Minor modifications related to introduction of integrated subissues and changes in Figure 2
Rev. 2	3.1/1	September 1999	Minor modifications to include information on new DOE design for EBS
Rev. 2	3.2/1	September 1999	Minor modification related to ISIs
Rev. 2	3.2.2/1	September 1999	Minor modifications due to new DOE design

Revision #	Section/Paragraph	Date	Modification
Rev. 2	3.2.5/all	September 1999	Revised to clarify issues related to performance
Rev. 2	3.2.6/1	September 1999	Revised to include updated DOE information
Rev. 2	3.3/1	September 1999	Minor modification to include reference
Rev. 2	3.3.1/2–5	September 1999	Revised to include updated information on TSPA-VA
Rev. 2	3.3.3/1–3	September 1999	Revised to include updated information on TPA 3.2
Rev. 2	3.4/1–4	September 1999	Major changes to include updated results of sensitivity analysis. Figures 3, 4, and 5 are incorporated.
Rev. 2	4.0/1	September 1999	Addition of ASTM Standard Practice for long-term behavior of EBS components
Rev. 2	4.1/Title	September 1999	Redefinition of subissue
Rev. 2	4.1.2/1	September 1999	Minor modification related to ENFE KTI
Rev. 2	4.2/Title	September 1999	Redefinition of subissue to include initial defects
Rev. 2	4.2.1/5	September 1999	Addition of a new acceptance criterion

Revision #	Section/Paragraph	Date	Modification
Rev. 2	4.2.2/1–3, 5, 6	September 1999	Revised to include modifications on DOE design and effect of initial defects
Rev. 2	4.3/Title	September 1999	Redefinition of subissue
Rev. 2	4.3.1/2–3	September 1999	Addition of two new acceptance criteria
Rev. 2	4.3.2/1–2	September 1999	Minor modifications related to environment inside WPs
Rev. 2	4.4/Title	September 1999	Redefinition of subissue
Rev. 2	4.4.1/2, 3	September 1999	Addition of two new acceptance criteria
Rev. 2	4.4.2/1, 2	September 1999	Minor modification related to environment inside WPs and scope of resolution
Rev. 2	4.5/Title, 1	September 1999	Redefinition of subissue according to performance based regulation
Rev. 2	4.5.1/1-7	September 1999	Revised to add new acceptance criteria
Rev. 2	4.5.2/1-7	September 1999	Revised to provide technical bases for new acceptance criteria
Rev. 2	4.6/Title, 1	September 1999	Revised to consider new DOE design
Rev. 2	4.6.1/5, 6	September 1999	Addition of two new acceptance criteria to consider effects of new DOE design

Revision #	Section/Paragraph	Date	Modification
Rev. 2	4.6.2/1, 5	September 1999	Revised to include modification of DOE design after VA
Rev. 2	4.7/1, 5	September 1999	Revised to include reference and importance of performance confirmation after VA review
Rev. 2	5.0/4	September 1999	Minor modification to include reference to NRC comments on VA
Rev. 2	5.1.1/Title, 1, 3	September 1999	Revised and shortened to consider changes in DOE design
Rev. 2	5.1.2/Title, 1, 3	September 1999	Revised and shortened to include TSPA-VA review and changes in DOE design
Rev. 2	5.1.3/Title,1, 2, 5, 10	September 1999	Revised and shortened to include TSPA-VA review and changes in DOE design
Rev. 2	5.1.4/Title, 1–5, 7,8,10	September 1999	Revised to include TSPA-VA review, progress in issue resolution and Figures 6 and 7
Rev. 2	5.2.1/Title, 1	September 1999	Revised and shortened to include changes in DOE design and progress in issue resolution

Revision #	Section/Paragraph	Date	Modification
Rev. 2	5.2.2/Title, 4–6	September 1999	Revised to include progress in issue resolution
Rev. 2	5.2.3/Title, 1	September 1999	Included in relation to new acceptance criterion
Rev. 2	5.3.2/1, 2	September 1999	Revised to include results of TSPA-VA review
Rev. 2	5.3.4.1/3, 7	September 1999	Revised to include information related to TSPA-VA review
Rev. 2	5.3.4.2/1	September 1999	Minor modifications of values
Rev. 2	5.3.4.3/1,2,5,6	September 1999	Revised to include information on TSPA-VA review
Rev. 2	5.4.4/1,2	September 1999	Revised to include progress in issue resolution
Rev. 2	5.5/All	September 1999	Revised to include progress in issue resolution
Rev. 2	5.6.1/Title, 1, 2	September 1999	New section to reflect DOE design changes
Rev. 2	5.6.2/Title, 1, 2	September 1999	New section to reflect DOE design changes
Rev. 2	5.6.3/Title, 1 2	September 1999	New section to reflect DOE design changes
Rev. 2	6.0	September 1999	New references added according to listed changes
Rev. 3	Acknowledgments	January 2001	Revised to include names of new authors and reviewers

Revision #	Section/Paragraph	Date	Modification
Rev. 3	Executive Summary	January 2001	Added to summarize status and path to resolution for the various subissues
Rev. 3	1.0/1	January 2001	Revised to update information on NRC regulation and staff issue resolution
Rev. 3	1.0/2	January 2001	Added to include categories of issue resolution
Rev. 3	1.0/6	January 2001	Revised to indicate displacement of acceptance criteria and review methods to the proposed YMRP
Rev. 3	1.0/8	January 2001	Revised to indicate modifications and addition of Appendixes B and C
Rev. 3	2.1/1	January 2001	Revised to indicate removal of acceptance criteria and review methods
Rev. 3	2.1/2-3	January 2001	Revised to indicate DOE design changes and updated references
Rev. 3	2.2/1	January 2001	Modified Figure 1 to change subissue components
Rev. 3	2.2/3	January 2001	Modified to include consolidated IRSR
Rev. 3	3.0/1	January 2001	Revised to introduce DOE Repository Safety Strategy (RSS) Revision 3

Revision #	Section/Paragraph	Date	Modification
Rev. 3	3.0/2	January 2001	Revised to introduce Appendix B showing relationships between ISIs and CLST subissues
Rev. 3	3.1/1	January 2001	Revised to introduce updated reference to DOE RSS
Rev. 3	3.2.1/2	January 2001	New references
Rev. 3	3.2.2/1	January 2001	Revised heading and text to include initial defects
Rev. 3	3.2.3/1	January 2001	Revised to include degradation of Zr cladding and DSNF
Rev. 3	3.2.6/1	January 2001	Revised to update reference to DOE RSS Revision 3
Rev. 3	3.3/1	January 2001	New references
Rev. 3	3.3.1/2-7	January 2001	Revised to clarify results of DOE sensitivity analyses
Rev. 3	3.3.2/1-3	January 2001	Revised to update EPRI PA
Rev. 3	3.3.3/1-2	January 2001	Revised to update information on NRC TPA codes
Rev. 3	3.4/1-2	January 2001	Revised to clarify aspects of sensitivity analysis for VA and EDA-II DOE designs
Rev. 3	3.4/3	January 2001	Revised to modify Figures 4 and 5, and list of models/parameters

Revision #	Section/Paragraph	Date	Modification
Rev. 3	4.0/1	January 2001	Revised to delete acceptance criteria
Rev. 3	4.1/1	January 2001	Revised to delete acceptance criteria
Rev. 3	4.1.1/1-2	January 2001	Modified to indicate DOE design change
Rev. 3	4.1.1.1/1-6	January 2001	Introduced as technical bases modified text originally in Section 5.1.4
Rev. 3	4.1.1.2/1-3	January 2001	Introduced as technical bases modified text originally in Section 5.1.4
Rev. 3	4.2./1	January 2001	Revised to delete acceptance criteria
Rev. 3	4.2.1/1	January 2001	Modified to indicate DOE design change
Rev. 3	4.2.1.1/1-5	January 2001	Introduced as technical bases modified text originally in Section 5.2.2
Rev. 3	4.2.1.2/1-2	January 2001	Introduced as technical bases modified text originally in Section 5.2.3
Rev. 3	4.3/1	January 2001	Revised to delete acceptance criteria
Rev. 3	4.3.1/2	January 2001	Added in this section for consistency from Section 5.3.1
Rev. 3	4.3.1.1/1	January 2001	Introduced as technical bases modified text originally in Section 5.3.1

Revision #	Section/Paragraph	Date	Modification
Rev. 3	4.3.1.2/1-3	January 2001	Introduced as technical bases modified text originally in Section 5.3.2
Rev. 3	4.3.1.3/1-4	January 2001	Introduced as technical bases modified text originally in Section 5.3.3
Rev. 3	4.3.1.4/1	January 2001	Introduced as technical bases modified text originally in Section 5.3.4
Rev. 3	4.3.1.4.1/1-5	January 2001	Introduced as technical bases modified text originally in Section 5.3.4.1
Rev. 3	4.3.1.4.2/1	January 2001	Introduced as technical bases modified text originally in Section 5.3.4.2
Rev. 3	4.3.1.4.3/1-5	January 2001	Introduced as technical bases modified text originally in Section 5.3.4.3
Rev. 3	4.3.1.5/1-8	January 2001	Introduced as technical bases modified text originally in Section 5.3.5
Rev. 3	4.3.1.6/1-3	January 2001	Introduced as technical bases modified text originally in Section 5.3.6
Rev. 3	4.4/1	January 2001	Revised to delete acceptance criteria
Rev. 3	4.4.1/2	January 2001	Added in this section for consistency from Section 5.4.1

Revision #	Section/Paragraph	Date	Modification
Rev. 3	4.4.1.1/1	January 2001	Introduced as technical bases modified text originally in Section 5.4.1
Rev. 3	4.4.1.2/1	January 2001	Introduced as technical bases modified text originally in Section 5.4.2
Rev. 3	4.4.1.3/1-4	January 2001	Introduced as technical bases modified text originally in Section 5.4.3
Rev. 3	4.4.1.4/1-2	January 2001	Introduced as technical bases modified text originally in Section 5.4.4
Rev. 3	4.4.1.5/1-3	January 2001	Introduced as technical bases modified text originally in Section 5.4.5
Rev. 3	4.4.1.6/1-3	January 2001	Introduced as technical bases modified text originally in Section 5.4.6
Rev. 3	4.5/1-2	January 2001	Revised to delete acceptance criteria and focus only on postclosure
Rev. 3	4.5.1.1/2	January 2001	Introduced to complete technical bases description
Rev. 3	4.5.1.2/2-4	January 2001	Introduced to complete technical bases description
Rev. 3	4.5.1.3/1	January 2001	Introduced to complete technical bases description

Revision #	Section/Paragraph	Date	Modification
Rev. 3	4.5.1.4/1	January 2001	Introduced to complete technical bases description
Rev. 3	4.5.1.5/1-2	January 2001	Introduced to complete technical bases description
Rev. 3	4.5.1.6/1	January 2001	Introduced to complete technical bases description
Rev. 3	4.5.1.7/1	January 2001	Introduced to complete technical bases description
Rev. 3	4.6/1	January 2001	Modified to indicate DOE design change and to delete acceptance criteria
Rev. 3	4.6.1/1	January 2001	Modified to indicate DOE design change
Rev. 3	4.6.1.1/1-3	January 2001	Introduced as technical bases modified text originally in Sections 5.6.1 and 5.6.3
Rev. 3	4.6.1.2/1-4	January 2001	Introduced as technical bases modified text originally in Section 5.6.2
Rev. 3	5.0/3	January 2001	Modified to indicate review of DOE documents
Rev. 3	5.0/4	January 2001	Included to list review of PMRs and AMRs
Rev. 3	5.0/5	January 2001	Introduced to add review of FEP tables as listed in Appendix C

Revision #	Section/Paragraph	Date	Modification
Rev. 3	5.1/All	January 2001	Revised to include progress in issue resolution
Rev. 3	5.2/All	January 2001	Revised to include progress in issue resolution
Rev. 3	5.3/All	January 2001	Revised to include progress in issue resolution
Rev. 3	5.4/All	January 2001	Revised to include progress in issue resolution
Rev. 3	5.5/All	January 2001	Revised to include progress in issue resolution
Rev. 3	5.6/All	January 2001	Revised to include progress in issue resolution
Rev. 3	6.0	January 2001	New references added according to listed changes
Rev. 3	Appendix A	January 2001	Revised to update status
Rev. 3	Appendix B	January 2001	Added to indicate ISIs and CLST subissues relationships
Rev. 3	Appendix C	January 2001	Added to list evaluated FEP

TABLE OF CONTENTS

TABLE OF CONTENTS (cont'd)

Section Page

TABLE OF CONTENTS (cont'd)

TABLE OF CONTENTS (cont'd)

Section | Page

TABLE OF CONTENTS (cont'd)

Section | Page

TABLE OF CONTENTS (cont'd)

FIGURES

TABLES

LIST OF ACRONYMS

AC — Acceptance criteria
ACM — Alternative conceptual method
AMR — Analysis model reports
ANL — Argonne National Laboratory
AOA — Area of applicability
ASTM — American Society for Testing and Materials
BWR — Boiling water reactor
CL — Critical limit
CLST — Container Life Source Term
CNWRA — Center for Nuclear Waste Regulatory Analyses
CP — Commercial purity
CPP — Cyclic potentiodynamic polarization
CRC — Commercial reactor criticals
CSNF — Commercial spent nuclear fuel
DCB — Double cantilever beam
DCCG — Diffusion-controlled cavity growth
DCF — Dose conversion factor
DHLW — Defense high-level waste
DOE — U.S. Department of Energy
DS — Drip shield
DSNF — DOE spent nuclear fuel
DWPF — Defense Waste Processing Facility
EAC — Environmentally assisted cracking
EB — Engineering barriers
EBS — Engineered Barrier Subsystem
EBSPAC — Engineered Barrier System Performance Assessment Code
EDA-II — Enhanced design alternative-II
ENFE — Evolution of the Near-Field Environment
EPRI — Electric Power Research Institute
FEIS — Final Environmental Impact Statement
FEP — Features, events, and processes
FM — Fissile material
FY — Fiscal year
HE — Hydrogen embrittlement
HIC — Hydride induced cracking
HLW — High-level waste
IA — Igneous activity
IRSR — Issue Resolution Status Report
ISI — Integrated subissues
KTI — Key technical issues
LA — License application
LANL — Los Alamos National Laboratories

LIST OF ACRONYMS (cont'd)

LCE	—	Laboratory critical experiments
LLNL	—	Lawrence Livermore National Laboratory
LRO	—	Long range ordering
LTCTF	—	Long-Term Corrosion Testing Facility
MDEB	—	Mechanical disruptions of engineered barriers
MIC	—	Microbially influenced corrosion
MSL	—	Master scenario list
MTHM	—	Metric tons heavy metal
NDE	—	Non-destructive examination
NG	—	Nuclear grade
NNPP	—	Naval Nuclear Propulsion Program
NRC	—	U.S. Nuclear Regulatory Commission
PA	—	Performance assessment
PCT	—	Product consistency test
PMR	—	Process model report
PNNL	—	Pacific Northwest National Laboratory
PWR	—	Pressurized water reactor
QA	—	Quality assurance
RAI	—	Request for additional information
RDTME	—	Repository Design and Thermal-Mechanical Effects
RH	—	Relative humidity
RIP	—	Repository Integration Program
RM	—	Review method
RT	—	Radionuclide Transport
RSS	—	Repository Safety Strategy
SCC	—	Stress corrosion cracking
SCW	—	Saturated concentrated water
SDS	—	Structural Deformation and Seismicity
SER	—	Safety evaluation report
SNF	—	Spent nuclear fuel
SR	—	Site recommendation
SS	—	Stainless steel
SSW	—	Simulated saturated water
TCP	—	Topologically closed-packed
THC	—	Thermal-hydrologic-chemical
TPA	—	Total-system Performance Assessment
TR	—	Topical report
TSPA	—	Total System Performance Assessment
TSPAI	—	Total System Performance Assessment and Integration
UT	—	Ultrasonic testing
VA	—	Viability assessment
WF	—	Waste form

LIST OF ACRONYMS (cont'd)

WP	—	Waste package
WPOB	—	Waste package outer barrier
YM	—	Yucca Mountain
YMP	—	Yucca Mountain Project
YMR	—	Yucca Mountain region
YMRP	—	Yucca Mountain Review Plan

ACKNOWLEDGMENTS

This Issue Resolution Status Report (IRSR) Revision 3 was prepared by the staffs of the U.S. Nuclear Regulatory Commission (NRC) and the Center for Nuclear Waste Regulatory Analyses (CNWRA). Primary authors of the report are Tae M. Ahn (NRC) and Gustavo Cragnolino (CNWRA). Other members of the Container Life and Source Term Key Technical Issue Team who have provided input to various sections of this IRSR and its previous revisions include B. Jennifer Davis (NRC), Richard Codell (NRC), Charles Greene (NRC), Meraj Rahimi (NRC), Vanice Perin (NRC), John Contardi (NRC), Tamara Bloomer (NRC), Narasi Sridhar (CNWRA), Darrell S. Dunn (CNWRA), Sean Brossia (CNWRA), Yi-Ming Pan (CNWRA), Vijay Jain (CNWRA), James Weldy (CNWRA), Roberto Pabalan (CNWRA), David Pickett (CNWRA), Osvaldo Pensado (CNWRA) and Kwai Chan (SwRI). The review efforts of Oliver Moghissi (CNWRA), William Murphy (CNWRA), Wes Patrick (CNWRA), Budhi Sagar (CNWRA), James Andersen (NRC), King Stablein (NRC), and William Reamer (NRC) are acknowledged. Editorial reviews by Barbara Long (CNWRA), Cathy Cudd (SwRI), Jim Pryor (SwRI), Alana Woods (SwRI), and Ellen Kraus (NRC) are also acknowledged. Janie Gonzalez (CNWRA) and Karen Valloch (NRC) provided secretarial support.

QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: The original data generated by CNWRA contained in this report meet the quality assurance requirements described in the CNWRA Quality Assurance Manual. Sources of other data should be consulted for determining the level of quality for those data.

ANALYSES AND CODES: The Total-system Performance Assessment (TPA) code Version 3.2, used for sensitivity analyses, was developed under CNWRA Technical Operating Procedure (TOP) 018.

EXECUTIVE SUMMARY

The Container Life and Source Term Key Technical Issue (CLST KTI) deals with the containers and the waste form as the primary engineered barriers, and the source term resulting from their degradation. It also considers other features of the engineered barrier subsystem (EBS), such as the drip shield, which in conjunction with the containers is designed to provide a significant contribution to the overall repository performance. This Issue Resolution Status Report (IRSR) is focused on evaluating the adequacy of the methodology, testing, and modeling used by the U.S. Department of Energy (DOE) in the investigations related to containers and waste forms. The potential for criticality inside the waste packages (WPs), arising from water penetration in breached containers, is also assessed in this IRSR.

The adequacy of the information on methodology, testing, and modeling developed by the DOE to select the materials and design the components of the WPs and other features of the EBS was evaluated to define the current status and the path to resolution of the six subissues of the CLST KTI. A thorough review of the available WP Degradation Process Model Report (PMR), the Waste Form Degradation PMR and the supporting Analysis Model Reports was conducted. Overall, the U.S. Nuclear Regulatory Commission staff believes that significant progress has been made by DOE in assessing the container life and source term. However, a series of questions and concerns arose from the review of the WP Degradation PMR and the corresponding AMRs regarding the methodologies for estimating the corrosion rate, localized corrosion, and stress corrosion cracking. More information is considered to be necessary for evaluating the influence of microbially influenced corrosion on WP performance. Although DOE has undertaken a limited study of the effect of welding on container performance, the methodology used for inclusion of the effects of welding and fabrication on the performance of container requires improvement. It was concluded that DOE also needs to better characterize the effects of closure welding (e.g., consider full-thickness welds) and post-weld treatments. Although DOE has included the effect of in-package chemistry on spent nuclear fuel (SNF) dissolution, as described in the Waste Form Degradation PMR, the lack of consideration of the spatial variation of the in-package aqueous environment on SNF dissolution and inadequate consideration of the corrosion of Zircaloy cladding may result in nonconservative estimates of some radionuclide release rates.

A series of agreements were reached during a DOE/NRC Technical Exchange conducted on September 12–13, 2000. The agreements covered all subissues, except Subissue 5 on the effects of in-package criticality. The technical exchange on criticality took place on October 23–24, 2000. Based on information presented by the DOE and agreements reached for additional information, the status of all subissues was changed to closed, pending. The status of resolution of the subissues is defined by the NRC as follows

- Closed—If the DOE approach and available information acceptably address staff questions such that no information beyond what is currently available will likely be required for regulatory decision making at the time of initial license application

- Closed, pending—If the NRC staff has confidence that the DOE proposed approach, together with the DOE agreement to provide the NRC with additional information (through

specific testing, analysis, etc.), acceptably addresses the NRC's questions such that no information beyond that provided, or agreed to, will likely be required at time of initial license application

- Open—If the NRC has identified questions regarding the DOE approach or information and the DOE has not yet acceptably addressed the questions or agreed to provide the necessary additional information in a potential license application

A subissue can be reopened and considered during licensing proceedings if new information is available that could potentially change the conclusions. The status of these CLST subissues and comments, regarding their path to resolution, as summarized in the following table, was abstracted from transcripts of the technical exchanges on CLST subissues[1] and criticality subissues[2] in which the agreements reached with the DOE are documented.

Subissue	Status	Path to Resolution
Effects of corrosion processes on the lifetime of the containers	Closed, pending	Provide information on range of water chemistries contacting WP and drip shield, including minor constituents. Provide data on general, localized, and microbially influenced corrosion of Alloy 22, using tests with improved sensitivity for corrosion rate measurements, including consideration of fabrication effects and, if needed, provide data obtained with alternative methods. Provide data for stress corrosion cracking (SCC) of Alloy 22, including cold worked, welded, and welded and thermally aged materials. Provide information in support of SCC mitigating treatments such as induction annealing and laser peening.

[1]Schlueter, J., Letter (October 4) to S. Brocoum, U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Key Technical Issue: Container Life and Source Term (ML003760868). Washington, DC: U.S. Nuclear Regulatory Commission. 2000.

[2]Schlueter, J., Letter (October 27) to S. Brocoum, U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting Related to Criticality (ML003763270). Washington, DC: U.S. Nuclear Regulatory Commission. 2000.

Subissue	Status	Path to Resolution
Effects of phase instability of materials and initial defects on the mechanical failure and lifetime of the containers	Closed, pending	Provide information on the effect of the entire fabrication sequence on phase instability of Alloy 22, including welding and postweld treatments. Provide information on the effect of rockfall and seismicity on mechanical failure. Provide information on the effect of initial defects in failure of closure welds.
Rate at which radionuclides in spent nuclear fuel are released from the engineered barrier subsystem through the oxidation and dissolution of spent fuel	Closed, pending	Provide documentation of modeling, including the effects of radiolysis, incoming water chemistry, corrosion products, and transient effects. Additional analysis and sensitivity studies will be conducted and, if testing is needed, tests plans will be provided to the NRC. Provide data addressing chloride-induced localized corrosion and SCC of Zircaloy cladding, considering in-package water chemistry modeling. Provide distributions of cladding temperatures and hoop stresses for evaluating hydride reorientation and SCC.
Rate at which radionuclides in high-level waste glass are leached and released from the engineered barrier subsystem	Closed, pending	Provide documentation on in-package water chemistry modeling for waste forms, including evaluation of the chemical form and concentration of iron corrosion products. Address: a) the inconsistency of the rates in the acidic pH region for the dissolution of high-level waste glass, b) the technical basis for using Si release rate in the calculation of radionuclide releases from glass, and c) clarification of the definition of long-term dissolution rate.

Subissue	Status	Path to Resolution
Effect of in-package criticality on waste package and engineered barrier subsystem performance	Closed, pending	Provide Disposal Criticality Analysis Methodology Topical Report, Rev. 01, addressing all 28 open items. Modify Disruptive Events Features, Events, and Processes (FEP) AMR; revise FEP database; and analyze to support screening of system-level FEP. Analyze probability of criticality before 10,000 yr. Validate reports and provide other documents as identified in the Technical Exchange. Conduct the "what-if" analysis for an early criticality event and sensitivity analyses that include the most significant probability consequence criticality scenario.
Effects of alternate engineered barrier subsystem design features on container lifetime and radionuclide release from the engineered barrier subsystem	Closed, pending	Provide corrosion rate data for Ti alloys from long-term corrosion test facility and alternative methods to measure corrosion rates or justification of current approach. Provide data on effects of fluoride anion and trace heavy metal cations on corrosion modes and rates for Ti alloys. Provide data from SCC testing, technical basis for the hydrogen pickup as a result of corrosion and justification for the use of 400-ppm hydrogen as a threshold. Provide rockfall calculations, taking into account drip shield wall thinning due to corrosion, hydride embrittlement, fall of multiple rock blocks, and seismic calculations considering temperature-dependent mechanical properties of Ti alloys. Demonstrate that the Tresca failure criterion bounds a fracture mechanics approach to mechanical failure of the drip shield.

1.0 INTRODUCTION

The U.S. Nuclear Regulatory Commission (NRC) strategic planning assumptions for the prelicensing period of the high-level radioactive waste (HLW) repository proposed at Yucca Mountain, Nevada, call for the early identification and resolution of issues at the staff level. A principal means for achieving this goal is through formal, and open-to-the-public, prelicensing consultation with the U.S. Department of Energy (DOE) regarding site characterization, experimentation, and design activities that are conducted consistent with the provisions contained in the proposed Title 10 of the U.S. Code of Federal Regulations, Part 63 (10 CFR Part 63), "Disposal of High-Level Radioactive Wastes in a Proposed Geologic Repository at Yucca Mountain, Nevada" (U.S. Nuclear Regulatory Commission, 1999a). All these consultations, required by law, occur in an open manner that permit observation by the State of Nevada, Tribal Nations, affected units of local government, and other interested members of the public. Obtaining input and striving for consensus from the technical community and interested parties help the issue resolution process. Staff issue resolution during the prelicensing consultation period is included in the proposed regulation specified in Part 63. This process of prelicensing issue resolution attempts to avoid having substantive technical issues open to resolution at the time of the NRC licensing review and, thus, streamline the review process.

Consistent with NRC regulations and a 1992 agreement with the DOE, staff-level issue resolution can be achieved during the prelicensing consultation period. The three categories of issue resolution defined by the NRC are

- Closed—If the DOE approach and available information acceptably address staff questions such that no information beyond what is currently available will likely be required for regulatory decision making at the time of initial license application.

- Closed, pending—If the NRC staff has confidence that the DOE proposed approach, together with the DOE agreement to provide the NRC with additional information (through specific testing, analysis, etc.), acceptably address the NRC's questions such that no information beyond that provided, or agreed to, will likely be required at time of initial license application.

- Open—If the NRC has identified questions regarding the DOE approach or information, and the DOE has not yet acceptably addressed the questions or agreed to provide the necessary additional information in a potential license application.

It should be noted that additional pertinent information could raise new questions or comments regarding a previously resolved issue. The issue may be re-opened and considered during licensing proceedings.

The NRC HLW program was realigned during fiscal year (FY) 1996–1997 in response to (i) a reduction in Congressional budget appropriations for NRC in FY 1996; (ii) the reorganization of DOE's geologic repository program for the proposed site at Yucca Mountain, Nevada; and (iii) a 1995 report issued by the National Academy of Sciences to advise the U.S. Environmental

Protection Agency regarding the technical bases for new geologic disposal standards for Yucca Mountain (YM). As a result of these developments, the NRC HLW program was realigned to focus prelicensing work on those topics most critical to the post-closure performance of the proposed geologic repository. These critical topics are identified as key technical issues (KTIs). This approach is summarized in Chapter 1 of the FY 1996 Annual Progress Report (U.S. Nuclear Regulatory Commission, 1997).

The NRC current approach is to focus most activities on issue resolution at the staff level. Division of Waste Management activities have been reprioritized to improve the integration of the technical work necessary to achieve staff-level resolution. Regulatory attention is focused on those technical uncertainties that have the greatest effect on the assessment of repository safety. This focus is accomplished by identifying KTIs, integrating their activities into a risk-informed approach, and evaluating their significance for postclosure repository performance. Early feedback among all parties is essential in determining what is known, what is not known, and if additional information is likely to make a significant difference in understanding future repository safety.

An important step in the NRC approach to issue resolution is to provide DOE with feedback regarding issue resolution before the potential LA submittal. Issue resolution status reports (IRSRs) are the primary mechanism used to provide DOE with feedback on KTI subissues. IRSRs focus on the status of issue resolution, listing the acceptance criteria (AC) for issue resolution, and include areas of agreement or comments or questions. Open public meetings and technical exchanges with DOE provide additional opportunities to discuss issue resolution, identify areas of agreement and disagreement, and develop plans to resolve such disagreements. This revision of the Container Life and Source Term (CLST) IRSR completely supersedes previous revisions. Previous IRSRs included (i) AC and review methods (RMs) for use in issue resolution and regulatory review, (ii) technical bases for the AC and RMs; and (iii) the status of resolution. The AC and the RMs are currently being included in the proposed Yucca Mountain Review Plan (YMRP).

Furthermore, the IRSRs were the basis for the review of information in the DOE viability assessment (VA) (U.S. Department of Energy, 1998a,b,c). Comments on the VA were intended to facilitate the DOE's efforts to focus its program and develop a high-quality LA. The preliminary design concept, the Total System Performance Assessment (TSPA), the LA plan, and supporting documents (U.S. Department of Energy, 1998a,b,c) were reviewed. Through these reviews, a set of technical comments regarding the supporting data and models within the TSPA was identified.

Each IRSR contains six sections. This Introduction is Section 1.0. Section 2.0 defines the KTI, all the related subissues, and the scope of the particular subissue that is the subject of the IRSR. Section 3.0 discusses the importance of the subissue to repository performance, including: (i) qualitative descriptions, (ii) relationship to total system performance, (iii) results of available sensitivity analyses, and (iv) relationship to the DOE Repository Safety Strategy (RSS) (CRWMS M&O, 2000a). Section 4.0 provides the technical basis for resolution of the subissue that will be used in subsequent reviews of DOE submittals. Technical bases for AC are

explained in detail to further document the rationale for the staff evaluations. Section 5.0 documents the application of AC to the current DOE design of the waste package (WP) and other features of the engineered barrier subsystem (EBS) for the site recommendation (SR), provides a review of the pertinent DOE process model reports (PMRs) and supporting analysis model reports (AMRs), and updates the status of resolution of the subissues. Section 6.0 presents a list of pertinent references. Appendix A lists the open items resulting from the analysis of the YM Site Characterization Plan (U.S. Nuclear Regulatory Commission, 1989). Items resolved at the staff level and those items remaining open are summarized. The open items of the NRC Site Characterization Analysis (SCA) are updated in this revision of the CLST IRSR. If all CLST KTI subissues could be resolved, all SCA items will be closed accordingly. Appendix B contains the relationships between integrated subissues and key technical subissues and Appendix C includes tables with the staff evaluation of features, events, and processes (FEP) excluded by the DOE.

2.0 KEY TECHNICAL ISSUES AND SUBISSUES

2.1 PRIMARY ISSUE

The primary KTI related to CLST is adequacy of the EBS design to provide reasonable assurance that containers will be adequately long-lived, and radionuclide releases from the EBS will be sufficiently controlled, such that container design and packaging of spent nuclear fuel (SNF) and HLW glass will make a significant contribution to the overall repository performance. The site-specific regulation for the proposed YM repository, to be issued as 10 CFR Part 63 (U.S. Nuclear Regulatory Commission, 1999a) after final Commission action, is a risk-informed, performance-based regulation. The staff is currently preparing the YMRP to facilitate the process of reviewing the potential LA for the proposed geological repository at YM. The RMs and AC for all the KTIs and subissues will be incorporated in the proposed YMRP. This IRSR is focused on the containers and waste forms (WFs) as the primary engineered barriers, but it also considers other engineered subsystem enhancements [e.g., drip shield (DS)] that may be incorporated as options in the EBS design. For the purpose of this IRSR, the physical boundary of the EBS is defined by the walls of the WP emplacement drifts.

The reference DOE design for the EBS in the VA (U.S. Department of Energy, 1998b) consisted of double-wall WPs placed on steel supports in concrete-lined drifts. The WP consisted of a 10-cm-thick outer overpack made of a corrosion-allowance material and a 2-cm-thick inner overpack made of a corrosion-resistant Ni-base alloy, in addition to the WF and other materials for criticality control, heat transfer, and structural support of fuel assemblies. The reference materials for the VA design of the WP were A516 grade 55 steel (a wrought C-Mn steel) for the outer overpack and Alloy 22 for the inner overpack. Additional metallic components, such as the pour canister for defense HLW glass and the canister for DOE or U.S. Navy SNF, both made of Type 316L stainless steel (SS), were present in some WP designs. The WP and EBS designs have been significantly revised after the completion of the VA. The reference WP design recommended for the proposed SR (CRWMS M&O, 1999a), called the enhanced design alternative II (EDA-II), consists of an outer overpack made of 2-cm-thick Alloy 22 surrounding an inner overpack made of Type 316 nuclear grade (NG) SS that is 5 cm thick. The main purpose of the inner overpack is to provide structural mechanical strength to the WP. Additionally, a mailbox-shaped DS, to be made of 1.5-cm-thick Ti grade 7 plates and structural members made of Ti grade 24 for long-term structural support, will be extended over the length of the emplacement drifts to enclose the top and sides of the WP (CRWMS M&O, 2000w). The drift will have steel sets and lagging (or in some cases, rock bolts and mesh) for ground support instead of the concrete liner proposed in the VA design. The WPs will be resting on an emplacement pallet made of two V-shaped supports fabricated with Alloy 22 plates and connected together by four square SS tubes (CRWMS M&O, 2000w). The design of the EBS in the EDA-II included the use of backfill to cover the DS; however, a design without backfill is currently being considered for the SR (CRWMS M&O, 1999b, CRWMS M&O, 2000w). In addition the EDA-II uses thermal management features, such as line loading, ventilation, and SNF assemblies blending, to limit peak temperatures of cladding, WP wall surface, and drift wall (CRWMS M&O, 1999b).

There are several design concepts for SNF and HLW glass containers (CRWMS M&O, 2000x). The canistered designs included in the VA were removed from the SR WP design configurations, and an updated analysis of the uncanistered fuel design has been presented (CRWMS M&O, 2000y). There are five different designs for the commercial spent nuclear fuel (CSNF) but these designs all have the same container materials and wall thicknesses. The length, diameter, and interior of the five designs vary to accommodate fuel assembly variations. The CSNF disposal containers will be fabricated in two sizes, for 21 and 12 pressurized water reactor (PWR) fuel assemblies, in which neutron absorber plates will be used. An additional WP design for 21 PWR fuel assemblies will contain control rods. The disposal containers for boiling water reactor (BWR) SNF will be fabricated in two sizes for 44 and 24 fuel assemblies, both using neutron absorber plates. There are two designs that differ in length to hold the U.S. Navy SNF, both consisting of a single canister inside a disposal container. There are two designs of the codisposal container, for DOE-owned SNF (DSNF) and HLW glass canisters, that only differ in length and will hold five HLW glass canisters surrounding a DSNF disposal canister inserted in the center of the container. The third WP design for the DSNF will accommodate two HLW glass canisters and two multi-canister overpacks (MCOs) containing DSNF canisters.

2.2 SUBISSUES

Figure 1 identifies six subissues deemed important to the resolution of this KTI.

1. The effects of corrosion processes on the lifetime of the containers,

2. The effects of phase instability of materials and initial defects on the mechanical failure and lifetime of the containers,

3. The rate at which radionuclides in SNF are released from the EBS through the oxidation and dissolution of SNF,

4. The rate at which radionuclides in HLW glass are leached and released from the EBS,

5. The effect of in-package criticality on WP and EBS performance,

6. The effects of alternate EBS design features on container lifetime and radionuclide release from the EBS.

Each of these six subissues may, in turn, be addressed by its principal components. Subissue 1 considers failure of the outer container as a result of various corrosion processes affecting WP materials, such as dry-air oxidation, humid-air and uniform aqueous corrosion, localized corrosion, microbially influenced corrosion (MIC), stress corrosion cracking (SCC), and hydrogen embrittlement (HE). Subissue 2 examines long-term degradation of mechanical properties of container materials as a result of prolonged exposures of the WPs (thousands of years) to elevated temperatures. Mechanical failure because of phase instability of WP materials is highly dependent on material chemical composition and processing history. Examples of material

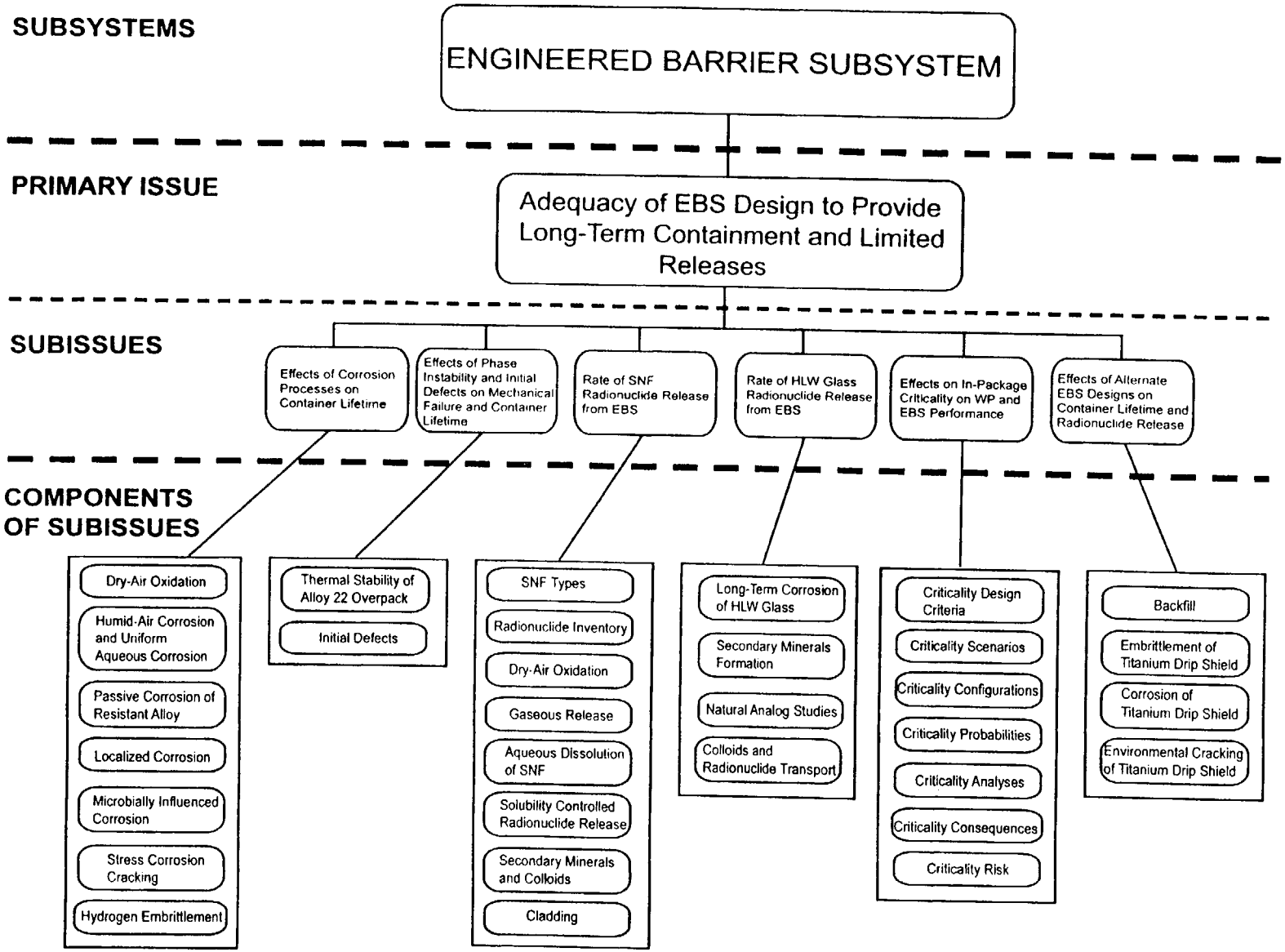

Figure 1. Flow diagram for container life and source term subissues

instability that can degrade mechanical properties include segregation of metalloid elements such as phosphorus and sulfur, precipitation of carbides or intermetallic phases, and long-range ordering (LRO). Fabrication defects that may lead to early failure of container materials are also the subject of this subissue, as well as the effects of disruptive events, such as seismicity, faulting, and igneous activity (IA). Mechanical failure of containers caused by disruptive events has been partially considered in repository design and thermal-mechanical effects (RDTME), structural deformation and seismicity (SDS), and IA IRSRs. Subissue 3 considers degradation of SNF and subsequent radionuclide release from SNF in both dry air and aqueous environments, after cladding failure. These processes involve radionuclide release by aqueous dissolution of the SNF matrix, limited by solubility or enhanced by colloid formation, and also includes dry-air oxidation of SNF and gaseous transport. In a similar manner, Subissue 4 deals with radionuclide release from the HLW glass form, following aqueous dissolution of the borosilicate matrix. The degradation of WPs may give rise to criticality problems, which may occur either within the WP or outside the WP after transport and redeposition of fissile radionuclides in the repository environment. Criticality inside the WPs is assessed as Subissue 5 in this IRSR taking into consideration as its components criticality design criteria, scenarios, configurations, probability, analysis, consequence, and risk. Criticality outside the WP is evaluated as a relevant subissue in both the evolution of the near-field environment (ENFE) and radionuclide transport (RT) IRSRs. Subissue 6 examines alternate design features of the EBS, such as DS and backfill, that DOE is considering for extending container life and decreasing radionuclide release from the EBS. Any other design feature adopted by DOE for improvement of the engineered barriers performance will be considered in this subissue.

This version of the IRSR addresses all subissues listed previously and describes the extent to which DOE has provided adequate technical bases for resolution of each subissue. Furthermore, in this and in the consolidated IRSR (planned to be issued in FY2001), the staff evaluates whether DOE's technical bases reflect important physical phenomena and processes, consistent assumptions and definitions, consideration of alternative models, bounding approaches, adequate abstraction of process models, appropriate expert judgments, and quality assurance (QA) documentation.

3.0 IMPORTANCE TO REPOSITORY PERFORMANCE

The DOE presented a strategy for waste containment and isolation at the proposed YM site that has evolved during the last few years. In 1998, prior to issuing the VA, the primary goals of the DOE RSS (U.S. Department of Energy, 1998d) were stated as the near-complete containment of radionuclides within the containers for several thousand years and acceptably low annual doses to the average member of a receptor group living near the site. The DOE RSS, Revision 03 (CRWMS M&O, 2000a), states that the safety case to protect the public from any unreasonable long-term risk after permanent closure will focus on the two categories of radionuclides that would dominate long-term performance. The first category includes those radionuclides sufficiently insoluble that only trace amounts can dissolve in the groundwater. The second category includes the small fraction of radionuclides that is relatively soluble and those radionuclides that may be transported attached to colloids. For this reason, the repository system would use a robust WP made of a highly corrosion-resistant material to prevent exposure of the waste to the water and a separate DS over the WP to provide defense in depth.

The staff is developing a plan for reviewing the performance assessment (PA) of a proposed HLW repository at YM. The elements of this plan, which will be used to review the LA and make a determination as to the acceptability of repository performance according to the proposed rule in Part 63, are defined as integrated subissues (ISIs). Figure 2 illustrates the ISIs for this KTI within the solid line block pertaining to the EBS. Table B-1 in Appendix B shows the relationships between the subissues of the CLST KTI listed in Section 2.2 and the ISIs, or the corresponding model abstractions. The AC, on which staff review of key elements in the DOE SR and LA will be based, and the corresponding RMs, are currently being developed as part of the proposed YMRP. As noted in Section 2.0 of this report, the subissues related to container lifetime and radionuclide release rates from the EBS are considered important factors in the repository performance. For DOE to adequately demonstrate and quantify the consequences that container failure and radionuclide release have on repository performance, its LA must include the effects of the near-field environment on corrosion of containers, the mechanical disruption of containers, the degradation effects of both the quantity and chemistry of the water contacting the various WFs, the processes that affect solubility, formation of colloids and radionuclide release rates, and the effects of potential criticality processes and events.

3.1 RELATIONSHIP OF SUBISSUES TO THE U.S. DEPARTMENT OF ENERGY REPOSITORY SAFETY STRATEGY

The performance of the engineered barriers after emplacement is extremely important in the DOE RSS for the proposed YM site (CRWMS M&O, 2000a). Among the principal factors for the postclosure safety case, the performance of the WP barriers and the performance of the DS are noted, as well as the solubility limits of the dissolved radionuclides. The staff needs to evaluate the CLST KTI subissues to determine the merits of each of these DOE principal factors and may then perform its evaluation using, as appropriate, methodologies independent of the ones used by DOE.

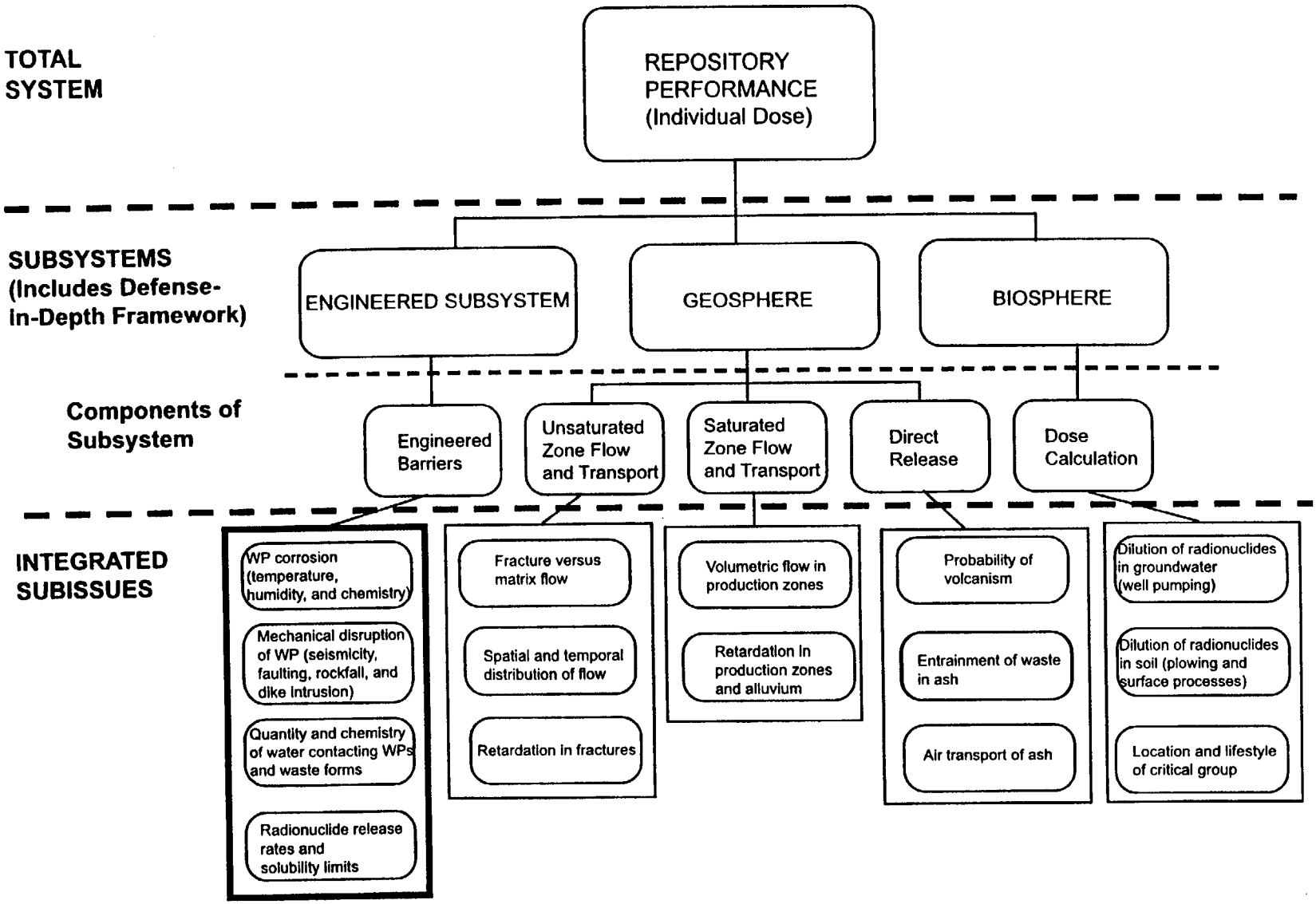

Figure 2. Flow diagram for total system performance assessment. The subissues of container life and source term provide input to the highlighted key elements.

3.2 IMPORTANCE OF SUBISSUES TO TOTAL REPOSITORY SYSTEM PERFORMANCE

Staff has implemented a strategy for assessing the performance of the proposed HLW repository at YM. The framework for this strategy is discussed in the Total System Performance Assessment and Integration (TSPAI) IRSR (U.S. Nuclear Regulatory Commission, 2000a). The four ISIs related to the performance of the engineered barriers and influenced by the subissues of the CLST KTI are highlighted in Figure 2. Figure 1 identifies the six subissues of the CLST KTI considered most important by NRC staff in determining the adequacy of container design, EBS features, and WF performance for long-term containment and limited radionuclide release. The container is the primary design element that provides radionuclide containment. After loss of containment, radionuclide release rates from the EBS are limited by WF characteristics and transport processes throughout the container and the EBS. The combination of long-lived containers and low-degradation-rate WFs can make a significant contribution to the performance of the repository system. The importance of the CLST subissues to repository performance is discussed in detail in the following sections.

3.2.1 Corrosion Effects—Importance to Performance

Under anticipated repository conditions, corrosion is expected to be the dominant failure mode limiting container life (Cragnolino and Sridhar, 1991, 1992; Sridhar, et al., 1995). Container life is defined as "...the time lapsed until through-wall penetration of both outer and inner metallic barriers by corrosion or by mechanical failure." Loss of containment allows the release of radionuclides to the environment surrounding the WPs. Mechanical failures associated with material instability and container failures resulting from disruptive events are both considered in Subissue 2.

In recent PA studies (Wilson, et al., 1994; CRWMS M&O, 1995, 1998a,b; U.S. Nuclear Regulatory Commission, 1995, 1999b; Mohanty and McCartin, 1998; Mohanty, et al., 1999; Kessler and McGuire, 1996; Shoesmith and Kolar,1998; U.S. Department of Energy, 1998c), container life is determined mainly by the failure time caused by the penetration of the outer and inner overpacks as a result of corrosion. Leaving aside those cases related to disruptive events and mechanical failure, it is assumed in these studies that radionuclide release cannot take place until the container is breached by through-wall penetration as a result of corrosion.

3.2.2 Materials Stability, Initial Defects, and Mechanical Failure—Importance to Performance

Thermal stability of corrosion-resistant Ni-base Alloy 22, proposed as the outer overpack material in EDA-II and the SR design, can be compromised by prolonged exposures to elevated temperatures (Cragnolino, et al., 1999). Generation of ordered structures or formation of brittle intermetallic phases may affect mechanical properties or facilitate degradation processes, such as HE. Degradation of mechanical properties leading to mechanical failure from residual and/or applied stresses can adversely affect container performance and, ultimately, performance of the

repository system. Initial or premature failure of containers, which occurs as a result of the presence of initial defects (presumably undetected during fabrication and handling operations), is considered within this issue because of its importance to performance. The consequences of disruptive events, such as seismic activity, volcanic activity, and faulting, and their effects on mechanical failure of WPs, which is part of this subissue, will be evaluated in the consolidated IRSR. Aspects of these disruptive events that may affect the mechanical integrity of containers are currently discussed in IRSRs on RDTME, SDS, and IA.

3.2.3 Spent Nuclear Fuel Degradation—Importance to Performance

After container failure, SNF will be exposed to the potentially degrading effects of the environment in contact with the WP. Possible degradation processes for CSNF include the breach of Zircaloy cladding, dry-air oxidation and aqueous dissolution of the irradiated UO_2 matrix, followed by the formation of colloids and secondary minerals, which can result in the mobilization of radionuclides and subsequent release from the EBS (Manaktala, 1993; Manaktala, et al., 1995; Ahn, 1996a,b). Although the total inventory of DSNF is relatively insignificant , it encompasses a variety of fuel types, some of which can exhibit dissolution rates much higher than that of CSNF. Resistance of the SNF to environmental degradation could contribute substantially to controlling radionuclide release from the EBS and could enhance overall performance of the repository.

3.2.4 High-Level Waste Glass Degradation—Importance to Performance

After container failure, the glass WF will be exposed to the potentially degrading effects of the environment in contact with the WP. A possible degradation process is dissolution of the borosilicate glass matrix, accompanied by the formation of colloids and secondary minerals, which can result in the mobilization of radionuclides followed by release from the EBS (Manaktala, 1992; Manaktala, et al., 1995). In this regard, the staff recognizes that glass wastes will constitute only about 3 percent of the total radionuclide inventory in the repository. However, if the glass WF performs poorly in the repository environment, it could conceivably make a significant contribution to the overall radionuclide source term from the EBS. Accordingly, the resistance of the glass WF to environmental degradation could contribute substantially to controlling radionuclide release from the EBS, enhancing the overall performance of the repository.

3.2.5 Criticality within the Waste Packages—Importance to Performance

Criticality within the WP during pre-closure and post-closure could have a significant effect on repository performance. The most likely effect of a criticality during the preclosure period would be an increase in dose to workers. Depending on the dynamics of the criticality condition, off-site releases could be possible. The likely effects of in-package criticality, with regard to repository post-closure performance, are increases in the radionuclide inventory, WP heat output, and WP degradation.

For in-package criticality, steady-state criticality events would lead to increased radionuclide inventories. However, repeated fast reactivity insertion over a long period of time could also be

important from a radionuclide production standpoint. Depending on the power level and duration of critical conditions, significant amounts of radionuclides, especially fission products including Tc-99, Np-237, and I-129, will be produced. The impact on the repository performance would be an increase in radionuclide inventory available for release from the WP, and a potential subsequent increase in dose to the critical group.

The second aspect of in-package criticality, with regard to the repository performance, is heat production, from the additional fission reactions taking place during criticality conditions, in addition to the expected decay heat. The additional heat produced could impact repository performance indirectly through its effect on the near field environment, and could increase WP corrosion rate.

The third aspect of in-package criticality is its impact on WP integrity, which includes the WF. This factor is directly linked to the repository performance. Configurations initiated by a sudden mechanical disturbance, such as an earthquake or rockfall, can result in a step reactivity insertion that could result in a mechanical failure of the already corroded WP and/or ruptures of the SNF cladding. The temperature and kinetic energy generated by the step reactivity insertion could also increase the exposed surface area and degradation rate of the SNF matrix. Other parts of the EBS could also be affected, including stability of the surrounding rock, which could then cause further damage to the WP.

3.2.6 Alternate Engineered Barrier Subsystem Design Features—Importance to Performance

The DOE discussed several major design alternatives in the VA (U.S. Department of Energy, 1998b). These alternatives include ceramic coating on containers, dual corrosion-resistant materials, DS, backfill over and under the DS, WP filler, steel-lined drifts, lower thermal loading, and ventilation. Subsequently, in EDA-II, the WP design proposed for the SR consists of a dual overpack with Alloy 22 as the outer overpack and Type 316 NG as the inner overpack (mainly to provide structural mechanical strength) (CRWMS M&O, 1999a,b). These design changes may have a significant effect on performance. For example, absence of a carbon steel outer overpack may obviate concerns related to thermal-aging-induced embrittlement and stresses arising from corrosion products. However, the thinner overpacks proposed for the SR design may give rise to greater radiolysis of the near-field environment and less mechanical strength to sustain the effects of seismic events, including rock fall. The DOE is considering alternate design features for improving the performance of the EBS. These features include the use of DS made of Ti grades 7 or 16 to avoid direct contact of water dripping on the WP surfaces, and backfill to modify the environment surrounding the WPs (CRWMS M&O, 1999b). The performance of the DS is one of the principal factors in the current strategy of the DOE for the safety case (CRWMS M&O, 2000a).

3.3 CONSIDERATION OF CONTAINER LIFE AND RADIONUCLIDE RELEASE IN PREVIOUS PERFORMANCE ASSESSMENTS

The evaluation of container life and radionuclide release from the EBS has been performed in recent PA studies for the proposed YM repository in which the horizontal drift-emplaced WP conceptual design was considered. These studies include DOE's TSPA-95 (CRWMS M&O, 1995); the Electric Power Research Institute (EPRI) YM TSPA, Phase 3 and 4 (Kessler and McGuire, 1996; Shoesmith and Kolar, 1998); the DOE TSPA-VA (U.S. Department of Energy, 1998c); the impending DOE TSPA-SR (CRWMS M&O, 2000o); and the NRC/Center for Nuclear Waste Regulatory Analyses (CNWRA) Total-system Performance Assessment (TPA).

3.3.1 U.S. Department of Energy Total System Performance Assessment

DOE evaluated container life in TSPA-95 (CRWMS M&O, 1995) using Version 1.0 of the stochastic WP degradation (WAPDEG) code (Atkins and Lee, 1996). WAPDEG is a probabilistic code designed to run stochastic simulations in which random values are sampled to represent parameters in the corrosion models for determining the WP failure time. This PA focused on WP failure by corrosion, and did not address WP degradation/failure resulting from mechanical stresses or juvenile failures.

The TSPA-VA (U.S. Department of Energy, 1998c), as well as the supporting technical basis document (CRWMS M&O, 1998a), included mechanical failure and juvenile failures, in addition to significant enhancements in the WAPDEG code for the consideration of corrosion processes. The main source data (i.e., corrosion rate) for evaluating WP performance in the TSPA-VA was obtained through the expert elicitation process.

Radionuclide release calculations were conducted as part of the calculations conducted with the Repository Integration Program (RIP), the computer code used for the PA of the repository (CRWMS M&O, 1998b). WP failure times, along with SNF matrix alteration/dissolution rates determined by using a parametric equation that depends on environmental factors, were used in the code to compute the rate at which radionuclides are released, taking into consideration their solubility as a constraint. The SNF matrix alteration/dissolution rates were determined by using a parametric equation from tests in Ca- and Si-free, sodium carbonate solutions for SNF and in simulated groundwater for HLW glass. The rates depend on environmental factors such as carbonate concentration, pH, temperature, and oxygen fugacity. The alteration/dissolution by the groundwater was assumed to take place under dripping conditions. In addition, cladding protection was considered for SNF, decreasing the exposed surface area of the bare SNF matrix. The mass transfer of dissolved radionuclides out of and away from the WPs was computed as a sequence of processes. By using certain simplifications, release and transport of colloids were also considered.

The sensitivity analyses included in TSPA-VA (U.S. Department of Energy, 1998c) indicated that uncertainty and variability in the Alloy 22 general corrosion rate were important for 10,000 and 100,000 years. Additional factors important to total system performance were the fraction of wetted surface area, pH, water chemistry, juvenile failures, and rate of cladding failure.

The DOE TSPA-SR (CRWMS M&O, 2000o) will further update the models used in the TSPA-VA to reflect design changes since the issuance of TSPA-VA, such as a dual-container model using Alloy 22 as the outer container material and Type 316 NG SS as the inner container material and the use of a Ti grade 7 (Ti-0.15Pd) DS. The TSPA-SR will also utilize, where possible, qualified experimental data as model parameter inputs. Based on the current materials for construction (Alloy 22 and Ti grade 7), dry-air oxidation of container materials is no longer considered an important failure mode (CRWMS M&O, 2000o). The failure modes that are expected to be considered in the upcoming TSPA-SR include humid air corrosion, general aqueous corrosion, crevice corrosion, pitting corrosion, stress corrosion cracking (SCC), hydride cracking, and long-term phase stability.

Humid air corrosion is distinguished from dry conditions through the use of a critical relative humidity (RH). The critical RH for the onset of humid air corrosion is considered to be a function of the presence and composition of salt deposits on the WP and DS surfaces. Once the critical RH is achieved, corrosion takes place. The corrosion rates used for humid-air corrosion are described by the same distribution used for general aqueous corrosion (CRWMS M&O, 2000b) and assumed to be constant with time. Above a higher critical RH, a thin, continuous aqueous layer is formed marking the onset of general aqueous corrosion. The rates used for general aqueous corrosion for both Alloy 22 and Ti grade 7are currently based on weight-loss measurements of specimens exposed in the Long-Term Corrosion Test Facility (LTCF). Two models are currently being considered for localized corrosion—one relying on a critical potential approach and the other relying on a critical temperature approach. For both cases, once the parameter of consequence (i.e., potential or temperature) exceeds the critical value, localized corrosion is considered possible. The rates of propagation for localized corrosion are also intended to originate from qualified laboratory data. Similar to localized corrosion, two conceptual models for SCC of Alloy 22 are being considered, the first using a critical stress intensity for initiation and the second using a finite stress level and a finite SCC propagation rate. Both models have been abstracted in a form that could be used in the WAPDEG code. Hydrogen-induced cracking of the Ti Grade 7 DS is dependent on the rate of the cathodic production of hydrogen, the quantity of hydrogen absorbed by the metal, and the critical hydrogen concentration needed to induced embrittlement.

Results of the TSPA-SR are not available at this time; however, several key sensitivity analyses have been planned to examine potentially important issues. These issues include percentage of WP and DS wetted by drips, cyclic wet and dry conditions, alternative water chemistries in contact with the WP and DS, alternative conceptual models for SCC, effects of microbial activity, alternative threshold potentials for localized corrosion, and the effects of rockfall and fabrication on WP and DS performance (CRWMS M&O, 2000o).

3.3.2 Electric Power Research Institute Performance Assessment

An alternative assessment of WP performance was conducted by EPRI examining the VA design in their YM TSPA, Phases 3 and 4, using the integrated multiple assumptions and release calculations code, as reported by Kessler and McGuire (1996) and Shoesmith and Kolar (1998) respectively. Similar to that developed in Phase 3 (Kessler and McGuire, 1996), the Phase 4 code

is a deterministic code in which an event tree approach is used and the container life is assumed to be governed by a series of Weibull distributions that are dependent on the heat transfer mechanism (conduction only, conduction and convection, and heat pipe) and the temperature history. Corrosion processes considered in this statistical approach are general corrosion; localized corrosion (pitting and crevice); SCC; degradation from a metastable microstructure; embrittlement caused by hydride formation; and MIC. Galvanic protection is not considered. The Weibull distributions employ a feature that allows for the possibility that a small fraction of the containers may have failed at emplacement, or shortly thereafter because of manufacturing flaws, construction errors, or emplacement mishandling. The parameters for the distribution in the case of aqueous corrosion processes were obtained in Phase 3 through correlations derived from underground corrosion tests in soils and in Phase 4 (Shoesmith and Kolar,1998) by examination of available literature data and reliance on the DOE WP Expert Elicitation results.

The source term is modeled as a set of compartments in which it is assumed that all WF surfaces are wetted immediately after the container fails. Advection and diffusion between the following compartments can be modeled: WF; corrosion products found in the corroded section of the container; gravel backfill below and, sometimes, above the container; concrete invert (concrete matrix and fracture); and the rock matrix and fractures immediately surrounding the drift. The flux entering the container is assumed to be 5 percent of the water percolation rate times the horizontal cross-sectional area of the container. An opening at the bottom of the container is assumed to be equal in size to the opening at the top, so a flow-through model is used to mobilize waste inside the container. Radionuclides are assumed to be released congruently with the degradation of cladding and dissolution/alteration of the SNF matrix, but are constrained by their solubilities.

Results of the container failure rate model used in this PA indicate container lifetimes in the range of 10^4 to 10^5 yr in Phase 3 that increased to from 10^4 to 10^6 yr in Phase 4, including the effects of temperature, humidity, and microbiologically influenced corrosion on WP degradation. Mechanical failures were not considered.

3.3.3 U.S. Nuclear Regulatory Commission/Center for Nuclear Waste Regulatory Analyses Total System Performance Assessment

The EBS failure (EBSFAIL) module in TPA Versions 3.1 and 3.2 (U.S. Nuclear Regulatory Commission, 1999b; Mohanty and McCartin, 1998) is designed to calculate the failure times of the WPs from various corrosion processes. Below a critical value of RH only dry-air oxidation takes place. Above this value, humid-air corrosion occurs and at a higher critical value, aqueous corrosion begins. The aqueous environments considered in EBSFAIL are those derived, adopting several simplifications, from coupled thermal-hydrological-chemical calculations. The aqueous corrosion processes for both the outer and inner overpack are governed by the corrosion potential and the critical potential required to initiate localized corrosion. This approach uses well-established electrochemical kinetics equations for calculating the corrosion potential, which depends on environmental variables, such as temperature, oxygen partial pressure, and pH, as well as experimentally measured values of the critical potentials. The repassivation potential (E_{rp}), which depends on temperature and chloride

concentration, is the critical potential conservatively used to define the occurrence of localized corrosion. Once the corrosion potential exceeds the E_{rp}, the initiation time for pitting corrosion is assumed to be negligible, but pit growth rates are calculated by using experimentally determined expressions and parameters. Failure of the WP is defined as penetration of both overpacks by a single pit or by general dissolution. Different container materials can be assessed by changing values of several input parameters. The E_{rp}, rates of uniform and localized corrosion, and threshold Cl^- concentration for localized corrosion can be listed, among others, as the corrosion-related parameters for the overpack materials. Yield strength and fracture toughness are the mechanical properties included as input parameters.

The EBS release (EBSREL) module in TPA calculates the time-dependent release of radionuclides after EBSFAIL determines the failure time of the containers. These release computations are based on the congruent dissolution of the SNF, limited by solubility. Four alternative models are considered for the dissolution of SNF. The first model consists of an empirical, parametric equation for the dependence of the dissolution rate on environmental factors obtained in flow-through tests conducted in pure carbonate solutions. These environmental factors are temperature, pH, carbonate concentration, and oxygen partial pressure. The dissolution rate in the second model is an Arrhenius-type dissolution rate with parameters selected to be consistent with experimental data under multiple environmental conditions. The third model allows for the use of a specified dissolution rate (e.g., derived from natural analogue studies or from drip tests). The fourth model is based on calculating the total U concentration considering five aqueous UO_2^{2+} species in equilibrium with a secondary uranyl phase, schoepite, assuming that most of the radionuclides contained in the SNF matrix are incorporated in this solid phase and released congruently. Release from a perforated container can be evaluated through either a WP bathtub or flow-through models, which are considered as alternative conceptual models for the source term. Advective and diffusive transport of radionuclides away from the EBS is computed based on radionuclide mass balance in the water contacting the WP. Both EBSFAIL and EBSREL are deterministic modules incorporated in the TPA code, which provides for sampling parameter distributions in a probabilistic framework.

3.4 SENSITIVITY ANALYSES

Sensitivity analyses were conducted using Version 3.2 of the NRC TPA code (Mohanty, et al., 1999). Specifically, the sensitivity of repository performance to the effects of container failure and radionuclide release was analyzed. These effects, as well as the importance of parameter values used in the various models, can be determined by systematically performing sensitivity analyses. (In this case, repository performance is defined as individual dose to an average member of the critical group.) Both process-level models and the abstracted models in the TPA code can be used to ascertain the effects of container failure and radionuclide release on the performance of the repository system. Process-level models are detailed models based on fundamental principles and empirical correlations or expressions that govern container failure and radionuclide release for the range of expected conditions at the repository. Abstracted models within the NRC TPA code are designed to represent the physical processes by extracting only higher-order effects identified in process-level models. The CLST process-level models have

been described in the Engineered Barrier System Performance Assessment Code (EBSPAC) Version 1.1, Technical Description and User's Manual (Mohanty, et al., 1997).

Results of sensitivity analyses obtained with the TPA code Version 3.2 to examine the performance of WPs, with particular emphasis on the behavior of Alloy 22,are summarized in the following paragraphs.

1. There are two parameters related to the conditions prevailing in the near-field environment that have a significant effect on container failure as a result of corrosion and, correspondingly, to radionuclide release from the EBS and to dose to an average member of the critical group. These parameters are oxygen partial pressure and chloride concentration in the water contacting the WPs. Their main effects are to reduce the lifetime of the Alloy 22 overpack after those parameters exceed the threshold values required to promote localized corrosion, instead of uniform corrosion. Although not directly evaluated, RH has an important influence on container life because containers become wet at an earlier time when RH is higher, promoting the occurrence of aqueous uniform or localized corrosion.

2. If localized corrosion does not take place, a key parameter is the passive corrosion rate of the outer overpack material. For Alloy 22, the outer overpack material selected by DOE in the SR design, the container failure time is significantly delayed, as demonstrated in the system-level sensitivity analysis. In this case, the effect of the range of values adopted for the passive corrosion rate is even more important for its influence on dose, as illustrated in Figure 3 by comparing the base case with the modified case. The results shown in Figure 3 were obtained using the TPA code Version 3.2 by eliminating the contribution to performance of the outer carbon steel container included in the VA design.

3. Other parameters that affect radionuclide release from failed containers and, as a consequence, dose, are SNF surface area as related to irradiated UO_2 particle or grain size, solubility of Am, and cladding as a barrier to release. Particles are fragments of irradiated UO_2 pellets, and a large number of grains in a particle can be exposed to groundwater during SNF dissolution. As expected, radionuclide releases assuming a fuel grain model are larger than those for a fuel particle model. Also, the presence of cladding significantly decreases radionuclide release by decreasing the exposed area of the bare SNF matrix.

4. The contribution of colloids (mainly Pu) to dose was also evaluated. The contribution of colloidal transport of Pu appears to be insignificant within the compliance time by considering the amount of Pu released from SNF in contact with J-13 well water. However, if Pu release increases as expected in the presence of altered groundwater, its contribution to dose can be significant.

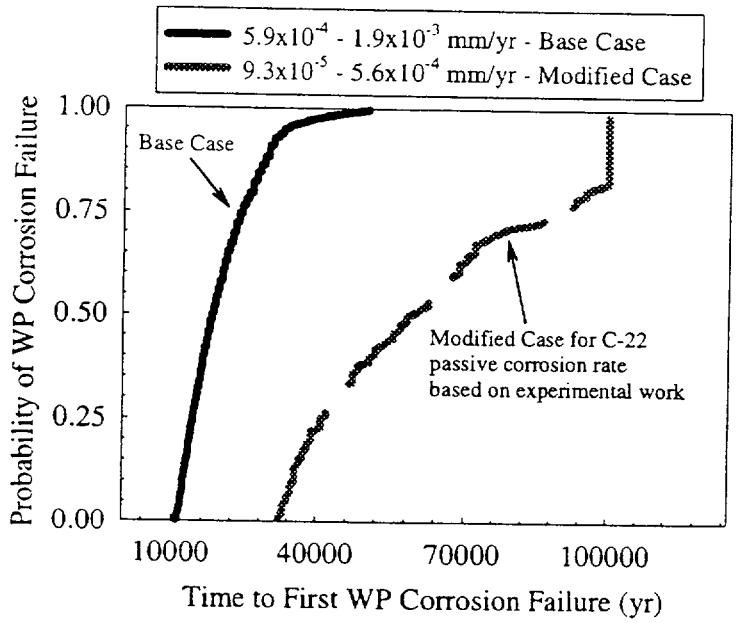

Figure 3. Effect of assumed passive corrosion rates for Alloy 22 on predicted waste package lifetime. Sensitivity analysis using TPA code Version 3.2.

Figure 4 shows the sensitivity of the peak mean doses at 10,000 and 50,000 years to the different dissolution models for SNF (see Section 4.3.1) and to various release-related parameters described above. Among others, the parameters include no retardation of Pu, Am, and Th (as a simulation of potential colloid contribution), flow-through conditions, dissolution of SNF grains in pure carbonate solution, dissolution of SNF particles in pure carbonate solution, dissolution of SNF particles in groundwater as regarded in the basecase, and cladding protection.

The list of model and parameters included in Figures 4a and b (Mohanty, et al., 1999) comprises

NoRet	No retardation for Pu, Am, and Th
Flwthru-1	The flow-through option for fuel dissolution Model 1
Flwthru-2	The flow-through option for fuel dissolution Model 2
Grain1	Model 1 dissolution plus UO_2 grain-size distribution
Model 1	Fuel dissolution model based on carbonate water
Focflow	Four times the flow to 1/4 the number of wetted WPs
Base	The base case
Matdif	Matrix diffusion in pathway analysis
Clad-M1	Cladding credit of 99.5 percent with Model 1 fuel dissolution model

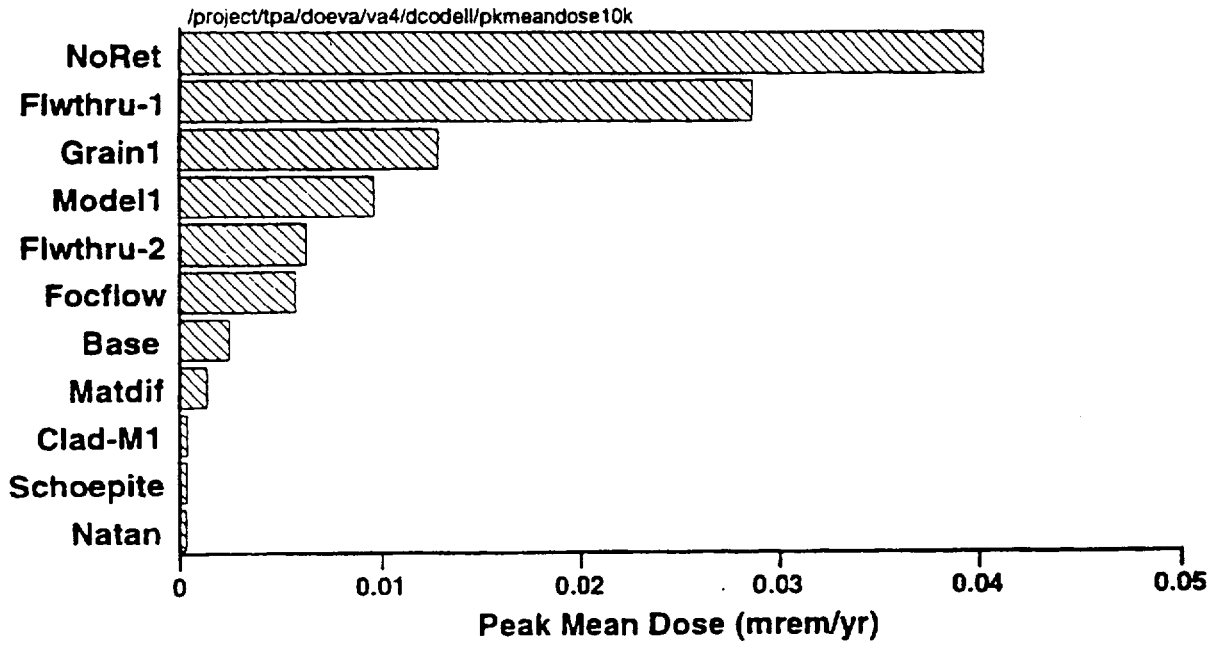

Figure 4a. Effect of several spent fuel dissolution models and various input parameters on the peak mean dose for 10,000 years (Mohanty, et al., 1999)

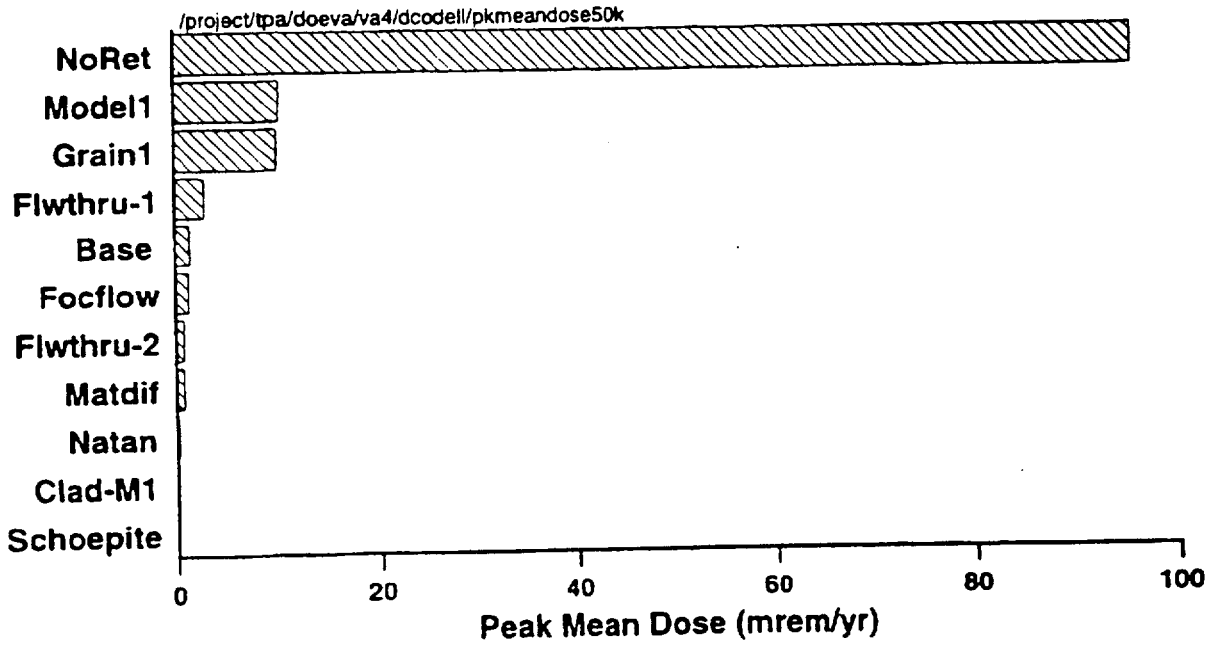

Figure 4b. Effect of several spent fuel dissolution models and various input parameters on the peak mean dose for 50,000 years (Mohanty, et al., 1999)

Natan	Release rate from fuel based on Peña Blanca natural analog
Sckoepite	Release rate form fuel based on solubility of schoepite

It is expected that sensitivity analyses completed with a new version of the TPA code will draw different conclusions because of the different repository design that it addresses (TPA code Versions 3.1 and 3.2 model the VA design). The code is being modified to model the SR design.

4.0 TECHNICAL BASES

The proposed 10 CFR Part 63.113 requires DOE to demonstrate that both engineered and natural barriers make a contribution to overall repository system performance such that isolation of radioactive material does not depend unduly on any single barrier, and as a result, is more tolerant to failures and external challenges. In this regard, the CLST primary issue (Section 2.0) relates to the contribution of the EBS to performance. Specifically, the adequacy of the EBS design will depend, in part, on DOE's demonstration that the containers will be sufficiently long-lived and that radionuclide releases will be sufficiently controlled such that the EBS contributes to overall repository system performance. DOE should address the six subissues described in Section 2.0, all of which relate directly to processes and events that affect container lifetime and radionuclide release. The staff developed AC that, if satisfied, would resolve the CLST primary issue, the six subissues and, ultimately, questions related to the adequacy of the EBS design. General and specific AC, as well as the corresponding RMs, are currently being developed. In this revision (Revision 3) of the CLST IRSR, detailed AC are cited in the discussion of the status of issue resolution in Section 5.0. The general AC are consistent with the methodology described in the American Society for Testing and Materials (ASTM) Standard Practice C-1174 for prediction of the long-term behavior of EBS components in a geologic repository (American Society for Testing and Materials, 1997a). The following sections provide the technical bases for all subissues listed in Section 2.0.

4.1 SUBISSUE 1: THE EFFECTS OF CORROSION PROCESSES ON THE LIFETIME OF THE CONTAINERS

This subissue relates to the adequacy of DOE's consideration of the effects of corrosion processes on the lifetime of the containers. Resolution of this subissue will be accomplished through the application of the AC, as presented in Section 5.1.

4.1.1 Technical Bases

Repository regulatory requirements recognize that the engineered barriers provided to isolate radioactive wastes for long periods of time will eventually degrade. It is anticipated that the primary cause for engineered barrier degradation under normal conditions (i.e., in the absence of disruptive events, such as seismicity, faulting, or volcanism) will be one or more corrosion processes. Both DOE and the staff evaluated the most likely forms of materials degradation for the candidate container materials of interest (Farmer, et al., 1988; Gdowski, 1991; Cragnolino and Sridhar, 1991, 1992; Geesey, 1993; Sridhar, et al., 1994; U.S. Nuclear Regulatory Commission, 1997; Cragnolino, et al., 1999). These degradation modes include dry-air oxidation of container materials during the initial hot, dry period following emplacement of the WPs in the drifts. After this initial period, the drift wall and container surface temperatures will decrease and the container materials will be subjected to humid-air corrosion and various modes of aqueous corrosion (i.e., general corrosion, localized corrosion, MIC, SCC, and HE). It is hypothesized that humid-air corrosion and aqueous corrosion can be initiated at times in which RH exceeds the respective critical value for each corrosion process. Under these conditions, it is expected that humid-air corrosion will occur in the presence of a thin surface film of condensed fluid in contact with water

vapor above the surface as in the case of atmospheric corrosion (Fyfe, 1994). As the temperature continues to decrease, aqueous corrosion will occur as a result of the formation of a thicker film of condensed fluid that behaves as bulk water. In addition, groundwater enriched in salts through evaporation and rock-water interactions may drip on the WPs through fractures in the rock. The influx of water is determined by various thermo-hydrological processes, such as heat-pipe effects, gravity-driven refluxing, and percolation of meteoric water. The importance of various modes of materials degradation and the corresponding effects on barrier performance are dependent on WP design and construction, materials selection, and the environment interacting with those materials. The chemical composition of the environment contacting the WP components depends on the evolution during the heating and cooling periods of the near-field environment. Information about this evolution is, therefore, a requirement for evaluating WP corrosion. A detailed discussion of the effects of coupled thermo-hydrological-chemical processes on the WP chemical environment is presented in the ENFE KTI IRSR.

Alloy 22, a Ni-Cr-Mo alloy, was selected by DOE as the candidate material for the outer overpack of the double-shelled WP in the proposed design for the SR surrounding an inner overpack of Type 316 NG SS, which will provide structural strength. The performance of Alloy 22 has become one of the most important factors in determining the performance of the repository system. Hence, this component of the subissue is discussed in greater detail. DOE is evaluating the advantage of taking credit for the performance of Type 316 NG SS in the proposed SR design as related to the reduction of the rate of radionuclide release from the degraded WP.

Resolution of Subissue 1 will necessitate identification of the most important modes of container degradation resulting from corrosion processes, numerical estimates of the effects of corrosion on container lifetime, assessment of the performance of the WPs, including material and fabrication methods for the containers, and adequacy and validity of the available corrosion database.

4.1.1.1 General and Localized Corrosion of Alloy 22

The corrosion behavior of the Ni-Cr-Mo alloys was reviewed in detail by the CNWRA on the basis of literature data (Cragnolino and Sridhar, 1991; Sridhar, et al., 1994) and the available information was recently updated (Cragnolino, et al., 1999). A similar review was conducted by DOE (Gdowski, 1991). Initially, Alloy 825 was the primary candidate material, replaced after several years by the more corrosion-resistant Alloy 625, and at the end of 1997, by the even more corrosion-resistant Alloy 22. In this context, corrosion resistance implies increasing resistance to localized corrosion (pitting and crevice) in chloride solutions promoted by the combined effect of Cr as the main alloying element (about 22 wt %) and the increasing Mo (and W for Alloy 22) content. To quantitatively assess the beneficial effect of these alloying elements and, in particular, to develop a methodology for PA, the CNWRA used the E_{rp} as a criterion for the occurrence of localized corrosion. This potential is measured in chloride-containing solutions simulating concentrated groundwater assumed to be present in the environment surrounding the WPs. Extensive experimental work was conducted on Alloy 825 to develop and confirm the validity of this methodology (Sridhar, et al., 1995; Dunn, et al., 1996, 2000a). A similar approach has been developed for Alloys 625 and 22 (Gruss, et al., 1998; Dunn, et al.,1999a, 2000b;

Cragnolino, et al., 2000). The short-term data on localized corrosion of these alloys at 95 °C (Figure 5) indicate that the E_{rp} for Alloy 22 is significantly higher than that of Alloys 825 and 625 at chloride concentrations less than about 4 M. At higher chloride concentrations, E_{rp} for Alloy 22 decreases significantly. As shown in Figure 6, E_{rp} decreases with increasing temperature at any chloride concentration.

The approach adopted by the CNWRA consists of measuring the E_{rp}, and comparing the values obtained, considering the associated uncertainties, with the corrosion potential expected over a wide range of environmental conditions. This approach was used in EBSPAC (Mohanty, et al., 1997) and in the TPA Version 3.2 code (Mohanty, et al., 1999) to determine the electrochemical conditions leading to the initiation of localized corrosion. Calculations conducted with Alloys 825 and 625 demonstrated the initiation of localized corrosion and the failure of the WP because of the pit penetration of both the outer and inner overpack in a few thousand years after repository closure. In the case of Alloy 22, however, computations reveal the absence of localized corrosion for more than 10,000 years. As a consequence, a precise determination of the rate of uniform corrosion under passive conditions becomes important to assess container life. Measured values of passive current densities, and the values of corrosion rates calculated using Faraday laws are shown in Table 1 in which the range of values assumed in the TPA Version 3.2 code are also listed. The values of passive current density listed are the result of a single determination using as received, base metal specimens (not welded). Uncertainties associated with the measurements of extremely low corrosion rates by weight loss preclude a reliable and precise prediction of container life. This calculation of container life becomes important for radionuclide release and the subsequent estimation of the average annual dose to the average member of the critical group. A reasonable approach to resolve these uncertainties could be the use of fundamental models describing the growth of anodic oxide films on metals. These models would at least establish an upper bound value for the rate of dissolution under passive conditions. Fundamental models for passive film growth can be compared to measured passive current

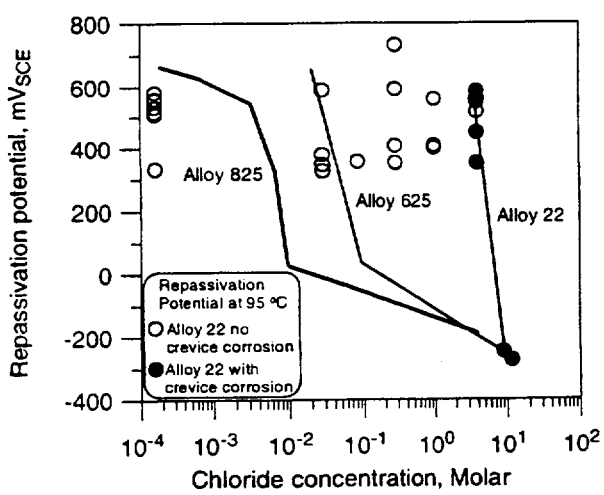

Figure 5. Effect of chloride concentration on repassivation potential of three different Ni-Cr-Mo alloys (Dunn, et al., 1999a)

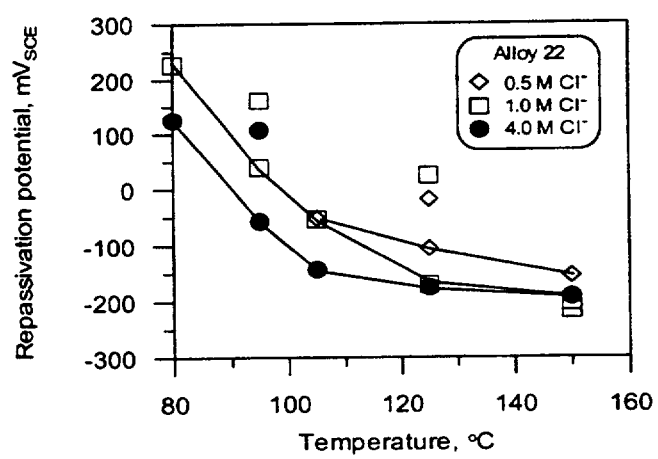

Figure 6. Effect of temperature on the repassivation potential for crevice corrosion of Alloy 22 in Cl^- solutions (Cragnolino, et al., 2000)

Table 1. Measured passive current density and calculated corrosion rates of Alloy 22 under various conditions (Dunn, et al., 1999b)

Starting Condition of Alloy 22	$[Cl^-]$ (M)	pH	Temp (°C)	Potential (mV_{SCE})	Anodic Current Density (A/cm^2)	Corrosion Rate (mm/yr)	Lifetime of 20-mm thick Waste Package Barrier (yr)
As received	0.028	8	20	200	2×10^{-9}	2×10^{-5}	~ 1,000,000
As received	0.028	8	95	200	3×10^{-8}	3×10^{-4}	~ 67,000
As received	0.028	0.7	95	200	7×10^{-8}	7×10^{-4}	~ 29,000
As received	4	8	95	200	3×10^{-8}	3×10^{-4}	~ 67,000
As received	4	8	95	200	4×10^{-8}	4×10^{-4}	~ 50,000
Low dissolution rate assumed in TPA 3.2 code					6×10^{-8}	6×10^{-4}	~ 34,000
High dissolution rate assumed in TPA 3.2 code					2×10^{-7}	2×10^{-3}	~ 10,000

density values. The development of models, to be validated experimentally over a period of few years, could be useful to evaluate if low passive corrosion rates can be sustained over periods of many thousands of years.

The specific consideration of corrosion modes associated with weldments is necessary because in many engineered structures and components, welded joints are more prone to corrosion failure than the base metal. The effect of welding on the localized corrosion resistance of Alloy 22 is being evaluated because the weld metal exhibits a critical temperature for pitting corrosion significantly lower than that of the base metal (Sridhar, 1990). The lower localized corrosion resistance of the weld metal has been related by Sridhar (1990) to the segregation of alloying elements, such as Mo and W in the interdendritic regions formed during the solidification of the fusion zone (Cieslak, et al., 1986). However, the E_{rp} values measured at 95 and 125 °C for welded material are approximately equal to those for the mill-annealed material, as shown in Figure 7 (Cragnolino et al., 2000). The passive current density increased on welded material with respect to the mill-annealed material, but it is only three times greater (Dunn, et al., 2000b), as shown in Figure 8. Because of its low carbon content, Alloy 22 is not susceptible to intergranular corrosion as a result of sensitization induced by carbide or intermetallic phase precipitation (Sridhar, 1990).

Inappropriate welding procedures, however, can result in increased susceptibility to intergranular corrosion (Cragnolino, et al., 1999). In addition, the effect of cold work followed by long-term thermal exposure on the localized corrosion of Alloy 22 should be evaluated, as also noted in Section 5.2.2, for the case of mechanical properties.

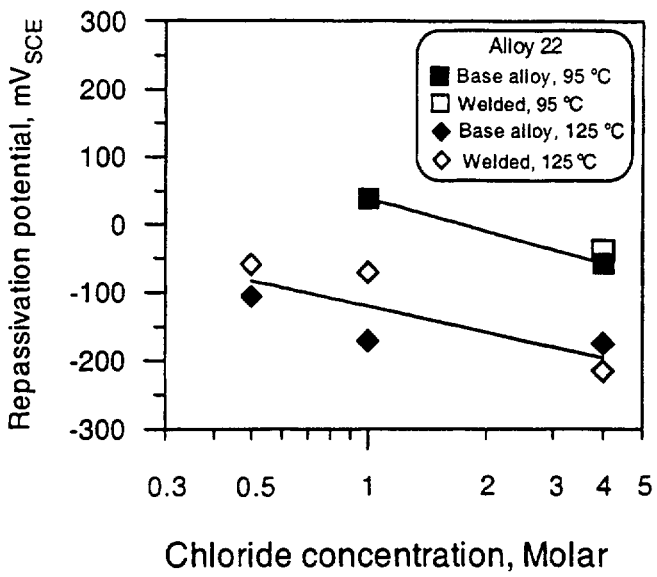

Figure 7. Repassivation potential for crevice corrosion measured on Alloy 22 specimens in Cl^- solutions (pH 8) (Dunn, et al., 2000b)

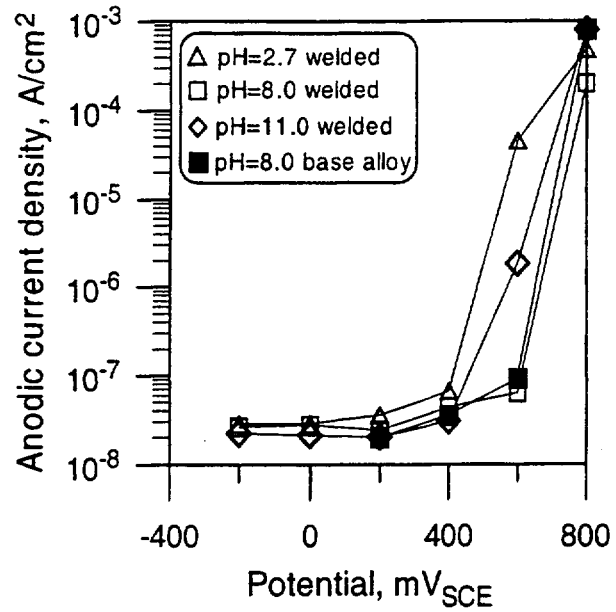

Figure 8. Steady-state anodic current densities measured for Alloy 22 in 4 M Cl^- solutions at 95 °C (Dunn, et al., 2000b)

MIC is currently acknowledged as a phenomenon that may affect the performance of WP materials (Geesey and Cragnolino, 1995). Microbial populations can survive exposures to temperatures on the order of 120 °C. They turn active only when the temperature declines and water and nutrients become available in sufficient quantities for bacterial growth. Classically, bacteria involved in MIC have been divided into three broad phenotypic groups: (i) acid-producing bacteria, (ii) sulfate-reducing bacteria, and (iii) iron-oxidizing bacteria (Little, et al., 1991). Bacteria representatives of each of these phenotypic groups have been identified as part of the natural flora at the proposed HLW repository site at YM (Pitonzo, et al., 1996; Horn, et al., 1998). Microbial biofilms are known to grow in environments where nutrients are present only at growth-limiting levels (Costerton, et al., 1995). Bacteria are able to grow because of the efficiency with which biofilms are capable of scavenging the available nutrients. However, as noted in the ENFE IRSR, before a determination of the effects of bacteria on corrosion of container materials, a nutrient and energy inventory calculation would be desirable to evaluate the potential for microbial activity.

Limited information is available on MIC of Ni-base alloys, with high Cr and Mo content, such as Alloy 22 (Geesey, 1993). It appears that the resistance of these alloys to MIC is related to their resistance to localized corrosion in abiotic environments. Owing to the high resistance of Alloy 22 to localized corrosion, MIC has not been reported for this alloy, but more information is needed to attain a definitive conclusion (Geesey and Cragnolino, 1995).

4.1.1.2 Stress Corrosion Cracking of Alloy 22

Ni-base alloys are quite resistant to SCC in hot chloride solutions and are used in many applications as a result of their exceptional corrosion resistance in a wide variety of aggressive environments. The resistance of these alloys to SCC has been reviewed (Staehle, et al., 1970; Jones and Bruemmer, 1990; Sridhar and Cragnolino, 1992) and has been demonstrated to be strongly dependent on the chemical composition of the alloy. Ni is the most important alloying element of Fe-Cr-Ni alloys conferring resistance to SCC in Cl^- environments. Additions of Cr and Mo also have significant effects on the SCC resistance, as well as the thermal history of the alloys. Aside from the alloy composition and thermal history, the composition and temperature of the environment are major factors determining SCC resistance. Elemental S, H_2S, or reduced S compounds are known to promote SCC. Most of the Ni-base alloys are susceptible to SCC above a critical temperature specific for each alloy.

As previously reviewed (Cragnolino, et al., 1999), Speidel (1981) examined commercial Fe-Ni-Cr alloys with 16 to 30 percent Cr, 1 to 73 percent Ni, and 0 to 4.5 percent Mo using compact tension specimens in boiling 22 percent NaCl (105 °C). In this solution, alloys with 20 percent Ni have the lowest threshold stress intensity for SCC, whereas, alloys with more than 30 percent Ni did not crack after 3 months of exposure at stress intensities of 60 $MPa \cdot m^{1/2}$. SCC testing of Alloy 22 and Type 316L SS using precracked double cantilever beam (DCB) specimens was completed to confirm the occurrence of SCC reported by investigators at the Lawrence Livermore National Laboratory (LLNL) in a N_2-deaerated 0.9 molal Cl^- (5 percent NaCl) solution at 90 °C acidified to pH 2.7 by the addition of HCl. Under equivalent experimental conditions to those used at LLNL, no crack growth (below a detection limit of 3×10^{-13} m/s) was observed in either material after more than 1 year of exposure (Dunn, et al., 2000c; Pan, et al., 2000a). In addition, no crack propagation was observed on Alloy 22 specimens after 1 year of exposure to a more aggressive solution (40 percent $MgCl_2$ at 110 °C) in which Type 316 L SS exhibited fast crack growth (about 1×10^{-8} m/s).

A review of SCC mechanisms, performed by Sridhar, et al. (1993), concluded that no one mechanism cou . satisfactorily explain the occurrence of SCC for the range of alloys and environment combinations where SCC is well documented. In addition, many SCC models have parameters that cannot be readily obtained. As a result, current models cannot be used to predict the SCC susceptibility of the candidate container materials over the long time intervals required for the proposed HLW repository. Hence, emphasis was placed on the evaluation of the concept of a critical potential such as the E_{rp} for localized corrosion to predict the electrochemical conditions for the initiation of SCC. The results of short-term tests with tensile specimens support the critical potential concept; however, long-term crack propagation measurements are necessary to demonstrate the validity of this approach that uses E_{rp} as a threshold parameter to assess SCC susceptibility (Cragnolino, et al., 1999). A similar concept but based in fracture mechanics considerations is applicable. In this case, the stress intensity threshold for SCC, K_{Iscc} can be used. However, as in the case of that based on E_{rp}, an extremely sensitive technique for measuring crack growth rates is necessary as a result of the long performance period (Sridhar, et al., 1993).

4.2 SUBISSUE 2: THE EFFECTS OF PHASE INSTABILITY AND INITIAL DEFECTS ON THE MECHANICAL FAILURE AND LIFETIME OF THE CONTAINERS

This subissue relates to the adequacy of the DOE consideration of container materials stability and mechanical failure. Container failures resulting from degradation of mechanical properties because of material instability, combined with the action of residual and/or applied stresses, can lead to release of radionuclides from the EBS. Resolution of this subissue will be through the application of the AC as presented in Section 5.2.

Disruptive events, such as seismic activity, volcanism, and faulting may promote premature failure of the containers through different processes. For example, as a consequence of seismic events, mechanical stresses may promote either brittle or ductile fracture of the container, depending on the degree of embrittlement of the container material and the magnitude and location (weldments, base metal) of the applied stresses. The component of this subissue related to the coupling of disruptive events and container material properties will be discussed in the consolidated IRSR.

4.2.1 Technical Bases

Repository regulatory requirements recognize that the engineered barriers provided to isolate radioactive wastes for long periods, in addition to being degraded by corrosion processes, may be affected by material instability (i.e., degraded mechanical properties) owing to prolonged exposure to relatively high temperatures. The staff evaluated the most likely processes affecting material stability for both outer and inner overpack materials considered in the VA design (Sridhar, et al., 1994; Cragnolino, et al., 1996, 1999).

Mechanical failure of containers caused by disruptive effects has been partially considered in other IRSRs (i.e., RDTME, SDS, and IA). The effect of phase instability on corrosion and SCC resistance is considered in Subissue 1.

Resolution of Subissue 2 will necessitate identification of the most important modes of mechanical failure, an evaluation of the potential for materials instability, and the effect of disruptive events on the probability of failures. Resolution will also require numerical estimates of the effect of these processes on container lifetime, assessment of the performance of the containers regarding materials selection and fabrication methods, adequacy and validity of the available database of mechanical properties, including toughness, and identification of appropriate nondestructive examination (NDE) methods.

4.2.1.1 Phase Instability of Alloy 22

Alloy 22, the material currently selected for the outer overpack, experiences an ordering transformation when heated in the temperature range of 250 to 550 °C (Sridhar, et al., 1994; Cragnolino, et al., 1999). The result is an increase in the work-hardening rate and, as a consequence, an enhanced susceptibility to SCC and HE. Another possible cause of thermal instability in Alloy 22 arises from the precipitation of brittle intermetallic phases. The effect of cold

work before thermal treatment on ordering transformation or intermetallic precipitation has not been studied extensively for Alloy 22. For Alloy 22, these effects are more likely to be a concern at high heat-loading. The thermal stability of Ni-Cr-Mo alloys under repository conditions has been reviewed by Sridhar, et al. (1994), Cragnolino, et al. (1999), and Gdowski (1991). Alloys such as Alloy 22 are prone to the formation of M_6C-type carbides and intermetallic phases, such as μ, σ, P, and Laves (Raghavan, et al., 1982).

All the Ni-Cr-Mo alloys of the class consisting of C-4, C-276, and Alloy 22 experience an ordering transformation when heated in the temperature range of 250–550 °C (Tawancy, 1981; Raghavan, et al., 1982; Hodge and Ahluwalia, 1993). Ordering in this temperature regime involves an initial short-range ordering followed by a LRO. The LRO follows the same type of crystallographic modification found in pure Ni_2Cr (Klein, et al., 1970) and involves formation of an orthorhombic crystal structure from the (420) or the (220) planes of the parent γ-phase. Six orientations of this orthorhombic structure are possible with respect to the parent γ-phase. Because of this definite orientation requirement, a twinning type deformation mode is preferred rather than dislocation slip. The result is an increase in the work hardening rate and, as a consequence, an increased susceptibility to SCC and HE. The effect of aging at lower temperatures for long periods on the mechanical properties was reported by Hodge and Ahluwalia (1993). A significant embrittlement as measured by the Charpy V-notch impact energy was found for specimens aged at 538 °C for 20,000 hours (2.3 years) and even at 425 °C for 45,000 hours. Rebak and Koon (1998) confirmed the existence of the LRO of Alloy 22 and the absence of the μ phase for aging times of 30,000 and 40,000 hours (3.4 and 4.6 years) at 425 °C. Hodge and Ahluwalia (1993) concluded, however, that long-range ordering in Alloy C-4 and related alloys is not likely under the thermal conditions expected in the repository (container temperatures lower than 250 °C) in a 1000-year period.

As noted by Sridhar, et al. (1994), cold-work before aging can increase markedly the kinetics of segregation of phosphorous to grain boundaries and LRO, as observed for Alloy 276 (Sridhar, et al., 1980a). Local areas of cold-work may occur in the containers through rock impingement, mechanical damage during handling, or on areas where surface defects, such as weld spatter, have been mechanically removed by grinding operations. Cold-work in the form of residual stresses can also result from fabrication during the cylinder rolling operations. Exposure to temperatures ranging from 200 to 500 °C may result in grain boundary segregation of metalloid elements, such as P (Berkowitz and Kane, 1980). Effects on mechanical properties and susceptibility to embrittlement of Ni-Cr-Mo alloys, however, have not been studied in sufficient detail. Issues related to weldments of Ni-Cr-Mo alloys have been briefly reviewed by Sridhar, et al. (1994). Segregation of Cr and Mo has been reported, but the effect on mechanical properties is unknown. Gdowski (1991) also concluded that long-term aging of Alloy 22 should be studied at temperatures of 250 °C or less, to determine the formation of intermetallic phases and the occurrence of LRO, as well as possible effects on mechanical properties and corrosion resistance. Although the studies of Hodge and Ahluwalia (1993) and Rebak and Koon (1998) suggested that repository temperatures are too low to promote degradation of mechanical properties, the effect of cold-work before long-term aging has not been addressed yet.

The necessary stresses for mechanical failure as a consequence of processes that cause material instability may arise from residual stresses generated as a result of welding operations; from stresses associated with the buildup of corrosion products in the gap between the outer and the inner overpacks once the outer container is breached; and applied stresses from the effect of disruptive events, such as seismic activity, volcanism, faulting, or a combination of these events.

4.2.1.2 Initial Defects in Alloy 22 Containers

The detection of fabrication defects associated, among other causes, with welding operations for both seam and closure welds requires the application of appropriate NDE methods. This factor is important in reducing the incidence of initial or premature failures in the performance of the WPs, a critical factor in calculated doses (Sridhar, 1999).

Initial or premature failures of containers are those initiated at one or more initial defects and occur essentially instantaneously (in comparison to the expected period of performance) These defects are considered to be undetected during fabrication, handling operations, and the preclosure period. Many of these defects are produced during fabrication, such as lack of fusion or weld penetration, surface contamination (e.g., poor degreasing), laps and iron contamination, improper filler metal in welds, voids, and inclusion/primary carbides. Other premature failures may be related to improper heat treatments (e.g., temperature evolution in large components leading to sensitization or temper embrittlement) or material mix-up. Improper handling operations may lead to dents or scrapes that may induce localized cold-work or become initiation sites for pits or cracks.

4.3 SUBISSUE 3: THE RATE AT WHICH RADIONUCLIDES IN SPENT NUCLEAR FUEL ARE RELEASED FROM THE ENGINEERED BARRIER SUBSYSTEM THROUGH THE OXIDATION AND DISSOLUTION OF SPENT FUEL

This subissue relates to the adequacy of DOE investigations on the rate of release of radionuclides from the SNF and the EBS. Resolution of this subissue will be through application of the AC, as presented in Section 5.3.

4.3.1 Technical Bases

It is expected that after the failure of the metallic container, there will be a gradual release of radionuclides from the EBS over long periods of time. Both DOE and the staff evaluated the most likely forms of SNF degradation (Manaktala, 1993; CRWMS M&O, 1998b; U.S. Nuclear Regulatory Commission, 1997). These degradation modes include dry-air oxidation of the fuel cladding and matrix inside any breached container (i.e., by juvenile failure) during the initial period following repository closure, when the environment contacting the WP is considered to be hot and dry air. After failure of containers by any of the various corrosion or mechanical processes described in Sections 4.1 and 4.2, the fuel cladding will be subjected to modes of failure somewhat similar to those anticipated for the failure of containers. As the cladding is breached, the fuel matrix consisting of irradiated UO_2 will be dissolved either by modified groundwater partially filling the failed containers, or by groundwater dripping on the SNF surfaces. As an

alternative process, fuel dissolution may occur by the action of humid air condensed as a thin film of water on the SNF. The chemical composition of the water inside breached WPs needs to be known or at least bounded to evaluate the dissolution of SNF. Initially, radionuclides in the gap between cladding and the SNF matrix and in the fuel grain boundaries will be released promptly. Following this prompt release, radionuclides will be released as the SNF matrix dissolves. Whereas high-solubility radionuclides, such as ^{99}Tc or ^{129}I will be released congruently with the dissolution of the matrix, U and low-solubility radionuclides, such as ^{239}Pu or ^{241}Am, will be reprecipitated on the surface of the irradiated UO_2 as secondary minerals. Consequently, the release of low-solubility radionuclides from the EBS will be determined thermodynamically by solubility limits or kinetically by steady-state concentration values controlled by the formation of secondary minerals. The low-solubility radionuclides may also form colloids that may become a vehicle for the mobilization of radionuclides in larger concentrations than those of soluble species limited by solubility. Once radionuclides are mobilized, they can be transported away from the EBS either by diffusion or by advection or both, depending on the various modes of groundwater contact with the SNF, such as dripping, partial or full immersion, or vapor condensation.

To evaluate the status of resolution of this subissue, several components need to be considered: (i) radionuclide inventory and distribution in the fuel; (ii) dry-air oxidation of the SNF and its effects on subsequent performance in aqueous environment; (iii) dissolution of SNF in aqueous environment, considering the in-package water chemistry; (iv) solubility of radionuclides; (v) secondary mineral formation and coprecipitation, considering natural analog studies; (vi) formation of colloids; (vii) cladding performance; and (viii) conceptual models for release. Each of these components is addressed in this section according to current knowledge and information needs for subissue resolution. Unlike the performance of container materials for which NRC generated independent experimental data, DOE generated most of the data regarding radionuclide release from SNF. The issue resolution in this context is achieved through examination of the adequacy of DOE data for determining the radionuclide release from SNF and consistency of the information with evidence generated by studies in other countries.

Resolution of Subissue 3 will require consideration of all the categories of SNF to be disposed, the identification of the most important modes of degradation owing to various forms of water contact and water chemistry inside WPs for the different types of SNF; numerical estimates of the rate of SNF dissolution and the rate of radionuclide release from the EBS; assessment of the effects of the compatibility of SNF and internal components of the WP on radionuclide release; and adequacy and validity of the available SNF database, including data on interactions with groundwater.

4.3.1.1 Spent Nuclear Fuel Types

It is anticipated that 70,000 metric tons heavy metal (MTHM) of waste, consisting of 63,000 MTHM CSNF; 2,333 MTHM DSNF; and 4,667 MTHM (equivalent) of vitrified HLW will be emplaced in the repository (U.S. Department of Energy, 1998a). The commercial fuels are nominally UO_2 pellets clad with Zircaloy. The DSNF, which falls into 34 groups (Duguid, et al., 1997), has been, for the purposes of TSPA-SR, grouped into 12 categories (CRWMS M&O, 2000c). Most of the DOE inventory is metallic fuel in the form of U or U alloyed with Al, C, or Si—the most predominant

being the N-reactor fuel from Hanford, which is metallic U. The cladding is either Al or Zr. These fuels have higher enrichment than the commercial fuels and are classified as high enriched (ranging from 20 to 95 percent) and low enriched (less than 20 percent). The highly enriched Al-based fuels may be diluted with depleted uranium and remelted (Westinghouse Savannah River Company, 1998). The commercial fuels, in contrast, have enrichments ranging from 2.5 to 4 percent. However, the radionuclide inventory of DSNF is small compared to that of CSNF. This revision of the CLST IRSR focuses on the commercial light water reactor fuels, although most of the subissues are valid for other fuels.

4.3.1.2 Radionuclide Inventory and Distribution in Spent Nuclear Fuel

The radionuclide inventory becomes distributed among the fuel matrix, boundaries between UO_2 particles (usually called grain boundaries), the fuel-cladding gap, the cladding itself, and corrosion products, such as crud deposited on the outer surface of the cladding during reactor operation, or secondary minerals formed after exposure of the fuel to the repository environment. The fractional distribution of the actinides in the fuel matrix is more than 99 percent, whereas up to 6 percent of the volatile fission products, such as ^{135}Cs and ^{129}I tend to migrate to the fuel cladding gap (Johnson and Tait, 1997). According to Johnson and Tait (1997), approximately 1 percent of ^{99}Tc accumulates at the gap and grain boundaries. Although part of the inventory of ^{99}Tc is apparently associated with ε-phase particles (Gray and Thomas, 1994), these particles are not very soluble. This circumstance explains the conclusion of Gray and Wilson (1995) that the inventory calculated from release at gap and grain boundaries is less than 0.2 percent. Although considerable uncertainties may exist regarding the grain boundary inventory of ^{99}Tc, the 2 percent approximation used in the TSPA-VA (CRWMS M&O, 1998b) may be conservative. More recent measurements of ^{129}I and ^{135}Cs (Gray, 1999) show wider variations in the gap and grain boundary inventories. The combined gap and grain boundary inventories of ^{129}I approximately equal the fission-gas release fraction. For ^{135}Cs the combined gap and grain boundary inventories are approximately one third of the fission-gas release fraction. Because the fission-gas release fractions vary as much as 20 percent, the gap and grain boundary inventories can vary by more than 20 percent for ^{129}I and more than 5 percent for ^{135}Cs.

Radionuclides important to system-level performance calculations depend on the assumptions regarding the flow pathways, transport parameters, and dilution (Jarzemba and Pickett, 1995). In the TSPA performed by NRC, the radionuclides contributing the greatest to the dose at 10,000 and 100,000 years were ^{237}Np, ^{234}U, ^{99}Tc, ^{129}I, ^{36}Cl, and ^{79}Se from a total of 20 radionuclides considered. In the DOE TSPA-VA (CRWMS M&O, 1998c), the six predominant radionuclides contributing to 99 percent of the dose after 1,000,000 years among the nine radionuclides considered were ^{99}Tc, ^{129}I, ^{237}Np, ^{234}U, ^{239}Pu, and ^{242}Pu. Similar order of radionuclides was presented by the DOE in the NRC/ DOE Technical Exchange on CLST as part of the TSPA-SR preliminary results.[1] The order of importance is a function of the time after emplacement. Resolution of the differences in the importance of specific radionuclides will depend on the

[1]C. Stockman. Key Technical Issue: Container Life and Source Term. *Presentation to the U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting.* September 12–13, 2000. Las Vegas, Nevada. 2000.

assumptions regarding radionuclide distribution between gap, grain boundaries, and matrix; releases including solubility and coprecipitation of certain radionuclides in secondary U minerals; and transport, including stability of colloids and sorption.

In the case of DOE fuels, distribution of radionuclides is dependent on the microstructure of the fuel material. At present, there is considerable uncertainty regarding distribution of radionuclides among the various metallurgical phases. The distribution is important because these fuels dissolve preferentially along the boundaries between the second-phase particles and matrix, releasing second-phase particles that could contain most of the radionuclides of importance to performance (Westinghouse Savannah River Company, 1997). A preliminary DOE PA indicates that ^{237}Np, ^{129}I, and ^{99}Tc are the most important radionuclides contributing to dose (Duguid, et al., 1997).

4.3.1.3 Dry-Air Oxidation of Spent Nuclear Fuel

The dry oxidation of SNF may be important if there is a premature container failure exposing the fuel to an oxygen-rich environment at temperatures higher than 100 °C with RH below approximately 30 percent. This process may occur if containers exhibit juvenile failures or fail as a result of seismicity-induced fracture. The effect of dry-air oxidation can be manifested as gaseous release of certain radionuclides (e.g., ^{14}C); alteration of the oxidation state of the SNF such that subsequent aqueous dissolution rate is enhanced; and spallation of SNF grains, caused by volume expansion, to increase the surface area. The contribution to dose from ^{14}C may be small because it is not a strong β-emitter. In addition to dissolving in the aqueous medium, it mixes in the gas phase and is released to the atmosphere. Two other radionuclides that may be released are ^{36}Cl and ^{129}I (Ahn, 1994).

The static air oxidation of SNF at temperatures ranging from 175 to 195 °C has been studied as a function of burnup, fission-gas release, and grain size (Einziger, et al., 1992). It was found that air oxidation of SNF is quite different from oxidation of unirradiated UO_2. Unirradiated UO_2 oxidizes by the formation of a surface layer of U_3O_7 that proceeds inward and is followed by the formation of U_3O_8 at the surface. SNF was shown to undergo grain boundary oxidation, which then progresses into the grain matrix. The oxide stoichiometry can be as high as $UO_{2.4}$ (U_4O_{9+x}), which causes a 3-percent reduction in volume compared to UO_2 (Thomas, et al., 1989). This reduction in volume can create small areas of grain boundary cracking. Additionally, because the oxide is hyperstoichiometric with respect to oxygen, it would be expected to be more electrically conductive than a stoichiometric oxide and, hence, dissolve more readily (Blesa, et al., 1994). Extrapolation of the kinetics of $UO_{2.4}$ from 175 °C to lower temperatures indicates that this oxide may not form for periods extending to several thousand years (Einziger, et al., 1992; Ahn, 1996b).

The effect of $UO_{2.4}$ formation on subsequent aqueous dissolution was examined by Gray, et al. (1993), who found that prior oxidation to $UO_{2.4}$ did not increase the intrinsic dissolution rate significantly in oxygenated, flowing carbonate solutions. The apparent dissolution rate (i.e., dissolution rate calculated by assuming the apparent particle area), however, was higher by a factor of 10 for the preoxidized SNF, possibly because of grain boundary opening (Gray, 1997). No difference in intrinsic dissolution rate was observed between oxidized and unoxidized SNF

particles on the basis of U release. Lack of sensitivity of the dissolution rate to prior oxidation may be consistent with the finding that the surface layer of UO_{2+x} attains an oxidation state dependent only on the corrosion potential of the fuel which, in turn, is determined by the redox condition of the environment (Shoesmith and Sunder, 1992). For example, in aerated solutions, Shoesmith and Sunder (1992) found that the surface oxidation state corresponded to $UO_{2.5}$.

Above 250 °C, irradiated $UO_{2.4}$ (with an average burnup of 28 to 48 GWd/MTU) oxidizes rather rapidly to U_3O_8, as observed by Einziger, et al. (1992) in laboratory tests, and the oxidation is accompanied by a volume expansion of about 36 percent. It appears there is a threshold temperature of approximately 250°C, below which U_3O_8 is not formed in 10,000 years as reviewed by Ahn (1996b). This threshold temperature increases at higher burnups (Hanson, 1998) and may decrease at lower burnups (Einziger and Cook, 1985). The volume expansion is expected to increase the surface area by two orders of magnitude. Preliminary experiments by Gray, et al. (1993) on unirradiated fuel oxidized to produce U_3O_8 showed that the effect of increased surface area due to the volume expansion on aqueous dissolution rate was, at most, a factor of 4. However, more recent results using a different fuel exhibited a tenfold increase in the intrinsic dissolution rate, resulting in a fractional release rate (rate for unit specimen weight) equal to 150 times that of unoxidized particles (Gray and Wilson, 1995). Oxidation of fuel to U_3O_8 can lead to disintegration of fuel into individual grains because of volume expansion. Nevertheless, tests of intact whole rod (fuel plus cladding) in inert and air atmospheres at 325 to 570 °C did not result in cladding rupture (Einziger, 1997), presumably because the cladding acted as an oxygen getter preventing pellet oxidation. Splitting of cladding was noted at low burnup ends of rods with defective cladding (Einziger, 1997).

Based on the limited data published by DOE (Gray, et al., 1993), prior dry-air oxidation to temperatures up to 250 °C would not be expected to significantly increase (at most, a factor of 10 in certain SNF) the subsequent aqueous dissolution rate. Such an expectation is consistent with the dissolution model proposed by Shoesmith and Sunder (1992), who argue that the surface oxidation state of SNF is conditioned by the redox nature of the aqueous environment contacting it, regardless of the prior oxidation state. Gaseous release of ^{14}C, ^{36}Cl, or ^{129}I is likely to occur during dry oxidation of SNF (Van Konynenburg, 1994; Ahn, 1994, 1996b). These releases may be important for premature failure of containers and cladding.

4.3.1.4 Radionuclide Release

The rate of release of U and other species from breached WPs is affected by the condition of the fuel cladding and controlled by a series of processes, such as transport of oxidants and flux of water, oxidative dissolution of SNF, uranyl mineral precipitation, uranyl mineral dissolution or transformation, and transport of radionuclides. Thermodynamic analysis of some of the secondary uranyl minerals indicates that their solubility may decrease with an increase in temperature, thus exhibiting retrograde solubility (Murphy, 1997). However, increasing temperature may increase the SNF dissolution and transport rates. This effect of temperature may mean that at high temperatures (e.g., in prematurely failed containers), radionuclide release will occur under conditions of fast dissolution rate of the SNF and low solubility of secondary minerals. If some radionuclides co-precipitate with secondary uranyl minerals, their release may

be governed by solubility of secondary minerals. At low temperatures, the dissolution and transport rates will be low, but the solubility may be high, leading to dissolution or transport-limited release of radionuclides. Lastly, fuel cladding may act as a partial barrier to radionuclide release.

4.3.1.4.1 Dissolution Rate Controlled Release of Radionuclides in Aqueous Environments

Under oxidizing conditions, UO_2 dissolves as uranyl species, which then react with other species in solution to form uranyl oxyhydroxides or silicates, depending on the chemistry of the solution (Wronkiewicz, et al., 1992; Finn, et al., 1998). The release of highly soluble radionuclides, such as ^{99}Tc and ^{129}I, occurs at a relatively constant fractional rate (Finn, et al., 1998) and, therefore, it has been assumed that the dissolution rate of the fuel matrix controls the release rate of highly soluble radionuclides (Wilson and Gray, 1990a). The dissolution behavior of SNF and the release of radionuclides depend on the mode of contact of water with the fuel (e.g., flow-through, full immersion, or dripping) and the chemistry of the water. Four different techniques have been used to determine the fuel dissolution rate: (i) flow-through tests (Gray and Wilson, 1995), where a column of the SNF particles is exposed to a solution whose flow rate is adjusted so the concentration of uranyl species is maintained below solubility limits; (ii) semistatic or, batch-type immersion tests, where fuel pellets or particles are exposed to replenished solutions for specific periods of time and the solution then analyzed (Wilson, 1990a,b); (iii) electrochemical tests, where rotating disc specimens are subjected to a potential scan and the electrochemical polarization behavior analyzed to yield a corrosion rate (Shoesmith, et al., 1989); and (iv) drip tests, where J-13 water equilibrated with tuff drips on fuel particles and the resultant effluent is collected periodically to measure radioactive release (Bates, et al., 1995; Finn, et al., 1998). Of these techniques, the electrochemical technique measures the total oxidation rate, including dissolution of the fuel matrix directly into the aqueous environment, whereas the other techniques estimate the matrix dissolution rate from the leachate analysis.

Using the flow-through system, UO_2 dissolution rates ranging from $(0.6 \pm 0.4) \times 10^{-14}$ to $(2.1 \pm 1.2) \times 10^{-14}$ moles/(cm^2·s) were measured in three laboratories [Whiteshell Laboratories, Pacific Northwest National Laboratory (PNNL), and LLNL], during a test period of 300 days in air-saturated 0.1 M NaCl plus 0.01 M $NaHCO_3$ solution (pH 9.0) at 25 °C (Gray, et al., 1994). By using electrochemical techniques, Shoesmith, et al. (1989) estimated steady-state corrosion rates of UO_2 at 25 °C. In air-saturated solutions ($[O_2] = 2.5 \times 10^{-4}$ M), rates ranging from 0.4×10^{-15} to 3.9×10^{-15} moles/(cm^2·s) were obtained in 0.1 M $NaClO_4$ at 25 °C. With the addition of 0.01 M and 0.5 M $NaHCO_3$, rates increased to 2.1×10^{-13} moles/(cm^2·s) and to 5.4×10^{-13} moles/(cm^2·s). On the other hand, in N_2-deaerated ($[O_2] < 3 \times 10^{-8}$ M), plain 0.1 M $NaClO_4$ solution, the corrosion rate was estimated to range from 4×10^{-21} to 4×10^{-19} moles/(cm^2·s). The corrosion rates in the flow-through tests (Gray, et al., 1994) are approximately one order of magnitude lower than those estimated by Shoesmith, et al. (1989) under almost equivalent environmental conditions. This difference in corrosion rates was attributed to variations in the value of E_{corr}. This value seems extremely sensitive to the reactivity of the surface, particularly in carbonate-containing solutions (Gray, et al., 1994). It appears that flow-through tests gave practically the same corrosion rate with and without the presence of NaCl in solution (Gray, et al., 1994). These observations suggest that, under the conditions of these

tests, the dissolution rate is kinetically controlled by charge transfer at the UO_2/solution interface rather than by mass transport processes in solution or by the solubility of U compounds.

The flow-through tests in sodium carbonate solution with or without the presence of NaCl in solution, are accelerated and conservative tests for the YM repository. The actual groundwater chemistry in the YM repository is expected to contain cations such as Ca and Si species, which may inhibit the dissolution rate of the primary phase (Wilson and Gray, 1990b). However, whether Ca and Si remain mainly in solution or interact with WP degradation products has not yet been demonstrated for SNF. Also, the flow-through tests are accelerated tests used to determine the intrinsic dissolution rate of the primary phase without involving secondary minerals. In addition, conditions in drip tests may be also severe, presumably giving rise to conservative estimations of dissolution rate compared with bathtub and immersion conditions. Some experimental results suggest that dissolution rates obtained under immersion conditions in J-13 well water and other groundwaters containing Ca and Si can be 10 to 100 times lower than those obtained under flow-through conditions in sodium carbonate solutions, as discussed by Ahn (1999).

The dissolution kinetics of the primary phase are dependent on the effective reactive surface area of SNF. The effective reactive surface area is determined by the volume of groundwater entering the failed container, the mode of contact of the water (i.e., immersion or drip conditions), the breached area of the cladding, the penetration of water into the gap between cladding and fuel, and the exposed grain boundary and subgrain boundary areas resulting from prior dry-air oxidation or corrosion. Additionally, it has been argued that if the RH is sufficiently high, all the SNF surfaces may be covered by a film of water, increasing the surface area.

Several environmental factors are known to affect the dissolution rate of UO_2 in aqueous environments.

1. The pH of the aqueous environment has an effect on the rate of dissolution of SNF. Under oxidizing conditions, only a slight dependence of corrosion on pH has been observed at pH values lower than 4.0, whereas at pH values between 4.0 and 8.0, the logarithm of the rate decreases linearly with pH (Grambow, 1989). At higher pH values, the rate of dissolution seems to be unaffected by pH changes. At the proposed YM repository, slightly alkaline pH levels are expected under nominal conditions. However, container corrosion (e.g., crevice corrosion) and cement dissolution will modify the pH that may range from acidic to alkaline, depending on location and conditions inside WPs.

2. Temperature increases the rate of dissolution of UO_2, although a functional dependence is not well established for a wide range of temperatures extending from ambient temperatures to the boiling point of water.

3. The nature and concentrations of the anionic species present in the groundwater are extremely important in determining the rate of corrosion of SNF. Anions, such as CO_3^{2-} that form stable soluble complexes with UO_2^{2+} cations, substantially increase the rate of oxidative dissolution (Needes, et al., 1975; Blesa, et al., 1994). At low CO_3^{2-}

concentrations (0.001 M), the rate of corrosion is proportional to the total concentration because the rate-determining step is the surface complexation of CO_3^{2-} (Blesa, et al., 1994). DOE's flow-through tests were conducted in the regime of low total carbonate concentrations that is expected at the YM repository (Gray, et al., 1992; Steward and Weed, 1994; Gray and Wilson, 1995). At intermediate concentrations (0.5 M), the corrosion rate depends on the square root of the total concentration because the solution transport of CO_3^{2-} to the surface is rate-controlling, or dissolution of an initially formed UO_2CO_3 film controls the overall rate (Grambow, 1989). At a high CO_3^{2-} concentration (1.0 M at 100 °C), the corrosion rate reaches a constant value, but at higher concentrations, the rate decreases, probably because of the formation of surface films that limit the overall rate (Needes, et al., 1975). The rate of corrosion increases in the sequence $Cl^- < SO_4^{2-} < F^- < CO_3^{2-}$, although, in the case of SO_4^{2-}, a maximum in the rate is observed at intermediate concentrations (approximately 1.5×10^{-2} M) (Blesa, et al., 1994). Other species, such as Ca^{2+}, $SiO_2(aq)$, $H_3SiO_4^-$, and $H_2SiO_4^{2-}$, which are able to induce the precipitation of complex uranyl silicates, tend to reduce the corrosion rates (Gray, 1992).

4. Corrosion products from metallic components, mostly in the form of metal cations, affect corrosion rates directly through precipitation reaction, forming secondary minerals that may slow down dissolution. However, corrosion rates can be increased by indirect action of corrosion products that may change the redox potential, the pH of the environment, or both. The redox potential can increase by the action of reducible cations, such as Fe^{3+}, whereas the pH can decrease by the hydrolysis of highly charged cations, such as Cr^{3+}, among others (Sridhar, et al., 1995). These two effects may lead to higher rates of SNF corrosion.

5. Both α- and γ-radiolysis of water may accelerate the corrosion rate of SNF via an increase in the E_{corr} because of the generation of H_2O_2, O_2, and short-lived oxidizing radicals (i.e., HO, HO_2). Except in the case of early failures, the γ-radiation fields may decay to almost negligible levels by the time (thousands of years) the containers fail and fuel contacts groundwater (Shoesmith and Sunder, 1992). Therefore, α-radiation appears to be the only significant source of radiolytic oxidants and may play a role even in occluded regions inside failed containers, in which reducing conditions could tend to prevail as a result of oxygen depletion caused by oxidation of steel WP components.

6. The presence of low molecular weight organic compounds, including carboxylic acid produced by degradation of vehicle fuels, lubricants, or other organic materials, either by chemical- or biochemical-mediated processes, may accelerate the rate of corrosion of SNF through the formation of complexing or chelating species. The same action can be exercised by humic substances, such as humic acid and fulvic acid that act as polyelectrolytic weak acids. On the other hand, detergents or similar compounds can act as inhibiting species by blocking active sites on the SNF surface. It has been claimed that the temperatures prevailing around WPs will promote the oxidation of organic substances, such as lubricants or vehicle fuels to CO_2, removing them from the media as potential nutrients for microbial activity (Meike, 1996; Wilder, 1996). Additional uncertainties arise

from the effect of biochemically mediated processes in the modification of the near-field environment once conditions are established for temperature and availability of water for microbial growth.

4.3.1.4.2 Solubility Controlled Release of Radionuclides

In DOE PA studies, the solubility of radionuclides, with the exception of Np species, is currently constrained by solubility values derived primarily from the expert elicitation supporting TSPA-93 and TSPA-95 (Wilson, et al., 1994; CRWMS M&O, 1995). For example, the solubility of Pu species varies from a minimum of 1×10^{-8} M to a maximum of 1×10^{-6} M (CRWMS M&O, 1998b). The uncertainties in the solubility of several radionuclides have been addressed by NRC (Murphy, 1991). For example, the Pu solubility varied from 5.63×10^{-13} to 6.6×10^{-7} M, depending on whether the mineral phase in equilibrium was assumed to be PuO_2 (at pH of 8.5) or $PuO_2(OH)_2$ (at pH of 6.9). Murphy (1991) recommended that a critical evaluation of near-field chemistry, including deviation from chemical equilibrium, be conducted, and that uncertainties in the thermodynamic database be assessed. The range of solubility values for Np species used in DOE TSPA-1993 and TSPA-1995 was about two orders of magnitude higher than that used in TSPA-VA. The higher value of solubility was attributed to the possible presence of metastable phases in the Np solubility experiments performed by Nitsche, et al. (1993, 1994). It was argued that the solubility measurements, which were performed using solutions supersaturated with respect to NpO_2, did not adequately represent the conditions for SNF dissolution or for fluid compositions similar to J-13 water that the DOE (U.S. Department of Energy, 1998c) has assumed to be present inside the WP. More recently, the distribution of solubility values for Np species was revised by DOE to lower values based on a review of experimental SNF dissolution and Np solubility measurements (Sassani and Siegmann, 1998). In the preliminary calculations in TSPA-SR, it is assumed the TSPA-95 Np solubility prior to 1,000 yr and the TSPA -VA solubility after 1,000 yr.[2] Experimental confirmation of the solid Np compounds assumed to be in equilibrium with the dissolved Np species is needed to validate the solubility estimates, and also co-precipitation data and more reliable thermodynamic data.

4.3.1.4.3 Effects of Secondary Minerals and Colloids on Radionuclide Release

Secondary minerals precipitate on or near the SNF surface through the reaction of uranyl species with other species present in the environment contacting the WP. Secondary minerals may mitigate radionuclide release by sequestering or coprecipitating other radionuclides, thus reducing their concentration in the aqueous environment, and by partially blocking the SNF surface, thus reducing the access of water. This effect could be particularly important in solutions containing Ca and Si species. It has been suggested (Wilson and Gray, 1990b) that a protective film can be formed under such conditions on unirradiated UO_2 surfaces. Since the molar volume of the uranyl minerals is higher than that of uraninite, periodic spallation of the dissolution products may occur, exposing fresh SNF surface to further dissolution. Tests of UO_2

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[2]C. Stockman. Key Technical Issue: Container Life and Source Term. *Presentation to the U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting.* September 12–13, 2000. Las Vegas, Nevada. 2000.

and SNF in dripping J-13 well water show that the predominant secondary mineral is Na-boltwoodite ($Na[(UO_2)(SiO_3OH)](H_2O)$; the other minerals being uranophane $Ca[(UO_2)$ $Ca[(UO_2)_2(SiO_3OH)_2](H_2O)_5$; dehydrated schoepite $(UO_2)(O)_{0.1}(OH)_{1.8}$; and presumably a Cs-Mo uranate (Wronkiewicz, et al., 1992; Finn, et al., 1998). The appearance of these minerals on the SNF surface is consistent with the secondary mineral formation on uraninite found in the natural analog site at Peña Blanca (Pearcy, et al., 1994). The drip tests indicate that Ru, Mo, Cs, Np, and Ba are incorporated in the alteration products, and Pu appears to be concentrated at the fuel surface (Buck, et al., 1998; Bates, 1998b).

Colloids may enhance or mitigate radionuclide release from the EBS, depending on composition, stability, and sorptive properties (Manaktala, et al., 1995; Ahn, 1996a). The formation and stability of colloidal material are examined briefly in this IRSR, and transport of colloidal material is addressed in the "Radionuclide Transport" (RT) IRSR (U.S. Nuclear Regulatory Commission, 2000d) and in the ENFE IRSR (U.S. Nuclear Regulatory Commission, 2000c). Sensitivity studies for colloid effects were performed using Version 3.2 of the NRC TPA code (Mohanty, et al., 1999). A bounding case for Pu and Am colloid transport showed minimal effect on dose in the 10,000-year compliance period. This minimum effect is largely due to the extended WP lifetimes.

Colloid formation during SNF dissolution was first identified in semistatic tests (Wilson, 1990a,b). Low-solubility radionuclides, such as ^{239}Pu, ^{240}Pu, ^{241}Am, and ^{244}Cm, were found as colloids when the aqueous medium, resulting from immersion tests in J-13 well water at 85 °C, was filtered through 0.4- and 1.8-μm pore filters. In drip tests at 90 °C, ^{239}Pu and ^{241}Am were retained after filtering the medium (Bates, et al., 1995).

Four different processes of colloid formation have been reported in the dissolution of SNF (Manaktala, et al., 1995; Ahn, 1996a). The first process is nucleation and condensation from supersaturated solutions leading to continuous colloid formation under near-static replenishing conditions. The second process is dispersion arising from the mechanical detachment or spallation of secondary minerals formed on the surface of the altered SNF. Colloids will form continuously by this process, independent of radionuclide concentration in groundwater. The third process is sorption of dissolved radionuclides onto preexisting colloidal material, such as corrosion products or colloids in the groundwater. Groundwater in the vicinity of YM is known to have about 0.3 to 1.4 μg/mL of colloids, ranging in size from 0.03 to 1.0 μm and composed mainly of silicate- or Fe-based minerals (Kingston and Whitbeck, 1991). The sources of corrosion products include containers, canisters, and basket materials. Significant amounts of iron oxide can potentially be generated by the corrosion of the steel WP and EBS components (Ahn and Leslie, 1998). A significant fraction of these corrosion products is expected to be present as colloidal matter. The fourth process is individual grain detachment from SNF by preferential dissolution of grain boundaries. This process decreases with time as the altered layer develops and covers the irradiated UO_2 surface (Wronkiewicz, et al., 1992).

After colloids are formed, they may flocculate and settle, depending on groundwater properties, such as pH and ionic strength (Manaktala, et al., 1995). DOE is using empirical correlations to evaluate the stability of colloidal suspensions in terms of ionic strength and pH (Triay, 1998).

4.3.1.5 Effect of Cladding on Release of Radionuclides

SNF cladding can act as a barrier to the release of radionuclides. Although cladding was not previously considered in PA codes, DOE (U.S. Department of Energy, 1998c) included cladding as an additional metallic barrier in the TSPA-VA. Several potential degradation mechanisms of Zircaloy cladding, such as localized corrosion, creep, delayed hydride cracking, HE, mechanical failure owing to rock fall, SCC, and fuel and cladding oxidation, can impair this beneficial action (Cragnolino, et al., 1999).

Pitting corrosion of Zr and Zr alloys (Zircaloy-2 and -4) occurs in acidic and neutral chloride solutions above a critical potential that is dependent on chloride concentration but independent of pH (Cragnolino and Galvele, 1978; Maguire, 1984). This potential, equivalent to the E_{rp} in the reported data, is easily reached in the presence of reducible species, such as Fe^{3+} ions, even at low concentrations (Maguire, 1984). Therefore, localized corrosion of fuel cladding may occur, depending on chloride concentration and temperature, in an oxidizing environment (as is presumably present around the SNF) if the corrosion potential is higher than the E_{rp}, which is about 0.34 V_{SHE} in 1 M NaCl solution at room temperature (Cragnolino and Galvele, 1978). If the corrosion potential is lower, the corrosion rate of Zircaloy would be extremely low as a result of the protective characteristics of the ZrO_2 passive film.

In addition, Zircaloy is susceptible to SCC in the presence of tensile stresses lower than the yield strength under the same environmental and electrochemical conditions that promote pitting (Cox, 1973; Cragnolino and Galvele, 1973; Mankowski, et al., 1984). Sufficiently high hoop stresses (60 to 70 percent of the yield strength) may be present in localized regions of the cladding as a result of fuel pellet expansion during irradiation. DOE has not considered the possibility of localized corrosion and SCC of Zircaloy in the presence of oxidizing chloride solutions taking into consideration the electrochemical and environmental factors involved. These processes in solutions simulating conditions inside the WPs and their effects on the integrity of fuel cladding, need to be evaluated or at least appropriately bounded to assure that cladding can be considered as a metallic barrier to radionuclide release.

Both PNNL (Levy, et al., 1987) and LLNL (Schwartz and Witte, 1987; Thomas and Schwartz, 1996) developed mechanistic creep models for predicting the creep rupture life of cladding under repository conditions. The PNNL model was developed under a DOE contract, whereas the LLNL model was supported by an NRC contract. The PNNL/DOE model is based on the deformation and fracture mechanism maps and treats several different creep deformation and failure modes (Chin, et al., 1986). For the low longitudinal stress and low temperature (< 350 °C) anticipated for the cladding in the repository, the potential dominant creep failure mechanism is diffusion-controlled cavity growth (DCCG). McCoy and Doering (1994) reviewed previous models and proposed several refinements. The LLNL/NRC model, which treats DCCG, has been recently upgraded (Thomas and Schwartz, 1996). Both models have the same basic form traceable to the original model of Raj and Ashby (1975) and should predict similar results, providing similar values are used for the model constants. As noted by Ahn, et al. (1999), there is general consensus that cladding failure by creep rupture is unlikely under repository conditions, assuming no backfill. Creep-rupture data from Germany (Peehs and Fleisch, 1986) are

consistent with this assessment. There is, however, a lack of direct comparison of DCCG model prediction against experimental data and a lack of experimental evidence for DCCG in Zircaloy cladding materials (Pescatore, et al., 1989). Disagreement exists on the pertinent values of some constants in the DCCG models and on the validity of extrapolating to lower stresses and temperatures the results of calculations performed using creep models. Failure prediction is sensitive to the effect of temperature.

Delayed hydride cracking is a time-dependent crack propagation process under sustained-load conditions, that results from diffusion of hydrogen to the crack tip, and is followed by the formation and fracture of hydrides in the near-tip region (Dutton, et al., 1977). Most of the relevant experimental data on delayed hydride cracking in the literature are for Zr-2.5 wt % Nb (Northwood and Kosasih, 1983); Zr, Zircaloy-2, and Zircaloy-4 appear to be less susceptible or even unsusceptible to delayed hydride cracking. Both DOE (Cunningham, et al., 1987) and NRC (Ahn, et al., 1999) reviewed the Canadian data and performed pertinent modeling. They concluded that delayed hydride cracking would not be important in the repository because the operating stress intensity, which is approximately 0.5 to 2 MPa·m$^{1/2}$ (Siegmann, 1997a), is less than the crack growth threshold, K_{IH}, for delayed hydride cracking. The value of K_{IH} decreases with hydrogen concentration in solid solution (Shi and Puls, 1994), and values ranging from 5 MPa·m$^{1/2}$ (Shi and Puls, 1994) to 12 MPa·m$^{1/2}$ (Cunningham, et al., 1987) have been reported. Based on the available evidence, it seems that delayed hydride cracking is not important under repository conditions, but this assessment can be confirmed if results regarding the probability of failure are quantified on the basis of the crack-size distribution in the cladding.

Zircaloy cladding generally contains some circumferential hydrides that have little or no effect on ductility or fracture toughness (Northwood and Kosasih, 1983). The amount of hydrogen pickup in the repository is expected to be small. As a result, hydride embrittlement has not been studied closely. The occurrence of hydride embrittlement depends on the presence or absence of hydride reorientation from the circumferential planes to the radial planes. A few years after emplacement, the maximum cladding temperature for the design basis WP in the VA design is expected to be approximately 330 °C (Siegmann, 1997b), which is above the solvus temperature of 290 to 300 °C (Northwood and Kosasih, 1983). On the other hand, the average temperature of the cladding is expected to be less than 237 °C (Siegmann, 1997b). Note that use of backfill would cause the temperature to increase. If the temperature of the cladding reaches more than 300 °C, the circumferential hydrides are expected to redissolve in the Zr matrix. As the temperature drops below the solvus temperature, radial hydrides can reprecipitate at slow cooling rates if the cladding stress exceeds a critical value. The value of the critical stress required for hydride reorientation to occur is not well defined, but values ranging from 35 to 138 MPa have been quoted (Einziger and Kohli, 1984). The low critical stress value of 35 MPa is for Zr-2.5Nb (Hardie and Shanahan, 1975), whereas the value for Zircaloy is approximately 84 to 95 MPa (Marshall, 1967; Bai, et al., 1994; Chan, 1996). The cladding stress in the repository is anticipated to be 60 to 100 MPa (Siegmann, 1997b; Ahn, et al., 1999). Under these stress levels, reorientation of hydride may be feasible at the slow cooling rates anticipated in the repository. The morphology of the radial hydrides formed under such conditions is conducive to embrittlement (Chan, 1996) and can lead to decreases in ductility and fracture toughness. Experimental data (Simpson and Cann, 1979; Kreyns, et al., 1996) indicate fracture toughness of Zircaloy cladding

is reduced from approximately 44 MPa·m$^{1/2}$ without hydrogen to 7.5 MPa·m$^{1/2}$ at 4,000 ppm hydrogen (Kreyns, et al., 1996); and to 1 MPa·m$^{1/2}$, at higher hydrogen contents (Simpson and Cann, 1979). Thus, HE may or may not be an important failure mechanism for fuel cladding in the repository environment, depending on the cladding temperature, which is a critical factor in determining the possibility of hydride reorientation.

Fuel and cladding oxidation are potential cladding failure mechanisms if the disposal container fails when temperatures of the fuel assemblies are relatively high (> 250 °C). Cladding oxidation would be the predominant failure mechanism if the fuel rods remain intact when the container fails, whereas dry or wet oxidation of the fuel pellets and the resulting volume increase would be the dominant cladding failure mode for perforated fuel rods. The possible failure of fuel rods by cladding and fuel oxidation, followed by cladding splitting, was examined by Einziger (1994), McCoy (1996), and Ahn (1996b). Cladding oxidation can be dismissed as a failure mechanism if the drifts are not backfilled because the rate of oxidation is not sufficiently fast at temperatures lower than 350 °C, as expected in the absence of backfilling. For perforated fuel rods, fuel oxidation is not expected to be a problem if the fuel temperature is lower than 250 °C because the fuel oxidation kinetics would be too sluggish. Above 250 °C, dry-air oxidation of irradiated UO_2 to U_3O_8, and the consequent volume increase, may split the cladding. Below this temperature, secondary mineral formations may occur in perforated fuels exposed to aqueous environments, leading to volume expansion and the potential for cladding failure.

4.3.1.6 Radionuclide Mobilization in Waste Packages

When radionuclides are released from the cladding, partially failed containers may be another barrier to radionuclide release. The effectiveness of the container materials in reducing radionuclide release depends on the size and distribution of corrosion pits, presence of through-wall cracks, and the effect of corrosion products in the pits. The size of pits depends on the material and near-field environment. In the case of carbon steels, the pits are likely to be wide and filled with voluminous corrosion products (mainly various hydrated ferric oxides, such as akaganeite, lepidocrocite, and magnetite) and concentrated solutions of ferrous chloride. In the case of SS and Ni-base alloys, the pits will likely be narrow and deep with corrosion products not as voluminous as those of carbon steels. The distribution of pits depends on a number of geometric factors (presence of crevices, manufacturing defects, such as laps and grind marks) and metallurgical defects (sulfide and oxide inclusions, second-phase precipitates). In addition to through-wall pits developing from the outside, pitting may occur from the inside of the inner overpack after water flows in, through accumulation of fission products, such as ^{129}I, and ionic species already present in the groundwater. Extreme-value statistical treatments have been attempted in different applications, based on relatively short-term tests or field experience, to calculate the areal fraction of pits on carbon steel and aluminum (Aziz, 1956; McNeil, 1987). These approaches have not yet been applied to estimate the area of penetration of containers under repository conditions. On the other hand, if uniform corrosion takes place with scattered groundwater drips on the container, larger penetrations in the form of corrosion patches may develop (Lee, 1998). Corrosion products inside perforations or holes could provide diffusion barriers as in cladding. Although models of diffusion and convection are available to analyze restricted radionuclide release through perforations or holes (CRWMS M&O, 1995; U.S. Nuclear

Regulatory Commission, 1995; Zwahlen, et al., 1990), experimental data are scarce to support the models. Wilson (1990a,b) compared the reduction of radionuclide release in J-13 well water from SNF with cladding defects in the form of pinholes or slit flaws.

For colloidal transport, if the suspension of colloids is stable, release would take place by the transport of colloids through perforations in containers. However, colloidal transport could be limited because the penetrations may be small pits or hairline cracks filled with corrosion products (Johnson, 1998; Lee, 1998), as discussed previously. DOE has not yet performed calculations to estimate the amount of colloids that could be transported through perforations. Bounding values could be acceptable if an appropriate scenario description is developed. Otherwise, calculations are not necessary if DOE does not take credit for retardation of colloids by the perforated WP.

Depending on locations of the penetrations, radionuclide release may be modeled by considering immersion (bathtub) or flow-through conditions (CRWMS M&O, 1995; U.S. Nuclear Regulatory Commission, 1995). In the bathtub model, the critical parameters are the locations of the entry and exit ports for the water that determine the volume of water accumulating inside the container (Mohanty, et al., 1997). There is great uncertainty regarding the likely geometry of these parameters because no relevant scale-down test exists to evaluate the location, morphology, and characteristics of corrosion penetrations.

4.4 SUBISSUE 4: THE RATE AT WHICH RADIONUCLIDES IN HIGH-LEVEL WASTE GLASS ARE RELEASED FROM THE ENGINEERED BARRIER SUBSYSTEM

This subissue relates to the adequacy of DOE's consideration of the effects of degradation of HLW glass, taking into account the rate of degradation and its effect on the rate of radionuclide releases from the EBS. Resolution of this subissue will be accomplished through the application of the AC, as presented in Section 5.4.

4.4.1 Technical Bases

After the failure of the metallic container, it is expected that the EBS would provide gradual release of radionuclides during long periods. It is anticipated that limited mobilization of radionuclides arising from the low rate of dissolution of HLW glass will contribute to the slow release of radionuclides from the EBS. Both DOE and NRC staffs evaluated the most likely modes of HLW glass degradation (CRWMS M&O, 1998b; Manaktala, 1992). These degradation modes include hydration and leaching of primary HLW glass phases and formation of secondary minerals and colloids. High-solubility radionuclides, such as ^{99}Tc, will be released at a rate similar to alkali or boron release rate. On the other hand, low-solubility radionuclides, such as ^{239}Pu or ^{241}Am, will be reprecipitated with secondary minerals on the surface of the primary HLW glass phase. Consequently, the release of low-solubility radionuclides will be controlled by solubility limits or steady-state values that are constrained by the solubility of secondary minerals. These low-solubility radionuclides may also form mobile colloids that can carry larger amounts of radionuclides than those transported in the form of dissolved species. Once radionuclides are mobilized, they will be transported either by diffusion or by advection, depending on the water

contact modes with the WP (i.e., dripping, partial or full immersion, or condensation of water vapor) under conditions that can be altered by backfill emplacement. The chemical composition of the water inside breached WPs should be known or properly bounded.

To evaluate the status of the resolution of this subissue, several components are important, including HLW glass dissolution processes, formation of secondary minerals, natural analog studies, effects of colloids and microbes, and radionuclide transport in the EBS. Unlike the metallic container materials for which NRC generated independent experimental data, DOE has generated most of the data regarding radionuclide release from HLW glass. Issue resolution in this context will be achieved through examination of the adequacy of DOE HLW glass data.

Resolution of Subissue 4 will require consideration of all types of HLW glass planned for disposal, identification of the most important modes of degradation of HLW glass, numerical estimates of the rates of HLW glass dissolution and radionuclide release from the EBS taking into consideration the water chemistry, and assessment of the effects of the compatibility of HLW glass and internal components of the WP on radionuclide release.

4.4.1.1 Importance of High-Level Waste Glass for the Source Term

Projected radionuclide inventory for the HLW borosilicate glass is about 3 percent of the total radionuclide inventory to be disposed at the YM repository (U.S. Nuclear Regulatory Commission, 1995). Therefore, based solely on this percentage of the inventory argument, HLW glass could be neglected in the source-term analysis. Contribution of the HLW glass to the source term could be significant, however, if the rate at which the radionuclides can be released and transported from the glass is higher than that from the SNF (e.g., radionuclides released in colloidal form). The contribution could also be significant if radionuclides contained in the hydrated layer (corrosion product layer adhering to the glass surface) are released in larger quantities as a pulse.

4.4.1.2 High-Level Waste Glass Corrosion Process

The HLW glass corrosion process involves (i) transport and contact of reactant (i.e., groundwater or water vapor) to the HLW glass surface, (ii) chemical reaction between the reactants and glass surface, and (iii) transport of reaction products away from the reaction zone.

The HLW glass corrosion rate is controlled by the combination of these three processes and depends on factors such as chemical composition of the glass and surrounding fluids solubilities of the reaction products, exposed surface area, temperature, pH, and RH. The long-term corrosion behavior can be divided into three distinct stages as reviewed by Ellison, et al. (1994). In stage I, referred to as "the short-term stage," the chemical potential gradient between the glass components and local environment is the steepest. The glass components are released into the local environment at a comparatively high rate. The soluble components, such as boron and alkalis, are released at a higher rate compared with components such as silica and aluminum oxide. This higher release rate results in the formation of a layer on the glass surface depleted of soluble components, compared with the bulk glass. This layer is often called "the altered surface

layer". In stage II, "the intermediate stage," the corrosion rate decreases as the concentration of reaction products, particularly silica, increases in the solution in close contact with the glass. In addition, the reaction products in the altered surface layer reach saturation concentration of their crystalline phases and result in the formation of secondary phases, such as zeolites and clays. In stage III, "the long-term stage," glass corrosion rate is further affected because of the reprecipitation of secondary phases that exceed solubility limits at the altered zone. Physical processes, such as crystallization, cracking, or exfoliation of the altered surface layers, that occur in stage III, could influence the glass corrosion rate, as well as the release and transport of colloids and radionuclides. The change in dissolution rate also depends on the identity, distribution, and surface area of the secondary phases. In most cases, the dissolution rate increases as a result of crystallization, exfoliation, and cracking of the altered surface layers. The transition from one stage to another is dependent on the glass composition and the local environment. A highly durable glass may take months to years to reach stage II, whereas a nondurable glass may reach stage II within hours or days.

4.4.1.3 Long-Term Glass Corrosion Studies

Several long-term HLW glass corrosion studies have been conducted in the previous 20 years, and research relevant to the proposed YM repository is currently conducted at Argonne National Laboratory on simulated HLW glasses, simulated glasses doped with plausible radionuclides, and fully radioactive glasses. Drip tests, designed to simulate slow flow through the breached canisters, have been used by Fortner and Bates (1996) and Fortner, et al. (1997) to study the long-term performance of actinide-doped West Valley Demonstration Project and Defense Waste Processing Facility (DWPF) HLW glasses. The long-term product consistency test (PCT)-B, designed to simulate fully immersed conditions, has been used by Ebert and Tam (1997) to study long-term performance of DWPF glasses. In addition, vapor hydration tests, designed to replicate a natural alteration process, are used by Luo, et al. (1997) to compare the dissolution behavior of DWPF glasses with that of naturally occurring basalt glasses. It is evident from the continuing studies at the Argonne National Laboratory (ANL) that the test conditions strongly influence glass corrosion rates, and it is prudent to develop different tests to characterize various conditions that may exist in the repository. Although the previous studies may provide insight into corrosion mechanisms, the abstraction model should bound the range of evolving environments in contact with the WPs at the proposed YM repository.

The dissolution rate of the HLW glass decreases as the groundwater environment in close contact with the WPs becomes saturated with glass matrix components, such as silica. Even though the glass corrosion studies discussed previously confirmed that net dissolution rate decreases as the surrounding environment becomes rich in HLW glass matrix components, the drip test studies show a steep increase in radionuclide release rate for Pu and Am after 400 weeks. The steep increase in radionuclide release rate was attributed to the spalling of radionuclide-containing colloids from the exposed HLW glass surface. The HLW glass abstraction models should account for such excursions in corrosion behavior. These excursions may have a significant effect on radionuclide release.

The dissolution kinetics of the primary phase, as commonly represented by the kinetics of B release, determine the release rate of high-solubility radionuclides, such as Tc. The rate is dependent on the effective reactive surface area of HLW glass. The higher the exposed surface area, the higher the radionuclide release. The methodology used for estimating the effective reactive surface area for HLW glasses in the WP should be developed incorporating the effect of surface area on the HLW glass dissolution rate.

4.4.1.4 Formation of Secondary Minerals During High-Level Waste Glass Corrosion

Long-term corrosion studies of HLW glasses indicate formation of secondary phases on the exposed surface of the HLW glasses. This process is dependent on the external environment. Long-term PCTs in J-13 water show formation of clay, Ca-phosphate, and (Th, U, and Ca) titanate as secondary phases (Bates, 1998a), whereas the vapor hydration tests show accumulation of clay, zeolites, Ca-silicates, weeksite, and K-feldspar as secondary phases (Bates, 1998a). Formation of different phases under diverse test conditions is attributed to varying solution chemistries. These test conditions represent two environments that may exist at different times at the proposed YM repository. The formation of secondary phases may also be influenced by the corroding container materials. Secondary minerals play an important role in radionuclide release because they can incorporate low-solubility radionuclides, such as Pu and Am, and control their solubility limits. They may also act to block the reactive surface area of the primary phase.

4.4.1.5 Natural Analog Studies of Glasses

Natural analog studies, coupled with experimental data and geochemical modeling, provide another method of gaining confidence in predicting long-term corrosion behavior of glasses. Natural analog studies are useful in evaluating the merits of extrapolating short-term experiments to longer time frames. Several natural glasses, especially basalt, have compositions comparable to the HLW glasses and have been subjected to conditions similar to those expected in the proposed YM repository (Ewing, et al., 1998; McKenzie, 1990). The characterization of secondary phases formed on these natural glasses can provide insights into the long-term dissolution behavior of HLW glasses.

A recent study by Luo, et al. (1997) compared formation of secondary phases in the naturally occurring Hawaiian basaltic glasses with the results of vapor hydration tests conducted for 7 years on simulated basaltic and HLW borosilicate glasses. Luo, et al. (1997) concluded that secondary phases formed on both simulated natural glasses and HLW borosilicate glasses were similar to secondary phases observed in naturally occurring basaltic glasses, and vapor hydration tests could be used to simulate naturally occurring conditions.

Field data on naturally occurring glasses, combined with experimental data and models on dissolution of HLW glasses, could be useful to demonstrate that long-term dissolution behavior under repository conditions can be represented by extrapolation of results from short-term laboratory tests. Such data can be important to supplement and support the validity of the existing glass-dissolution data, generally obtained by short-term experiments.

4.4.1.6 Colloids, Microbes, and Radionuclide Transport in the Engineered Barrier Subsystem

Secondary phases formed on the HLW glass surface could be released as colloids and transported through the EBS (Manaktala, et al., 1995; Ahn, 1996a). These colloids could be hosts to radionuclides released from the glass. Sensitivity studies for colloid effects were performed using Version 3.2 of the NRC TPA code (Mohanty, et al., 1999). A bounding case for Pu and Am colloid transport showed minimal effect on dose in the 10,000-year compliance period.

Recent research by Fortner, et al. (1997) and Fortner and Bates (1996) has not only shown formation of colloids in the alteration phases, but also the transport of 100 percent of the actinides as colloids to the environment. Thus, colloids could lead to sudden increases in actinide concentrations in the environment present in the emplacement drifts. DOE has identified dominant colloid formation processes under anticipated repository conditions but has not modified the long-term dissolution models to account for such events. Currently, DOE has adopted empirical correlations of the colloidal suspension based on the ionic strength and pH (Triay, 1998). If the suspension of colloids is stable, release would take place by the transport of colloids through perforations in containers. However, colloidal transport could be limited because the penetrations may be small pits or hairline cracks filled with corrosion products (Johnson, 1998; Ahn, 1994; Lee, 1998). DOE has not performed calculations to estimate the amount of colloids that can be transported through perforations.

Studies conducted to date have ignored the corrosion of HLW glasses by the action of microbes. The effect of microbes in the dissolution of natural glasses can be significant (Thorseth, et al., 1992). Microbes can also change the solubilities of radionuclides by the increased production of organic acids. The effects of microbial activity on HLW glass corrosion should be studied if the viability and nature of the microbial activity at the proposed YM repository are demonstrated through the use of calculations based on a mass balance of nutrients and energy-generating chemical reactions, as indicated in the ENFE IRSR.

4.5 SUBISSUE 5: THE EFFECTS OF IN-PACKAGE CRITICALITY ON WASTE PACKAGE AND ENGINEERED BARRIER SUBSYSTEM PERFORMANCE

This subissue addresses whether DOE has sufficiently analyzed the effects of potential in-package nuclear criticality on WP and EBS performance during the postclosure time frame of interest. If the WP is designed to prevent any nuclear criticality over the postclosure period, the adequacy of the design of the WP and other components of the EBS must be demonstrated. If the in-package criticality probability is greater than or equal to the event probability defined in the proposed 10 CFR Part 63, the consequences of the in-package criticality and the contribution to total repository risk must be determined. Resolution of this subissue will be through the satisfactory implementation of the ACs for in-package criticality.

4.5.1 Technical Bases

The following sections provide the technical bases for the AC relevant to in-package criticality for the postclosure period.

4.5.1.1 Criticality Design Criteria

The majority of the SNF currently planned to be placed in the WP is commercial PWR, BWR, and some mixed oxide fuel. U.S. Navy SNF and DSNF, which includes SNF from research reactors, are also planned to be placed in the repository. Vitrified HLW glass logs with, and without, excess weapons fissile materials (FM) are other types of DOE waste that may be disposed of in the proposed repository.

To minimize the potential for, and consequences of, criticality, DOE should develop a set of design criteria to support a demonstration that the design of the WP and EBS is adequate. Given the different types of waste to be placed in the WPs, the DOE may choose different design criteria for different waste types.

4.5.1.2 Criticality Scenarios

DOE must identify all the FEP having the potential to increase the reactivity of the in-package system. DOE needs to consider the features of the site that would expedite or delay the processes resulting in in-package criticality. The amount, rate, temperature, and chemistry of water precipitating at the site, percolating through the unsaturated zone, seeping and flowing into the drifts, and entering into the WP need to be considered.

Events such as IA (extrusive and intrusive), seismic shaking (high-frequency, low-magnitude, and rare large magnitude events), tectonic evolution (slip on existing faults and formation of new faults), and climatic change (change to pluvial conditions) mentioned in the Total System Performance Assessment and Integration IRSR (U.S. Nuclear Regulatory Commission, 2000a) must be evaluated by their effect on WP geometry and content with respect to in-package criticality.

Processes such as corrosion of internal basket and poison materials need to be considered. The loss of reactivity-reducing isotopes from WP criticality control systems and the SNF matrix are among the processes that should be considered in developing criticality scenarios.

4.5.1.3 Criticality Configurations

Parameters associated with package configurations that exhibit uncertainties resulting from events and processes must be identified. Selection of the distribution and range of values for these parameters associated with a configuration must be technically defensible. For example, the value chosen for the amount of iron oxide produced from corrosion of the WP internal components remaining inside the WP may be important for criticality calculations. If models are

used to predict the iron oxide inventory in the WP, the acceptability of the model must be established through validation and verification.

4.5.1.4 Criticality Probability

The probabilities for those configurations that result in critical conditions must be determined for screening purposes. In developing the approach for the probability calculations, DOE needs to consider the range of parameters that could affect the probability distribution. If the parameter values are based on expert elicitation and the values are skewed towards the nonconservative end of the distribution, the resulting estimate of probability of criticality may be incorrect. Any approach selected in developing the probability values for critical configurations must be based on technically defensible ranges of parameter values.

4.5.1.5 Criticality Analyses

In performing criticality analyses, the effective neutron multiplication factor (k_{eff}) of the system of interest is calculated. To estimate k_{eff} of the WP, DOE could use a deterministic or probabilistic model. In either case, the biases and associated uncertainties that may exist must be quantified through appropriate benchmarks.

If DOE chooses to take credit for the burnup of SNF, any biases and uncertainties associated with depletion and k_{eff} computer codes must be identified and taken into account. The approach in incorporating these biases and uncertainties must have a sound and defensible basis.

4.5.1.6 Criticality Consequences

The consequences of criticality must be determined if DOE cannot screen criticality on the basis of low probability. In determining the consequences of critical (i.e., exceeding the subcritical limit established under design criteria) and supercritical configurations, different processes could cause an increase in k_{eff}, leading to varying rates of reactivity insertion that may cause a criticality event. Criticality must be analyzed under steady-state, transient, and autocatalytic conditions if it is credible that these conditions exist within the WP. The rate of reactivity insertion must be determined and consequence calculations performed under slow and step insertion conditions if these conditions are credible. The consequences for critical and supercritical configurations must be analyzed with respect to radionuclide production, heat generation, and WP and WF degradation. The consequences of additional heat generation and large energy release over very small time frames must be analyzed in terms of their potential effects on the WP, EBS, and repository environment.

4.5.1.7 Criticality Risk

If DOE determines that it is necessary to calculate the risk that may result from in-package criticality, DOE must consider the direct and indirect consequences as well as the probabilities associated with them. Increase in radionuclide inventory, production of additional heat, and increase in WP and WF degradation are the direct consequences of configurations that may

result from criticality events. Indirect effects include those affecting other components of the EBS and the near-field environment that could result in additional release of radionuclides. For example, a step reactivity insertion could affect the rock stability, especially when there is no backfill. Further instability of the rock formation would result in higher probability of rockfall on the WP. Therefore, the calculated risk must be based on the primary and the secondary consequences of the critical configurations.

4.6 SUBISSUE 6: THE EFFECTS OF ALTERNATE ENGINEERED BARRIER SUBSYSTEM DESIGN FEATURES ON CONTAINER LIFETIME AND RADIONUCLIDE RELEASE FROM THE ENGINEERED BARRIER SUBSYSTEM

This subissue is designed to address the effects of alternate EBS design features, such as backfill, DS, and any other design option, on container lifetime and radionuclide release from the EBS. These design features were presented as options for the improvement of the EBS performance in the VA (U.S. Department of Energy, 1998b). Consideration of this subissue in CLST IRSR, Revision 3 is based on the proposed SR design according to the most recent information available after the selection of EDA-II (CRWMS M&O, 1999b). As a result of the elimination of carbon steel as a material of choice for the disposal containers in EDA-II, ceramic coatings are currently not being considered as an alternative feature for improving the performance of the WPs. Most recently, backfill has been eliminated in the current design of the EBS to avoid a significant temperature increase in the WP surface and SNF cladding as a result of its emplacement at the time of repository closure. Resolution of this subissue will be through the application of the AC, as presented in Section 5.6.

4.6.1 Technical Bases

Use of a DS design option is intended to minimize the possibility of water dripping on containers. Corrosion of the containers can be enhanced by the presence of flowing liquid water that may also remove soluble corrosion products facilitating localized penetration. In addition, liquid water can mobilize and advectively transport most radionuclides. Where active flowing fractures in the repository couple with sharp drift wall edges, seeps (drips) into the drift can occur. It is the function of the DS to divert these drips from the WP surface. The current EDA-II design calls for the DS to be constructed of a Pd-bearing Ti alloy, such as Ti grades 7 or 16, and to be 15 mm in thickness. Although moisture condensation between the WP and the DS cannot be prevented, DS will reduce water contact arising from fracture flow. If the diverted seepage flux is drained without passing through the part of the invert contaminated by the radionuclides from failed WPs, transport of radionuclides will be reduced within the EBS, resulting in a considerable reduction in the release within the EBS, and dose rates will be greatly reduced.

Resolution of Subissue 6 will require identification of the effects of selected design option(s) on WP lifetime and the release of radionuclides from the EBS.

4.6.1.1 Thermal Embrittlement and Environmentally Assisted Cracking of Ti Drip Shield

Similar to ferritic-pearlitic low-alloy steels, α-Ti alloys, such as Ti grades 7 and 16, can also suffer from thermal embrittlement (Cragnolino, et al., 1999). Both temper embrittlement of steels and thermal embrittlement of α-Ti alloys occur as a result of a thermally activated redistribution of barely soluble impurities from grain interiors to grain boundaries (Nesterova, et al., 1980). Both phenomena are characterized by (i) embrittlement of the material, (ii) nominally constant strength with widely variable ductility, and (iii) increased intergranular boundary fracture. Unlike temper embrittlement of iron in which only equilibrium segregation of impurities (i.e., P, As, and Sn) occurs, impurity segregation in α-Ti results in the precipitation of finely dispersed particles at the grain boundaries (Nesterova, et al., 1980; Kryukov, et al., 1981; Ushkov, et al., 1984, 1995).

Commercial purity (CP) Ti exhibits a minimum impact toughness after heat treatment in the temperature range of 350 to 600 °C after exposure for 500 hours. Embrittlement susceptibility starts at approximately 350 °C and, at higher temperatures, reaches a maximum (minimum in toughness) near 500 °C, decreasing at even higher temperatures. At temperatures greater than 700 °C, the embrittlement effect disappears, and the impact toughness approaches its original value. Similar results are shown for other Ti alloys (e.g., Ti-2Al-1.5Zr) (Nesterova, et al., 1980). For Al-bearing α-Ti alloys, embrittlement occurs partially as a result of decomposition of the Al in solid solution with Ti and the precipitation of α_2 (Ti_3Al) throughout the interior of grains, which results in embrittlement of the grains themselves (Nesterova, et al., 1980; Ushkov, et al., 1984, 1995). For CP Ti and α-Ti alloys that contain trace amounts of Fe and Ni as impurities,[3] embrittlement results from the precipitation of sub-μm size face-centered-cubic Ti intermetallics in the form of $Ti_2(Fe,Ni)$. The effect of longer thermal holds (> 500 hours) on embrittlement has received little attention, but has revealed significant segregation of Fe and Ni at grain boundaries at temperatures as low as 350 °C (Ushkov, et al., 1984). The temperature experienced by the Ti DS is likely to be lower than that of the containers. Nevertheless, considering the long exposure period, the susceptibility to enhanced mechanical failure by embrittlement may be a possibility.

Environmentally assisted cracking (EAC) of Ti-Pd alloys has not been extensively examined as concluded in a recent review of alternative EBS designs (Cragnolino, et al., 1999). Many Ti alloys are susceptible to EAC due to HE associated with the precipitation of hydrides ahead of the crack tip. However, the Ti-Pd alloys may be highly resistant to EAC, especially those that have a low equivalent oxygen content (high O_{equiv} leads to higher strength and greater susceptibility). The addition of Pd to Ti has also been thought to enhance EAC resistance because hydrogen evolution as H_2 would preferentially take place at Pd-rich sites, thereby decreasing the available atomic hydrogen that could be absorbed into the Ti lattice. It is unclear if this mechanism is operable. In any event, the relatively few reported EAC failures of Ti-Pd alloys may be a result of slow crack propagation rates, which become important in engineering structures intended to maintain functionality for extremely long periods of time.

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[3]As impurities, typical concentrations for Fe and Ni in α-Ti alloys are ≤ 0.05 wt % and ≤ 0.005 wt %, respectively (Nesterova, et al., 1980; Ushkov, et al., 1984).

4.6.1.2 Uniform and Localized Corrosion of Ti Drip Shield

Ti alloys have been long recognized as highly resistant to corrosion because of their ability to form a protective oxide film when in contact with oxygen or water (Schutz, 1992). The presence of oxidizing agents, such as nitric and chromic acids, and the dissolved salts of iron, nickel, copper, and chromium can act as inhibitors and decrease corrosion. The oxidizing agents likely inhibit corrosion by accelerating growth of the oxide film because they increase the potential into the region of thermodynamic stability of TiO_2. The pH and chloride concentration have been found to have a relatively minor influence on the uniform passive dissolution rate of some Ti alloys, although data are limited in this area. Decreasing the pH from near neutral to 1 in 0.6 M sodium chloride solutions raised the passive dissolution rate of Ti-15V-3Cr (a β-Ti alloy) only by a factor of two. When tested in 5 M HCl, the passive current density increased only by an order of magnitude compared to that measured in 0.6 M NaCl (Kolman and Scully, 1994). In other work on pure Ti thin films, it was observed that the pH and chloride concentration had little to no influence on the passive dissolution rate (Kolman and Scully, 1996). Similar observations that pH and chloride concentration do not affect general corrosion rates have been made during industrial experience using Ti alloys in geothermal and desalination plant applications (Conover, et al., 1980).

A critical review of the literature on the localized corrosion of Ti alloys (Cragnolino, et al., 1999) indicates that, although Ti alloys can be susceptible to crevice corrosion, insufficient experimental data under relevant conditions are available for Ti-Pd alloys, such as Ti grades 7 and 16, to adequately determine the conditions for various corrosion modes and their propagation rates. Crevice corrosion of CP Ti has been observed under conditions that could develop in the repository. At reasonably achievable potentials for the repository (-0.1 V_{SCE}), the minimum temperature at which crevice corrosion was observed is approximately 170 °C at a chloride concentration of 0.034 M, 80 °C at 0.2 M chloride, and 50 °C at 1 M chloride (Tsujikawa and Kojima, 1993). Based on these reported results, crevice corrosion of Ti is possible in the repository. The addition of Pd to Ti, though, improves the crevice corrosion resistance of Ti in chloride solutions. Even at elevated temperatures (>165 °C), values of E_{rp} for Ti grade 7 in highly concentrated chloride solutions (> 4 M) are well above 1 V_{SCE} (Brossia and Cragnolino, 2000a). However, the presence of fluoride promotes accelerated corrosion in chloride solutions.

Also of importance are the possible interactions with other materials present in the repository and the effects of fabrication on degradation processes. Galvanic coupling of Ti to iron and carbon steels, SS, and Ni-base alloys may lead to conditions that enhance the propagation rates of processes already occurring, such as hydrogen absorption. Though some evidence shows that fabrication processes would not significantly affect material performance, the resolution limit of the methods used may mask propagation rates (in terms of SCC and HE crack propagation) that would be relevant on the time scale of repository performance.

In EDA-II, which has been recommended to DOE for the SR, a design consisting of a 2-cm thick Alloy 22 outer overpack surrounding a 5-cm-thick Type 316 NG SS overpack that provides structural strength was adopted. The introduction of a thinner overpack as compared to the VA design raises concerns related to the effect of γ-radiolysis and the resulting oxidizing conditions.

Additionally, the presence of steel beams on the floor, instead of concrete, despite the possible addition of a nonelectrically conductive ballast, may result in differences in the electrochemical conditions in the interface of the WPs and the DS with other EBS components and the aqueous environment (including the effects of corrosion products) that need to be considered.

5.0 STATUS OF SUBISSUE RESOLUTION AT THE STAFF LEVEL

Issue resolution is being pursued through continuation of the ongoing prelicensing consultation and interaction with the DOE. In prior years, staff raised detailed concerns and questions about DOE's site characterization and PA program in areas related to this KTI. These concerns and questions were documented in NRC Staff Site Characterization Analysis of the U.S. Department of Energy's Site Characterization Plan, Yucca Mountain Site, Nevada (U.S. Nuclear Regulatory Commission, 1989). The current status of the open items from this analysis is presented in Appendix A.

In 1995, the staff recognized the need to refocus the prelicensing repository program on resolving issues most significant to repository performance. The status of the staff refocused efforts, including general descriptions of the primary issues and concerns in the HLW program areas of interest (i.e., KTIs), was documented in NRC High-Level Radioactive Waste Program Annual Progress Report: Fiscal Year 1996 (U.S. Nuclear Regulatory Commission, 1997).

Additional comments and concerns related to several KTIs were reported in two documents related to DOE's 1995 iterative PA: (i) NRC/CNWRA Audit Reviews of DOE's TSPA-95 (Austin, 1996a,b,c), and (ii) NRC/CNWRA Detailed Review of Selected Aspects of TSPA—1995 (Baca and Jarzemba, 1997). Also, staff has reviewed the following items: the DOE site characterization progress reports, in relation to the further development of container design and materials selection; EBS design documents, such as the Mined Geologic Disposal System Advanced Conceptual Design Report (CRWMS M&O, 1996); and, recently, the Viability Assessment of a Repository at Yucca Mountain (U.S. Department of Energy, 1998a,b,c). Comments arising from the review of the DOE VA were documented in the attachment to the letter to Barrett from Paperiello.[1]

Continuing staff efforts to resolve the issues, concerns, and questions identified in these reports resulted in further refinement and clarification of the primary issue and subissues in the CLST KTI described in Section 2.0 of this IRSR. In the following sections, the status of resolution for each of the subissues described in Section 2.0, and whose technical bases were provided in Section 4, is presented. In conducting this review, the staff relied on information provided in the DOE VA (U.S. Department of Energy, 1998c), as well as on information presented in the Waste Package Degradation Process Model Report (CRWMS M&O, 2000b), Waste Form Degradation Process Model Report (CRWMS M&O, 2000c), Engineered Barrier System Degradation, Flow, and Transport Process Model Report (CRWMS M&O, 2000d), and related analysis model reports (AMRs). Progress in resolving the CLST subissues was reviewed during a NRC/DOE technical exchange and agreements were reached regarding the scope and schedule of additional data and analyses that will be provided by DOE to close issues. As a result, five of the six CLST subissues were closed pending. The subissue on in-package criticality was also defined as closed pending in a separate technical exchange with the DOE. Because many of the additional

[1]Paperiello, C. Letter (June 2) to L. Barrett concerning U.S. Nuclear Regulatory Commission Staff Review of the U.S. Department of Energy Viability Assessment for a High-Level Radioactive Waste Repository at Yucca Mountain, Nevada. 1999.

analyses and data DOE agreed to provide are scheduled prior to LA, continued interactions between the NRC and the DOE on these topics are needed to ensure implementation of paths to resolution.

NRC evaluation of DOE rationale for exclusion of FEP related to WP performance and radionuclide release, as well as in-package criticality, is summarized in Table C-1 in Appendix C. The "included" FEP are generally not evaluated.

5.1 SUBISSUE 1: THE EFFECTS OF CORROSION PROCESSES ON THE LIFETIME OF THE CONTAINERS

This subissue relates to the adequacy of DOE's approach to addressing the degradation of the WPs as a result of environmental exposure after emplacement in the proposed repository environment. Significant degradation modes include dry-air oxidation, humid-air corrosion, and aqueous corrosion processes such as uniform corrosion, localized corrosion, SCC and HE. Model abstractions that apply to this subissue are

- ENG1 Degradation of Engineered Barriers
- ENG2 Mechanical Disruption of Engineered Barriers
- ENG3 Quantity and Chemistry of Water Contacting the WPs and WFs

5.1.1 Description of the U.S. Department of Energy Approach

The description of the DOE approach in the following sections is based on the WP Degradation PMR and supporting AMRs. In the NRC/DOE Technical Exchange and Management Meeting on CLST,[2] DOE agreed to provide additional information through revised AMRs or other documents prior to or at the time of the LA, as described in detail in Section 5.1.3.

5.1.1.1 Dry-Air Oxidation of the Alloy 22 Waste Package Outer Barrier

The DOE TSPA-VA focused on dry-air oxidation of carbon steel because this was the proposed material for the WP outer barrier (WPOB) in the VA design (U.S. Department of Energy, 1998b). Dry-air oxidation of Alloy 22 was not considered in the VA design because the corrosion resistant material was placed inside the carbon steel outer barrier. The TSPA-SR WP design is expected to be very similar to the EDA-II, which uses Alloy 22 as the WPOB (CRWMS M&O, 2000b). As a result of this change in design, dry-air oxidation of carbon steel is no longer an issue for WP performance.

DOE considers that dry-air oxidation of the Alloy 22 WPOB will occur when the RH of the repository environment is less then the critical relative humidity ($RH_{critical}$) for the initiation of humid-air corrosion (CRWMS M&O, 2000b,e). The rate of dry-air oxidation is considered to be

[2]NRC/DOE Technical Exchange and Management Meeting on the Key Technical Issue: Container Life and Source Term, Las Vegas, NV, September 12–13, 2000.

limited by mass transport of reacting species through the tightly adhering passive oxide film and is modeled assuming a parabolic growth law where the film thickness is proportional to the square root of time. The oxide film thickness as a function of time (x) is given as

$$x = \sqrt{x_0^2 + k \cdot t} \tag{1}$$

where x_0 is the initial oxide film thickness, k is a temperature dependent rate constant, and t is time. Calculations for Alloy 22 using a x_0 of 20 nm (0.020 μm) and a k value of 8.61×10^{-5} μm^2 y^{-1} at 350 °C, indicate that the initial growth rate during the first year is 9.2 nm y^{-1} (CRWMS M&O, 2000b). The value of k and the oxide growth rate are reduced as temperature decreases. It is concluded that the oxidation rate is low, and dry-air oxidation does not appear to limit WP lifetime.

5.1.1.2 Humid-Air Corrosion of the Alloy 22 Waste Package Outer Barrier

Humid-air corrosion is assumed to occur when the RH is greater than the $RH_{critical}$ (CRWMS M&O, 2000f). The $RH_{critical}$ is based on the deliquescence point (lowest RH at which a saturated solution of the salt can be maintained at a given temperature) for sodium nitrate (CRWMS M&O, 2000f) defined by

$$RH_{critical} = -3.5932\times10^{-5}T^3 + 5.9649\times10^{-3}T^2 - 0.45377T + 81.701 \tag{2}$$

where T is in °C. At 20 °C the deliquescence point for $NaNO_3$ occurs at an RH of 75 percent, whereas at 90 °C, the deliquescence point is lowered to an RH of 65 percent. The DOE model of corrosion of the Alloy 22 WPOB assumes that the corrosion rate and the distribution of corrosion rates under these conditions are the same as for aqueous corrosion and are independent of time (CRWMS M&O, 2000b).

5.1.1.3 General and Localized Corrosion of the Alloy 22 Waste Package Outer Barrier

Aqueous corrosion is classified into two corrosion modes: general corrosion and localized corrosion. For corrosion resistant Ni-Cr-Mo alloys such as Alloy 22, general corrosion in the assumed WP environments occurs in the form of passive corrosion, whereas localized corrosion is limited to pitting and crevice corrosion. SCC is considered independently of these localized corrosion modes.

Two environmental conditions are considered for the stabilization of an aqueous film on the WP surface. In one case, the presence of an aqueous environment is expected when the RH in the emplacement drift is greater than the deliquescence point of any salts deposited on the WP surface and, in the other case, when dripping of condensed water occurs on the WP. Below 100 °C the composition of water that contacts the WP surface is assumed to be simulated J-13 concentrated water (SCW). Simulated saturated water (SSW) is assumed to be present above 100 °C. Basic saturated water has also been identified as another plausible water chemistry that may develop on the WP surface as a result of dripping and evaporation. Compositions of the water chemistries are provided in Table 2. In addition, it is assumed that γ-radiolysis can

Table 2. Concentration of key species in simulated concentrated water (SCW), simulated saturated water (SSW), and basic saturated water (BSW) (CRWMS M&O, 2000f)

Species	SCW (M)	SSW (M)	BSW (M)
K^+	0.09	3.62	1.75
Na^+	1.78	2.12	4.84
F^-	0.07	0	0.071
Cl^-	0.19	3.62	3.8
NO_3^-	0.10	2.11	2.3
SO_4^{2-}	0.17	0	0.149
HCO_3^-	1.15	0	0
pH	—	—	11-13

increase the corrosion potential (E_{corr}) of Alloy 22 by 100 mV, based on short-term exposures of specimens to solutions containing hydrogen peroxide (H_2O_2).

General passive corrosion is assumed when the E_{corr} is less than the critical potential ($E_{critical}$) for the initiation of localized corrosion. The general corrosion rates are derived from data obtained from the long-term corrosion test facility (LTCTF) where numerous test specimens have been exposed to aqueous solutions based on modifications of J-13 water (CRWMS M&O, 2000e; McCright, 1998). Corrosion rates of specimens exposed in the LTCTF were calculated by measuring the weight loss of the specimens (American Society for Testing and Materials, 1997b) after exposures of at least 6 months. Weight gain was observed on 25 percent of the Alloy 22 weight loss specimens as a result of the deposition of silicates (assumed to be amorphous SiO_2) on the surface of the specimens. Data from specimens with weight gains were not used to determine the distribution of corrosion rates that ranged from 0 nm y^{-1} at the 0th percentile, 27 nm y^{-1} at the 50th percentile, 98 nm y^{-1} at the 90th percentile, and 730 nm y^{-1} at the 100th percentile. It has been suggested, based on atomic force microscopy measurements, that weight gain caused by the deposited silicate can be corrected by adding a value of 63 nm y^{-1} to the entire corrosion rate distribution (CRWMS M&O, 2000b,e). The abstracted general corrosion rate for the Alloy 22 WPOB was distributed between 10^{-6} and 7.3×10^{-5} mm y^{-1}.

An enhancement factor, normally distributed between 1 and 2.5, is used to model the corrosion rate of thermally aged Alloy 22 and is based on the passive current density of the thermally aged specimen (700 °C for 173 hours) measured in a potentiodynamic polarization test (CRWMS M&O, 2000b). Acceleration of the corrosion rates as a result of microbial activity is also treated using an enhancement factor, G_{MIC}. For Type 316 NG, a G_{MIC} of 10 is used, based on results

obtained with Type 304 SS. For Alloy 22, experimental results indicate a G_{MIC} of 2, based on the corrosion rate measured in short-term exposure tests (CRWMS M&O, 2000b,e).

Localized corrosion of Alloy 22 is assumed to occur when the E_{corr} is greater than the $E_{critical}$. Critical potentials for localized corrosion of Alloy 22, reviewed in the general corrosion and localized corrosion of WPOB AMR (CRWMS M&O, 2000e), are limited to pitting repassivation potential data obtained using a lead in pencil geometry (Gruss, et al., 1998). Initiation and repassivation potentials as a function of temperature, obtained in cyclic potentiodynamic polarization (CPP) tests using a variety of electrolytes based on modifications of J-13 water, were also used as values for $E_{critical}$ obtained from anodic polarization curves. Crevice corrosion stabilization and repassivation potentials measured in 5 M LiCl solutions from 60 to 95 °C (Kehler, et al., 2000) were not used as $E_{critical}$ values because the concentrated solutions were not deemed to represent any plausible repository environment (CRWMS M&O, 2000b). Although the $E_{critical}$ for a thermally aged specimen decreased by 100 mV, the susceptibility of the thermally aged specimens to localized corrosion was not increased with respect to the base alloy because it is assumed that the corresponding reduction of the E_{corr} will prevent the initiation of localized corrosion.

The rate of localized penetration of Alloy 22 was estimated using corrosion rates in highly corrosive environments such as 10 percent $FeCl_3$ at 75 °C; dilute boiling HCl; and a solution containing 7 vol%, H_2SO_4, 3 vol % HCl, 1 wt % $FeCl_3$ and 1 wt % $CuCl_2$ at 102 °C. The distribution of localized corrosion rates is centered around the highest passive current density of 10 μA cm^{-2} that corresponds to a corrosion rate of 100 μm y^{-1}. The cumulative distribution of penetration rates for localized corrosion is 12.7 μm y^{-1} for the 0th percentile, 127 μm y^{-1} for the 50th percentile, and 1,270 μm y^{-1} for the 100th percentile (CRWMS M&O, 2000b,e).

5.1.1.4 Stress Corrosion Cracking of the Alloy 22 Waste Package Outer Barrier

SCC susceptibility is one of the potential failure modes of the Alloy 22 WPOB. DOE proposed two models for SCC susceptibility evaluation: the SCC threshold model and the slip dissolution/film rupture model (CRWMS M&O, 2000b). The SCC threshold model is based on fracture mechanics concepts that suggest that for SCC to occur, the stress intensity (K_I) at a flaw or defect must be equal to or greater than the threshold stress intensity factor for the initiation of SCC (K_{Iscc}).

$$K_I \geq K_{Iscc} \tag{3}$$

The stress intensity factor can be calculated with a simplified expression:

$$K_I = \beta\sigma\sqrt{\pi a} \tag{4}$$

where β is the geometry factor, σ is the tensile stress, and a is the flaw size. K_{Iscc} is a material and environment dependent parameter below which an existing crack will not grow. A mean K_{Iscc} value for Alloy 22 was measured to be 33 MPa·m$^{1/2}$ using wedge-loaded precracked DCB

specimens in a deaerated, acidic 5 wt % NaCl solution at 90 °C (Roy, et al., 1998; McCright, 1998).

Weld residual stress is the only type of stress assumed to be relevant under repository conditions in the SCC susceptibility evaluation conducted by the DOE. Finite element analyses of the outer barrier lid welds indicate that while the stress intensity factors associated with circumferential flaws are less than the K_{Iscc}; the maximum stress intensity factor for radial flaws may exceed the K_{Iscc} (CRWMS M&O, 2000g). Thus, the calculations predict through-wall radial cracking based on the SCC threshold model and the experimentally measured values of K_{Iscc}.

The slip dissolution/film rupture model relates crack advance to the metal anodic oxidation that occurs when the protective film at the crack tip is ruptured as a result of a tensile stress. In this model, a simple expression relates the crack propagation rate (V_t) with the crack tip strain rate ($\dot{\varepsilon}_{ct}$) according to a power law relationship:

$$V_t = A(\dot{e}_{ct})^n \tag{5}$$

where A and the repassivation slope n are dependent on the material and environment. Two empirical relationships, adopted from the work of Ford and Andresen (1988), provide the dependance of A on n, defining the effects of the electrochemical and material factors, and the dependance of $\dot{\varepsilon}_{ct}$ on K_I, to account for the mechanical factors under constant load conditions, according to the following expressions:

$$A = 7.8 \times 10^{-3} n^{3.6} \tag{6}$$

$$\dot{\varepsilon} = 4.1 \times 10^{-14} K_I^4 \tag{7}$$

While it is suggested that these parameters can be determined from repassivation rate measurements under potentiostatic conditions, empirical data obtained for Types 304 and 316 SS in typical BWR environments and previous crack propagation rates for Alloy 22 are actually used to predict crack propagation rates as a function of K_I. For constant load conditions, which are assumed for the WP, V_t is given by

$$V_t = \overline{A}(K_I)^{\overline{n}} \tag{8}$$

where

$$\overline{A} = A(4.1 \times 10^{-14})^n \tag{9a}$$

and

$$\overline{n} = 4n \tag{9b}$$

For Alloy 22, crack propagation rates from exposures in 5 percent NaCl at 90 °C and A values obtained from SS in BWR environments were used to estimate a value of n of 0.84. Considering the uncertainty associated with the determination of n, 0.75 and 0.84 are selected to represent the lower and upper bounds of n (CRWMS M&O, 2000g). It is apparent from Eqs. (6) and (7) that V_t increases as the K_I increases and n decreases.

For both the slip dissolution/film rupture model and the SCC threshold model, through-wall radial cracking is predicted as a result of the high values of the calculated stress intensity factor. The approach adopted by the DOE to mitigate or eliminate the possibility of crack growth is to reduce the residual stresses associated with welding. One method consists of localized annealing of the weld region using induction heating. The other method proposed involves the use of laser peening to introduce compressive stresses on the surface using multiple passes of the laser beam (CRWMS M&O, 2000b).

5.1.2 Staff Evaluation of the U.S. Department of Energy Approach

5.1.2.1 Dry-Air Oxidation of the Alloy 22 Waste Package Outer Barrier

Acceptance Criteria

- The description of engineered barriers, design features, degradation processes, physical phenomena, and couplings that may affect the degradation of the engineered barriers is adequate. For example, it includes materials and methods used to construct the engineered barriers and considers degradation processes such as uniform corrosion, pitting corrosion, crevice corrosion, stress corrosion cracking, intergranular corrosion, microbially influenced corrosion, dry-air oxidation, hydrogen embrittlement, as well as the effects of wet and dry cycles, material aging and phase stability, welding, and initial defects on the degradation modes for the engineered barriers.

- Parameters used to evaluate the degradation of engineered barriers in the safety case are adequately justified (e.g., laboratory corrosion tests, site-specific data such as data from drift scale tests, in-service experience in pertinent industrial applications, and test results not specifically performed for the Yucca Mountain site, etc.). DOE describes how the data were used, interpreted, and appropriately synthesized into the parameters.

NRC Staff Evaluation

Previous investigations on thermal oxidation indicate logarithmic kinetics for Ni in the range of 40 to 300 °C. Parabolic growth has been observed when the nickel oxide thicknesses are greater than 3 to 4 nm (Fehlner, 1986). Oxidation of chromium has been observed to obey Mott and Cabrera (inverse logarithmic law) kinetics at low temperatures and parabolic kinetics above 450 °C (Fehlner, 1986). The assumption of parabolic growth of oxides on SS and Ni-Cr-Mo alloys is not supported by either DOE data or independent tests performed outside the HLW disposal program. However, parabolic oxidation kinetics result in greater oxide penetration compared to either logarithmic or inverse logarithmic kinetics (Fehlner, 1986). At the

temperatures expected for the proposed repository, oxide penetration of the Alloy 22 WPOB by uniform oxidation is not expected. Physical processes that lead to accelerated oxidation rates, such as spalling of the oxide layer or mechanical abrasion of the oxide layer, are not expected for Alloy 22 in a repository environment.

The approach used by DOE assumes the formation of uniform oxide film and does not consider the possible preferential oxidation along grain boundaries. Intergranular oxidation has been observed at temperatures above 600 °C on a Fe-10Cr-34Ni alloy (Newcomb and Stobbs, 1991) and in the range of 800 to 1000 °C for Alloys 800H and 825 (Wei and Scott, 1989). Formation of intergranular oxides of Cr and Fe has been observed on primary-side Alloy 600 steam generator tubing after 9 years of normal operation at temperatures of about 300 °C (Bruemmer, et al., 2000). The oxides were found to penetrate grain boundaries well in advance of intergranular SCC. The mechanism for intergranular oxidation of Ni-base alloys was concluded to be different than high-temperature oxidation (Simonen, et al., 2000). Enhanced oxidation at the grain boundaries was proposed to be a result of the nonequilibrium vacancy injection into the alloy and subsequent increases in the diffusion of substitutional solutes and ingress of interstitial oxygen through vacancy-oxygen interactions rather than accelerated diffusion of chromium and oxygen along the grain boundaries.

Additional information is needed in the case of dry-air oxidation. The DOE assumption of parabolic oxidation of Alloy 22 is reasonable but should be supported by empirical evaluations of Alloy 22 and similar Ni-Cr-Mo alloys. An evaluation of the possibility of preferential oxidation at grain boundaries would be desirable based on the apparent susceptibility of Ni-base alloy to enhanced intergranular oxidation, which has been shown to be a factor in SCC of steam generator tubing (Bruemmer, et al., 2000).

5.1.2.2 Humid-Air Corrosion of the Alloy 22 Waste Package Outer Barrier

Acceptance Criteria

- The description of engineered barriers, design features, degradation processes, physical phenomena, and couplings that may affect the degradation of the engineered barriers is adequate. For example, it includes materials and methods used to construct the engineered barriers and considers degradation processes such as uniform corrosion, pitting corrosion, crevice corrosion, stress corrosion cracking, intergranular corrosion, microbially influenced corrosion, dry-air oxidation, hydrogen embrittlement, as well as the effects of wet and dry cycles, material aging and phase stability, welding, and initial defects on the degradation modes for the engineered barriers.

- Parameters used to evaluate the degradation of engineered barriers in the safety case are adequately justified (e.g., laboratory corrosion tests, site-specific data such as data from drift scale tests, in-service experience in pertinent industrial applications, and test results not specifically performed for the Yucca Mountain site, etc.). DOE describes how the data were used, interpreted, and appropriately synthesized into the parameters.

- For those degradation processes that the Total System Performance Assessment abstraction indicates are significant to the performance of the engineered barriers, DOE provides appropriate parameters based on techniques that may include laboratory experiments, field measurements, industrial analogs, and process-level modeling studies conducted under conditions relevant to the range of environmental conditions within the WP emplacement drifts. DOE also demonstrates the capability to predict the degradation of the engineered barriers in laboratory and field tests.

- For the selection of parameters used in conceptual and process-level models of engineered barrier degradation that can be expected under repository conditions, assumed range of values and probability distributions are not likely to underestimate the actual degradation and failure of engineered barriers as a result of corrosion.

NRC Staff Evaluation

The approach used by DOE, assuming that the corrosion rates under humid-air conditions are the same as those under aqueous conditions, appears to be conservative as indicated. A comparison of aqueous and humid-air corrosion rates for Type 316L (CRWMS M&O, 2000b) reveals that the humid-air corrosion rates are almost an order of magnitude less than the aqueous corrosion rates.

The use of the deliquescence point for $NaNO_3$ as the criteria for the $RH_{critical}$ is supported by a review of empirical data (CRWMS M&O, 2000f). Other salts that may be deposited on the surfaces of the WPs have deliquescence points corresponding to higher values of RH. The deliquescence point for NaCl, for example, is not strongly dependent on temperature within the range of 0 to 80 °C and occurs at a RH of 74 to 76 percent (CRWMS M&O, 2000f).

The DOE assumption of humid-air corrosion rates of Alloy 22 bounded by aqueous corrosion rates is acceptable. It would be useful to have additional data obtained outside the Yucca Mountain Project (YMP) using information for Alloy 22 and similar Ni-Cr-Mo alloys.

5.1.2.3 General and Localized Corrosion of the Alloy 22 Waste Package Outer Barrier

Acceptance Criteria

- The description of engineered barriers, design features, degradation processes, physical phenomena, and couplings that may affect the degradation of the engineered barriers is adequate. For example, it includes materials and methods used to construct the engineered barriers and considers degradation processes such as uniform corrosion, pitting corrosion, crevice corrosion, stress corrosion cracking, intergranular corrosion, microbially influenced corrosion, dry-air oxidation, hydrogen embrittlement, as well as the effects of wet and dry cycles, material aging and phase stability, welding, and initial defects on the degradation modes for the engineered barriers.

- Sufficient technical bases for the inclusion of FEP related to degradation of engineered barriers in the Total System Performance Assessment abstractions are provided.

- Parameters used to evaluate the degradation of engineered barriers in the safety case are adequately justified (e.g., laboratory corrosion tests, site-specific data such as data from drift scale tests, in-service experience in pertinent industrial applications, and test results not specifically performed for the Yucca Mountain site, etc.). DOE describes how the data were used, interpreted, and appropriately synthesized into the parameters.

- Degradation models for the processes that may be significant to the performance of the engineered barriers are adequate. For example, DOE models consider the possible degradation of the engineered barriers as a result of uniform and localized corrosion processes, stress corrosion cracking, microbial influenced corrosion, hydrogen embrittlement, and incorporate the effects of fabrication processes, thermal aging, and phase stability.

- For those degradation processes that the Total System Performance Assessment abstraction indicates are significant to the performance of the engineered barriers, DOE provides appropriate parameters based on techniques that may include laboratory experiments, field measurements, industrial analogs, and process-level modeling studies conducted under conditions relevant to the range of environmental conditions within the WP emplacement drifts. DOE also demonstrates the capability to predict the degradation of the engineered barriers in laboratory and field tests.

- For the selection of parameters used in conceptual and process-level models of engineered barrier degradation that can be expected under repository conditions, assumed range of values and probability distributions are not likely to underestimate the actual degradation and failure of engineered barriers as a result of corrosion.

- DOE uses alternative modeling approaches consistent with available data and current scientific understanding, and evaluates their model results and limitations using tests and analyses that are sensitive to the processes modeled. For example, for processes such as uniform corrosion, localized corrosion, and stress corrosion cracking of the engineered barriers, DOE considers alternative modeling approaches to develop its understanding of environmental conditions and material factors are significant to these degradation processes.

- Numerical corrosion models used to calculate the lifetimes of the engineered barriers are adequate representations, considering the associated uncertainties in the expected long-term behaviors, the range of conditions (including residual stresses) and the variability in engineered barrier fabrication processes (including welding).

- Evidence is sufficient to show that models used to evaluate performance are not likely to underestimate the actual degradation and failure of engineered barriers as a result of corrosion or other degradation processes.

- Mathematical models for the degradation of engineered barriers are based on the same environmental parameters, material factors, assumptions, and approximations shown to be appropriate for closely analogous engineering or industrial applications and experimental investigations.

NRC Staff Evaluation

The DOE approach relies on passive dissolution rates of Alloy 22 determined via weight loss measurements. Because the passive corrosion rate of Alloy 22 is quite low, the change in mass is also small. For a typical 50 mm × 50 mm × 3.175 mm test specimen with an area of 56.35 cm^2 and a weight of 68.97 g, a corrosion rate of 26.6 nm y^{-1} (DOE 50th percentile) is equivalent to a passive current density of 2.6×10^{-9} A/cm^2 or a mass loss rate of 0.00125 g y^{-1}. For a 1-year exposure, the change in weight is less than 2×10^{-3} percent.

Such small changes in weight can be determined provided there is not substantial interference from a competing process. In the case of the DOE LTCTF data, the deposition of silicate was shown to interfere with weight loss data. The suggested correction (CRWMS M&O, 2000b,e) to the corrosion rate distribution (i.e., addition of 63 nm y^{-1}) may lead to a nonconservative estimation of the actual corrosion rates by overcorrecting the measured rates because it does not account for the time-dependent changes in corrosion rate that must have occurred after the silicate deposition. In addition, the value of the correction factor is more than twice the value of the median corrosion rate.

The distribution of passive corrosion rates used by the DOE is not supported by the electrochemical measurements conducted within the YMP and is lower than corrosion rates measured in a variety of service environments. The low passive corrosion rate of Alloy 22 is the result of the formation of a protective chromium oxide passive film. Kirchheim, et al. (1989) reported a passive current density of 0.014 μA/cm^2 (corrosion rate of 9.68×10^{-5} mm y^{-1}) for pure Cr in 1 N H_2SO_4. Higher corrosion rates were observed for Fe-Cr alloys. Smailos (1993) reported corrosion rates of Alloy C-4 brine environments containing 25.9 percent NaCl at 150 °C calculated from weight loss measurements after 18-month exposures to be in the range of 6×10^{-5} to 7×10^{-5} mm y^{-1}. In brines with 26.8- and 33-percent $MgCl_2$, the welded C-4 had a corrosion rate of 5×10^{-3} to 6×10^{-3} mm y^{-1}. Bickford and Corbett (1985) measured corrosion rates of Alloy 22 in environments containing 20,000-ppm Cl^-; 2,300 ppm F^-; and 1,400-ppm SO_4^{2-}. In solutions with a pH of 1.6, the corrosion rates were 0.005 mm y^{-1} at 40 °C and 0.05 mm/yr at 90 °C, whereas, in solutions at pH 6, the corrosion rates were 0.005 mm y^{-1} at 40 °C and 0.012 mm/yr at 90 °C. Harrar, et al. (1977, 1978) reported the corrosion rates of Alloys C-276 and 625 exposed to chloride containing groundwater at the Salton Sea geothermal field (100 °C brine containing 12-percent chloride at a pH of 3.4). General corrosion rates calculated using linear polarization were 0.0015 mm y^{-1} for Alloy C-276 and 0.007 mm y^{-1} for Alloy 625.

The corrosion rate data used by the DOE do not consider the effects of long-term changes to the composition of the oxide films. Previous investigations (Lorang, et al., 1990) indicated that the composition of the oxide film, that acts as a barrier for mass transport, becomes enriched in Cr

and depleted in Mo and Ni. The long-term effects of preferential dissolution of alloying elements may include changes to the oxide film composition that could, in turn, alter the passive corrosion rate, or promote an increase in the susceptibility of the alloy to localized corrosion. Information on the preferential dissolution of alloying elements has not been obtained from LTCTF specimens.

The relative corrosion rates of welded and base metal Alloy 22 were also determined using weight loss specimens. While the welded specimens are exposed along with the base alloy, the area of the welded region is quite small (approximately 10–15 cm^2) and accounts for less than 25 percent of the total specimen surface area. As a result, accelerated corrosion rate of the welded region would be masked by the much larger area of the base alloy.

The enhancement factor for the thermally aged specimens is based solely on short-term data and does not consider the effects of preferential corrosion that may occur at the grain boundary regions as indicated in previous investigations (Heubner, et al., 1989). Reductions in the $E_{critical}$ value are a strong indication that thermal aging increases the susceptibility of the alloy to localized corrosion and more appropriate values of $E_{critical}$ such that the crevice corrosion initiation and repassivation potentials are necessary for a proper evaluation of thermal aging effects on localized corrosion. The increased current density, measured during an anodic polarization scan of an Alloy 22 specimen thermally aged for 173 hours at 700 °C, was averaged over the entire exposed surface area. In light of the increased susceptibility of thermally aged Ni-Cr-Mo alloys to intergranular corrosion, the increased current density observed in the DOE test may be the result of preferential dissolution at grain boundaries rather than an overall increase in the corrosion rate. Such preferential attack, mainly confined to the grain boundary regions, would result in a true enhancement factor much greater than 2.5.

The enhancement factor for MIC, G_{MIC}, was calculated from the results of exposures to sterile and inoculated solutions (CRWMS M&O, 2000b,e). No information is provided on the possible preferential dissolution of alloying elements or on localized corrosion susceptibility as a result of microbial activity. In addition, the effect of temperature on the value of G_{MIC} is not available.

Determination of the Alloy 22 localized corrosion susceptibility by comparing the corrosion potentials and initiation potentials measured in short-term tests may not be acceptable. However, selection of the critical potential should be based on the most likely corrosion mode for the alloy and must consider environmental effects of temperature, solution chemistry, and the presence of microbes, as well as the effects of material property variations caused by fabrication, welding, thermal aging, and long-term evolution of the oxide film composition and characteristics. In addition, the range of environmental effects such as radiolysis and water chemistry, material factors such as the formation of thermal oxide films, and the long-term evolution of the oxide film composition should be included in the bounding analyses of the corrosion potential. The present set of data referenced in the WP PMR (CRWMS M&O, 2000b) used as criteria to evaluate the localized corrosion susceptibility of the WPOB is limited to localized corrosion initiation potentials, pitting corrosion repassivation potentials, and potentials associated with the evolution of oxygen. The latter potentials are not relevant to corrosion processes unless they are also associated with transpassive dissolution of the alloy.

The determination that the localized corrosion susceptibility of Alloy 22 is not affected by thermal aging based on the difference between the E_{corr} and the $E_{critical}$ may be nonconservative. The selected value of the $E_{critical}$, which may be a combination of pit initiation or oxygen evolution, is misleading because it does not compare other possible values of $E_{critical}$ such as the initiation and repassivation potentials for crevice corrosion with E_{corr}. The reduction of the pit initiation potential observed for the thermally aged specimen is a strong indication that thermal aging reduces the localized corrosion susceptibility of Alloy 22. Previous investigations identified the formation of topologically closed-packed (TCP) phases in both thermally aged (Heubner, et al., 1989) and welded (Cieslak, et al., 1986) Alloy 22. Observations of preferential initiation of localized corrosion in weldments and at grain boundary attack on the thermally aged material (Heubner, et al., 1989) as well as lower critical pitting temperature for welded Alloy 22 (Sridhar, 1990) do not support the DOE conclusion of no reduced susceptibility to localized corrosion after thermal aging. The reduction of the E_{corr} after thermal aging suggests an increase in the passive current density. As previously indicated, this increase may be a result of significantly enhanced dissolution at grain boundaries.

Localized corrosion rates assumed by the DOE, obtained from literature data using acidic chloride and acidic oxidizing chloride solutions, appear to correspond to measured localized corrosion penetration rates obtained in service environments as reviewed by Cragnolino, et al. (1999). Smailos (1993) reported a maximum pit depth of 0.90 mm in Alloy 625 after 18 months in 33-percent $MgCl_2$ at 150 °C, corresponding to a localized corrosion penetration rate of 0.6 mm y^{-1}. Carter and Cramer (1974) reported that pit penetration rates for Alloy 625 were 0.22 mm y^{-1} after 45 days in 105 °C brine containing 155,000 ppm chloride with 30 ppm sulfur. Oldfield (1995) observed crevice corrosion of Alloys 625 and C-276 in both natural and chlorinated seawater at ambient temperature. The average penetration rate for Alloy 625, following a 2-year exposure, was 0.049 mm y^{-1}.

The DOE data from the LTCTF for the corrosion rates of Alloy 22 are not reliable because of the deposition of silicate and the limitations of the weight loss measurements to evaluate the effects of welding. Additional tests, where interference from deposition processes do not occur, should be performed to confirm or correct the results obtained using LTCTF specimens. The determination of passive corrosion rates from weight loss may be possible in solutions that do not contain dissolved silica, divalent cations such as calcium, or other species that can precipitate from solution and deposit on the test specimens. As an alternative to weight loss, steady-state anodic current density measurements obtained under potentiostatic conditions can be used to determine corrosion rates according to ASTM G102 (American Society for Testing and Materials, 1999). A more substantiated discussion about the long-term validity of low passive corrosion rates is needed to provide support to the assumptions in the model abstractions used in WAPDEG. The selection of the values of $E_{critical}$ should be confirmed by long-term electrochemical testing. In addition, the value of $E_{critical}$ should be based on the possible occurrence of crevice corrosion because this has been identified as the most significant localized corrosion degradation mode. Similarly, the effects of thermal aging and welding need to be included in the determination of $E_{critical}$. An evaluation of preferential grain boundary dissolution is necessary for thermally aged Alloy 22. Determining enhancement factors for MIC and thermal

aging is based on few data obtained in short-term exposures. In both cases, the possibility for preferential dissolution of alloying elements and localized corrosion needs to be evaluated.

5.1.2.4 Stress Corrosion Cracking of the Alloy 22 Waste Package Outer Barrier

Acceptance Criteria

- The description of engineered barriers, design features, degradation processes, physical phenomena, and couplings that may affect the degradation of the engineered barriers is adequate. For example, it includes materials and methods used to construct the engineered barriers and considers degradation processes such as uniform corrosion, pitting corrosion, crevice corrosion, stress corrosion cracking, intergranular corrosion, microbially influenced corrosion, dry-air oxidation, hydrogen embrittlement, as well as the effects of wet and dry cycles, material aging and phase stability, welding, and initial defects on the degradation modes for the engineered barriers.

- Parameters used to evaluate the degradation of engineered barriers in the safety case are adequately justified (e.g., laboratory corrosion tests, site-specific data such as data from drift scale tests, in-service experience in pertinent industrial applications, and test results not specifically performed for the Yucca Mountain site, etc.). DOE describes how the data were used, interpreted, and appropriately synthesized into the parameters.

- Degradation models for the processes that may be significant to the performance of the engineered barriers are adequate. For example, DOE models consider the possible degradation of the engineered barriers as a result of uniform and localized corrosion processes, stress corrosion cracking, microbial influenced corrosion, hydrogen embrittlement, and incorporate the effects of fabrication processes, thermal aging, and phase stability.

- For those degradation processes that the Total System Performance Assessment abstraction indicates are significant to the performance of the engineered barriers, DOE provides appropriate parameters based on techniques that may include laboratory experiments, field measurements, industrial analogs, and process-level modeling studies conducted under conditions relevant to the range of environmental conditions within the WP emplacement drifts. DOE also demonstrates the capability to predict the degradation of the engineered barriers in laboratory and field tests.

- For the selection of parameters used in conceptual and process-level models of engineered barrier degradation that can be expected under repository conditions, assumed range of values and probability distributions are not likely to underestimate the actual degradation and failure of engineered barriers as a result of corrosion.

- DOE uses alternative modeling approaches consistent with available data and current scientific understanding, and evaluates their model results and limitations using tests and analyses that are sensitive to the processes modeled. For example, for processes such

as uniform corrosion, localized corrosion, and stress corrosion cracking of the engineered barriers, DOE considers alternative modeling approaches to develop its understanding of environmental conditions and material factors are significant to these degradation processes.

- Numerical corrosion models used to calculate the lifetimes of the engineered barriers are adequate representations, considering the associated uncertainties in the expected long-term behaviors, the range of conditions (including residual stresses) and the variability in engineered barrier fabrication processes (including welding).

- Evidence is sufficient to show that models used to evaluate performance are not likely to underestimate the actual degradation and failure of engineered barriers as a result of corrosion or other degradation processes.

- DOE uses appropriate methods for nondestructive examination of fabricated engineered barriers, the type, size, and location of fabrication defects that may lead to premature failure as a result of rapidly initiated engineered barrier degradation. DOE specifies and justifies the allowable distribution of fabrication defects in the engineered barriers and assesses the effects of defects that cannot be detected on the performance of the engineered barriers.

- Sufficient data have been collected on the geology of the natural system, engineering materials, and initial manufacturing defects to establish initial and boundary conditions for the Total System Performance Assessment abstraction of mechanical disruption of engineered barriers.

NRC Staff Evaluation

The DOE modeling of SCC of the Alloy 22 outer container considers the expected WP environments and the closure lid weld stresses. Two SCC models, the threshold model and the slip dissolution/film rupture model, are developed (CRWMS M&O, 2000g). The DOE models evaluate SCC susceptibility of Alloy 22 using model parameters obtained from LLNL data. Evaluation of these two alternative models reveals that while a K_{Iscc} value of 33 MPa·m$^{1/2}$, determined by Roy, et al. (1998), is adopted in the threshold model, the slip dissolution/film rupture model predicts crack propagation at K_I values less than the experimentally determined value of K_{Iscc}.

The residual stress analyses performed by the DOE, using a finite element method, indicate that given the calculated maximum stress intensity factors from weld residual stress and a K_{Iscc} determined by LLNL, a radially oriented flaw perpendicular to weld may initiate SCC of the Alloy 22 outer container. In contrast, no SCC initiation at a circumferentially oriented flaw parallel to weld is expected to occur based on the threshold value. These arguments are based on the threshold or minimum stress intensity criterion. K_{Iscc}, however, could be lower in a different environment than that tested (Speidel, 1981). The validity of K_{Iscc} as a bounding parameter for

performance should be assessed through an appropriate combination of experimental and modeling work.

K_{Iscc} values ranging from approximately 8 to 20 MPa·m$^{1/2}$ have been observed for Types 304, 304L, 316, and other similar austenitic SS in chloride-containing solutions at temperatures ranging from 80 to 130 °C (Cragnolino and Sridhar, 1992). As expected, the values in the lower end of that range are observed with both increasing temperatures and chloride concentration. It is also recognized that K_{Iscc} values are affected by the electrode potential. Eremias and Marichev (1980) demonstrated that an increase in potential of about 350 mV, with respect to the open-circuit potential, decreases K_{Iscc} from 12 to 2 MPa·m$^{1/2}$ for an austenitic SS in boiling, concentrated LiCl solution. A cathodic overpotential of 50 mV, on the other hand, increases K_{Iscc} up to 16 MPa·m$^{1/2}$. On the basis of these observations, it is apparent that the composition of the environment is another constraint that must be considered when using K_{Iscc} as a bounding parameter for the initiation of SCC.

The lack of SCC on either Alloy 22 or Type 316L SS DCB specimens tested under equivalent conditions to those used at LLNL, along with the fracture surface analysis of the Alloy 22 control specimen that was fatigue precracked, heat-tinted, and mechanically overloaded to failure, suggests that the apparent crack growth observed in the tests conducted at LLNL was an artifact induced by mechanical fracture of the specimens after the completion of the SCC tests (Dunn, et al., 1999b). These results indicate that selection of appropriate test methods and representative environmental conditions is critical in assessing the susceptibility to SCC. Variations in the intergranular SCC behavior of different heats of Type 304 SS also showed pronounced differences in the time to failure (Szklarska-Smialowska and Cragnolino, 1980). No clear dependence of the time to failure on the composition and mechanical properties of the various heats was reported. The effect of heat-to-heat differences in Alloy 22 susceptibility to SCC has not been evaluated. From this perspective, concerns exist regarding the procedures used and the results obtained in the SCC testing of Alloy 22 at LLNL.

The effects of WP fabrication processes (i.e., welding and heat treatments) on SCC of candidate container materials still remain as major concerns. Residual stresses from WP fabrication or applied stresses resulting from seismic events combined with the necessary electrochemical conditions may be sufficient to cause SCC. High residual stresses from fabrication processes suggest that the mechanical component necessary for SCC will be present in every WP placed in the repository. However, the effects of welding and heat treatments on the SCC susceptibility as well as the K_{Iscc} value of Alloy 22 have not been evaluated. Additionally, the DOE's SCC models consider weld residual stress the only stress significant to the SCC (CRWMS M&O, 2000b). Other sources of stress are assumed to be either insignificant such as dead load stress or temporary like seismic stress. Accordingly, the effects of other possible types of stress in the repository have not been assessed.

In the slip dissolution/film rupture model, the DOE adopted a value of 0.84 for the repassivation slope, n, for Alloy 22 (CRWMS M&O, 2000g). This specific n value is calculated using the assumption of constant load conditions. The input for the model includes an average crack growth rate of 2.1×10^{-8} mm/s and two empirical relationships as expressed in Eqs. (4) and (5),

both adopted from Ford and Andresen (1988). The crack growth rate shown in Figure 26 in the cited AMR, however, was measured under cyclic loading. An average crack growth rate of 1.3×10^{-7} mm/s from Table 1 of Roy, et al. (1998) under static loading is not considered in the model.

As for the empirical relationships used by Ford and Andresen (1988), the two interdependent model parameters (*n* and *A*) used to define the crack propagation rate/crack tip strain rate relationship in the slip dissolution/film rupture model are dependent on material properties and the environment at the crack tip, as previously reviewed by Sridhar, et al. (1993). From the analysis of the extensive work conducted by Ford and Andresen (1988), it can be concluded that most of the final expressions for calculating crack propagation rates and crack tip strain rates requires the input of field data to adjust several of the parameters included in the model. This is particularly true in the case of the parameter *n*. The model parameters that successfully predict SCC of sensitized Type 304 SS in oxygenated BWR water environments are largely empirical correlations on the basis of a combination of laboratory experimental results and field observations. Therefore, adaption of these empirical relationships to Alloy 22 requires a more complete database specifically for Alloy 22.

Recently, Barkatt and Gorman (2000) reported SCC of Alloy 22 in concentrated J-13 well water of 0.5 (acidified with HCl) containing Pb at relatively high concentrations (~1,000 ppm). Tests were conducted at 250 °C using U-band specimens. Although the test conditions were extremely severe in terms of Pb concentrations, temperature and stress and the results are preliminary, the concern regarding the role of impurities such as Pb, Hg, or As requires further evaluation.

In addition to environmental effects, the DOE evaluation of the SCC susceptibility of Alloy 22 should consider the effects of variations in material properties, fabrication and welding, and long-term exposure to elevated temperatures. These variations are not easily correlated with compositional variations or differences in mechanical properties. Segregation of alloying elements and the formation of TCP phases in the welded regions has been shown to occur for Alloy 22 (Cieslak, et al., 1986), and thermal aging has been shown to increase localized corrosion susceptibility (Heubner, et al., 1989). Long-term exposure of the WP to elevated temperatures expected in the proposed repository may result in microstructural alterations that may be equivalent to aging for 100 hour at 700 °C (CRWMS M&O, 2000b).

The models for the SCC of Alloy 22 need to be justified using an appropriate combination of testing and calculations. The use of source data in the models appears to be inconsistent. While the K_{Iscc} value determined by Roy, et al. (1998) is adopted in the threshold model, different source data for the crack growth rate is used in the slip dissolution/film rupture model. In addition, the environments used to evaluate the SCC susceptibility of Alloy 22 using the SCC threshold model are not consistent with the environments expected on the DS and WP (CRWMS M&O, 2000f). K_{Iscc} values used to determine SCC susceptibility should be based on measurements conducted in environments that may be expected in the proposed repository because K_{Iscc} values are strongly dependent on both the material and the environment (Speidel, 1981). At present, the slip dissolution/film rupture model for Alloy 22 uses a combination of parameters derived from SS in BWR environments (Ford and Andresen, 1988; Ford, 1990) and limited amount of data obtained

from laboratory tests (Roy, et al., 1998; McCright, 1998; CRWMS M&O, 2000g). Although the model is theoretically based on fundamental parameters such as the repassivation rate, in practice, the critical parameters are empirically derived using a substantial volume of data obtained in BWR environments (Ford and Andresen, 1988; Ford, 1990) that are not available for Alloy 22 in the potential WP environments.

The effects of the post-weld annealing treatment proposed for the dual lid WPOB on the SCC susceptibility of Alloy 22 should also be evaluated. The proposed annealing treatment relies on rapid heating and cooling cycles (CRWMS M&O, 2000b). Because only the end of the WP is elevated to temperatures above 1,000 °C, significant thermal gradients will exist that may result in the exposure of some portions of the WPOB to temperatures that favor the formation of detrimental TCP phases. Variations in the annealing parameters may exacerbate microstructural alterations and further reduce the SCC resistance of the alloy.

5.1.3 Status and Path to Resolution

This subissue is closed, pending further information. DOE agreed to provide the necessary information to close the subissue at the time of submitting the LA. The path to resolution is based on the DOE's presentation and agreements reached in the NRC/DOE Technical Exchange and Management Meeting on CLST regarding this subissue. Any NRC concern not specifically covered in this section is dealt with a risk-informed approach (i.e., the concern may not be important in PA). The agreements summarized below are abstracted from the transcripts of the meeting.[3]

Regarding the environment in contact with the WP and the drip shield, DOE will establish the credible range of water chemistries, evaluate the effect of materials introduced during site characterization and construction on the water chemistry, determine the chemical form and likely concentrations of minor constituents in YM waters, characterize the waters with respect to the parameters (e.g., pH, redox potential, concentration of aggressive anions, and buffer species) that define the type of aqueous solutions that would evolve, and evaluate periodic evaporation of dripping water. This information will be provided in a revision of the AMR titled Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier (ANL-EBS-MD-000001).

DOE agreed to continue testing in the LTCTF to evaluate general and localized corrosion of Alloy 22 WP outer barrier, adding two new bounding water test environments, installing specimens with a larger surface area/volume ratio to increase the sensitivity of the measurements, using high-sensitivity probes for on-line measurements, and monitoring changes in corrosion rates with time. In addition, DOE agreed to conduct tests in environments containing heavy metal concentrations (e.g., Pb, As, Hg) to evaluate the effect on critical potentials. It is anticipated that testing will continue during the performance confirmation period. DOE agreed to

[3]Schlueter, J., Letter (October 4) to S. Brocoum, U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Key Technical Issue: Container Life and Source Term (ML003760868). Washington, DC: U.S. Nuclear Regulatory Commission. 2000.

provide additional details on sensitivities, resolution of measurements, limitations, and deposition of silica for the high-sensitivity probes. DOE also agreed to document the results obtained with the high-sensitivity probes, including limitation and resolution of measurements as affected by silica deposition, and the results of testing in the absence of silica deposits. DOE agreed to implement alternative methods to measure the corrosion rate of the WP material (e.g., ASTM G-102 testing) or provide justification for the current approach.

DOE stated that it will perform surface analyses of corrosion film topography using the atomic force microscope and provide data that characterizes the passive film stability, including welded and thermally aged specimens. To delineate the regime of passive film stability, DOE stated that it will calculate potential-pH diagrams for Alloy 22; study oxide films grown at higher temperatures (90 to 175 °C) in air, in aqueous systems using autoclaves, and/or electrochemically under anodic polarization; determine the kinetics of film growth and the possibility of spalling; and determine chemical, structural, and mechanical properties of films. All the data characterizing passive film stability will include data obtained using welded and thermally aged specimens. DOE agreed to provide all this documentation in a revision to the AMR titled General Corrosion and Localized Corrosion of Waste Package Outer Barrier (ANL-EBS-MD-000003) prior to LA.

DOE stated that it will consider the possibility of dealloying of welds as a result of MIC. Surface elemental analysis will be conducted to determine the occurrence of selective dissolution, using welded specimens. In addition, DOE has agreed to provide the technical basis for the selection of the critical potentials as bounding parameters for localized corrosion taking into account MIC. The critical potential for localized corrosion will be determined for welded, and welded and thermally aged Alloy 22. The values measured will be compared with those for the base metal to evaluate the effect of alloying element segregation on the localized corrosion susceptibility. DOE indicated that it will conduct measurements of the corrosion potential in the LTCTF to determine any evolution of this potential toward critical potentials for localized corrosion. DOE agreed to provide the documentation regarding localized corrosion, including MIC, in a revision to the AMR (ANL-EBS-MD-000003) prior to LA.

DOE stated that it will provide SCC data for base metal, welded, welded and aged, and cold-worked Alloy 22, including the effect of laser peening and induction annealing on such range of metallurgical conditions to qualify and optimize these two SCC mitigation processes. DOE agreed to provide data characterizing the stress distribution (compressive and tensile) generated as a result of laser peening and induction annealing, including the size of the compressive zone resulting from induction annealing. Documentation on the thermal profile of the WP measured during induction annealing will be provided. DOE agreed to continue SCC testing using the slow strain rate technique, and fracture mechanics tests in which crack growth rate is measured using the potential drop method. These tests will be performed in the same type of environments, using specimens with the same metallurgical treatments. DOE stated that scaling and weld process factors will be evaluated to relate thin coupons with dimensions in actual welded WP containers, including thermal/metallurgical structural effects arising from multipass weld processes. Repassivation constants to be used in the slip dissolution/film rupture model will be determined. The SCC resistance of full thickness material with welds obtained from the mock-ups of the SR design will be evaluated. DOE agreed to provide the documentation in revisions to

the AMRs titled Abstractions of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier Hydrogen Induced Corrosion of Drip Shield (ANL-EBS-MD-000004) and Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier and the Stainless Steel Structural Material (ANL-EBS-MD-000005) prior to LA. In addition, DOE agreed to provide justification for not including the rockfall effect and deadload from the collapse of the emplacement drift on the SCC analysis. Documentation will be included in ANL-EBS-MD-000005.

DOE stated that it will provide additional details on acceptance testing, in the form of guidance and criteria in the next revision of the Technical Guidance Document (TGD) for LA. The development of the LA sections and associated programs and process controls for the procurement and fabrication of WP materials and components will be included, incorporating consideration of the required controls for compositional variations in Alloy 22. DOE will issue the TGD revision in June 2001, contingent on publication of the final Part 63 and the YMRP.

5.2 SUBISSUE 2: THE EFFECTS OF PHASE INSTABILITY AND INITIAL DEFECTS ON THE MECHANICAL FAILURE AND LIFETIME OF THE CONTAINERS

This subissue is related to the adequacy of the DOE's consideration of the phase stability of the container materials. The combined effects of thermal exposure, during both fabrication and after emplacement into drifts in the proposed repository, residual stresses, and applied stresses as a result of seismic activity, and rockfall may lead to mechanical failure of the WP.

The following model abstractions are applicable to this subissue:

- ENG1 Degradation of Engineered Barriers
- ENG2 Mechanical Disruption of Engineered Barriers

5.2.1 Description of U.S. Department of Energy Approach

The description of the DOE approach in the following sections is based on the WP Degradation PMR and supporting AMRs. In the NRC/DOE Technical Exchange and Management Meeting on CLST,[4] DOE agreed to provide additional information through revised AMRs or other documents prior to or at the time of the LA, as described in detail in Section 5.2.3.

5.2.1.1 Phase Instability of Alloy 22

The phase stability of Alloy 22 is modeled assuming the precipitation of secondary TCP phases, such as μ, σ, and P-phase, which is dependent on time and temperature. Alloy 22 specimens, exposed to temperatures in the range of 427 to 800 °C for periods up to 40,000 hours, were analyzed for precipitation of TCP phases and LRO (CRWMS M&O, 2000h). An activation energy

[4]NRC/DOE Technical Exchange and Management Meeting on the Key Technical Issue: Container Life and Source Term, Las Vegas, NV, September 12–13, 2000.

for the precipitation of TCP phases has been determined to be near 280 kJ mol^{-1}. Based on the results of specimens analyzed thus far, bulk precipitation of TCP phases is not predicted in 10,000 years at 300 °C (CRWMS M&O, 2000b). The formation of grain boundary precipitates is deemed a worst-case scenario that would be equivalent to a 100-hour exposure at 700 °C. Using a similar Arrhenius type relationship, it is predicted that the LRO may occur after 1,000 years at 300 °C. However, no LRO is predicted to occur if the temperature remains below 260 °C.

5.2.1.2 Initial Defects in Alloy 22 Containers

In the VA, DOE defined the probability of early failure to be the probability of generating a through-wall defect in a container. Based on analyses of pressure vessels and the assumption that the combined probability for a double-walled WP developing a through-wall is the product of the individual probabilities of through-wall defect, DOE estimated that there will be 1 to 10 WPs with a through-wall manufacturing defect among approximately 10,500. Therefore, for the expected case one WP was assumed to fail, with a range of one to ten potentially failing at the end of the first 1,000 years after closure

In the WP PMR (CRWMS M&O, 2000b) and its associated AMR (CRWMS M&O, 2000l), a more detailed analysis of the probability of initial defects in the WP was performed. In analyzing the early failures, DOE estimated the probabilities of flaws of various sizes to be introduced on the WP due to different processes. In contrast to TSPA-VA, where a certain fraction of WPs were assumed to have completely failed at the end of 1000 years, the cumulative distribution of initial defects estimated from analyses of various fabrication and handling processes were then provided as input to a SCC model, which was used to propagate these defects through the container wall. In this abstraction, the DOE assumed the only defects that are important were defects exposed to the outer WP surface. Defects that were either completely enclosed within the container walls or exposed only to the inner diameter of the container were ignored on the basis they would propagate only under cyclic loading, a process that was not considered plausible under repository conditions. The effect of initial defects on other corrosion and mechanical failure processes was also ignored.

DOE conducted a review of the literature pertaining to defect generation in various fabricated components. The literature reviewed included boiler and pressure vessels, nuclear fuel rods, underground storage tanks, cesium capsules fabricated as part of the Hanford radioactive waste concentration processes, dry storage casks for SNF, and tin-plate cans. Literature pertinent to aerospace structures and chemical process industries was not included. Based on this review of literature, several sources of defects in fabricated components were identified:

- Weld flaws
- Base metal flaws (not arising from heat treatment)
- Improper weld material
- Improper heat treatment (related only to improper thermal controls)
- Improper weld flux material
- Poor weld joint design
- Contaminants (introduced essentially after fabrication)

- Mislocated welds
- Missing welds
- Handling/installation damage
- Administrative/operational error

Of these, improper weld flux was eliminated as a source of defects because the current WP design does not involve welding processes utilizing flux. Poor weld joint design was eliminated from consideration because of the belief that significant amount of development and testing will have gone into the final closure weld joint design (to date there has not been any significant effort in development or testing of weld joints simulating actual WP closure welds). Missing welds were eliminated from consideration because of low probability of occurrence observed in the fabrication of fuel cladding (less than 10^{-7} per rod). Mislocated welds were eliminated from consideration because it was felt that any significant mislocation of electrode will prevent the arc from striking and would be detected.

The probability of weld flaw was calculated using a spreadsheet model that is based on distribution functions developed by more detailed computer models. Several assumptions were made in calculating the probability distribution of weld flaw. The most important assumption was that the weld flaw distribution developed for SSs on the basis of inspection records and expert elicitation can be used for deriving the flaw size distribution for Alloy 22. The cumulative distribution of weld flaws (probability of surface intersecting weld flaw versus flaw depth) was calculated by multiplying linear flaw density of welds (number of flaws per unit length of weld), flaw size distribution (fraction of total number of flaws versus depth of flaw), and the inspection reliability (probability of not detecting a particular size of flaw by ultrasonics) combined with the fraction of flaws intersecting the surface. These distributions were modified by weld thickness as well as prior inspection. It should be noted that the inspection reliability data was based on ultrasonic testing (UT) of intergranular SCC and not weld flaws.

The base metal flaw probability was estimated based on human error data developed for nuclear reactors. It was assumed that base metal flaws occur because of an operator not following written procedures and a QA inspector missing this failure to follow procedures. Therefore, the probability of flaw in base metal is the product of linear flaw density in the base metal (assumed to be one order of magnitude lower than that in weld), probability of human error on failure to follow procedure (estimated to be 0.01 from reactor studies), and probability of human error in not detecting the failure to follow procedure (estimated to be 0.1). The size distribution of flaws was assumed to be same as in the case of welds. Therefore, the cumulative probability distribution of weld flaws had the same shape as that of the weld, but was lower by four orders of magnitude.

The improper weld material probability was estimated through a survey of prior experience involving Babcock and Wilcox in the Crystal River 3 project. A mean probability of improper weld filler material was estimated to be 3.5×10^{-5} per pound of weld. This value was multiplied by the probability of human error in verifying filler metal composition prior to fabrication. The human error probability was taken to be the same as the probability of error in checking a digital display (0.001 from reactor experience). Thus, the total probability of flaw from improper weld was estimated to be 3.5×10^{-8} per pound of weld or 1.5×10^{-5} per WP.

The probabilities of improper heat treatment, surface contamination after fabrication during emplacement, and improper handling were estimated through an event tree calculation involving various elementary processes included in these operations. A bounding estimate of probabilities for these defects was also calculated assuming human errors only. The flaws from administrative error arose from not loading the WP within the thermal loading design basis and from misplacing the DPs over the WP such that a gap was created allowing premature dripping of water on the WP.

In summary, the DOE estimates of probabilities for initial defects in the WP from various sources range from 10^{-8} to 10^{-3} per WP.. In the specific case of weld flaw, the probability of initial through-wall defect (i.e., defect size larger than 20 mm) is estimated to be less than 10^{-11} per WP for the top lid closure weld of Alloy 22. The consequence of this initial flaw is calculated in terms of SCC growth.

5.2.2 Staff Evaluation of the U.S. Department of Energy Approach

5.2.2.1 Phase Instability of Alloy 22

Acceptance Criteria

- The description of engineered barriers, design features, degradation processes, physical phenomena, and couplings that may affect the degradation of the engineered barriers is adequate. For example, include materials and methods used to construct the engineered barriers and considers degradation processes such as uniform corrosion, pitting corrosion, crevice corrosion, stress corrosion cracking, intergranular corrosion, microbially influenced corrosion, dry-air oxidation, hydrogen embrittlement, as well as the effects of wet and dry cycles, material aging and phase stability, welding, and initial defects on the degradation modes for the engineered barriers.

- For those degradation processes that the TSPA abstraction indicates are significant to the performance of the engineered barriers, DOE provides appropriate parameters based on techniques that may include laboratory experiments, field measurements, industrial analogs, and process-level modeling studies conducted under conditions relevant to the range of environmental conditions within the WP emplacement drifts. DOE also demonstrates the capability to predict the degradation of the engineered barriers in laboratory and field tests.

- The description of geological and engineering aspects of design features, physical phenomena, and couplings that may affect mechanical disruption of engineered barriers is adequate. For example, the description may include materials used in the construction of engineered barrier components, environmental effects (e.g., temperature, water chemistry, humidity, radiation, etc.) on these materials, and mechanical failure processes and concomitant failure criteria used to assess the performance capabilities of these materials. Conditions and assumptions in the TSPA abstraction of mechanical disruption

of engineered barriers are readily identified and consistent with the body of data presented in the description.

- The TSPA abstraction of mechanical disruption of engineered barriers uses assumptions, technical bases, data, and models that are appropriate and consistent with other related DOE abstractions. For example, assumptions used for mechanical disruption of engineered barriers are consistent with the TSPA abstraction of degradation of engineered barriers. The descriptions and technical bases provide transparent and traceable support for the abstraction of mechanical disruption of engineered barriers.

- Engineered barrier mechanical failure models for disruption events are adequate. For example, these models may consider effects of prolonged exposure to the expected emplacement drift environment, material test results not specifically designed or performed for the YM site, and engineered barrier component fabrication flaws.

- Process-level models used to represent mechanically disruptive events within the emplacement drifts at the proposed YM repository are adequate. Parameter values are adequately constrained by YM site data such that the effects of mechanically disruptive events on engineered barrier integrity are not underestimated. Parameters within conceptual models for mechanically disruptive events are consistent with the range of characteristics observed at YM.

NRC Staff Evaluation

Modeling of TCP phase and LRO using Arrhenius relationships is acceptable if sufficient data are available. The activation energy value is reasonable if associated with the diffusion of Cr in the γ-phase matrix (Chen, et al., 1989; Pruthi, et al., 1977). Emphasis has been placed on long-term, low-temperature (T < 300 °C) precipitation rather than short-term, high-temperature TCP phase formation. The selection of the low-temperature emphasis is based on predictions of WP temperature after emplacement in the repository and the observation of few precipitates in the heat-affected zones of a welded sample and a welded and aged sample (427 °C for 40,000 hours). The evaluation of the effects of time and temperature on the phase stability of Alloy 22 is in line with the methodology presented in the TSPA-VA (U.S. Department of Energy, 1998b). The present modeling approach (CRWMS M&O, 2000b,h) is consistent with the previous investigations on the phase stability of Alloy 22 and other Ni-Cr-Mo alloys (Cieslak, et al., 1986; Raghavan, et al., 1982).

The precipitation of TCP phases is dependent on time, temperature, and alloy composition. Cold-work may also alter the phase stability of the alloy and the precipitation kinetics. Thin, welded specimens used in the DOE evaluation do not represent the dimensions of the final closure weld for the WP and, as a result, are likely to have substantially different thermal cycling and lower heat input compared to the actual WPs. In addition, the effects of heat-to-heat variations in alloy composition have not been evaluated. Precipitation of TCP phases in welds and thermally aged Ni-Cr-Mo alloys, including Alloy 22, are sensitive to the concentrations of Fe and W (Tawancy, 1996). Heat-to-heat variations have a significant effect on fracture toughness,

as measured by Charpy impact energy, of thermally aged Alloy 22 (Edgecumbe-Summers, et al., 1999).

Thermal aging is assumed to have an effect on the mechanical properties and corrosion resistance of the WPOB (CRWMS M&O, 2000b,h). Other failure modes, which may be enhanced by thermal aging such as increased HE susceptibility (Asphahani, 1977; Kane, et al., 1977; Sridhar, et al., 1980a,b) as a result of thermal aging at temperatures where ordering reactions and impurity segregation are known to occur, have not been addressed. However, these phenomena may not be so important in affecting performance.

Additional data and evaluations are necessary to properly model the effects of thermal aging on the intergranular and crevice corrosion susceptibility of Alloy 22 as discussed in Sections 5.1.2.3 and 5.1.3. The additional evaluations should include the effects of variations in base alloy composition, cold-work, and water chemistry. In addition, the effects of welding parameters such as welding method, heat input, joint geometry, number of passes, and weld filler metal composition must be considered.

The effect of thermal aging on fracture toughness parameters should be known to estimate the potential for mechanical failure of Alloy 22 containers. Mechanical failure of containers caused by disruptive effects has been partially considered in other IRSRs (i.e., RDTME, SDS, and IA).

5.2.2.2 Initial Defects in Alloy 22 Containers

Acceptance Criteria

- DOE uses appropriate methods for nondestructive examination of fabricated engineered barriers, the type, size, and location of fabrication defects that may lead to premature failure as a result of rapidly initiated engineered barrier degradation. DOE specifies and justifies the allowable distribution of fabrication defects in the engineered barriers and assesses the effects of defects that cannot be detected on the performance of the engineered barriers.

- Sufficient data have been collected on the geology of the natural system, engineering materials, and initial manufacturing defects to establish initial and boundary conditions for the Total System Performance Assessment abstraction of mechanical disruption of engineered barriers.

- Data on geology of the natural system, engineering materials, and initial manufacturing defects used in the Total System Performance Assessment abstraction are based on appropriate techniques. These techniques may include laboratory experiments, site-specific field measurements, natural analog research, and process-level modeling studies. As appropriate, sensitivity or uncertainty analyses used to support the DOE Total System Performance Assessment abstraction are adequate to determine the possible need for additional data.

NRC Staff Evaluation

As DOE acknowledged, despite a much more detailed analysis than before, most of the information is based on experience unrelated to WP fabrication and emplacement. Additionally, some sources and types of initial defects are not considered based on inadequate justification. While surface intersecting flaws are more important for SCC than completely enclosed flaws, the stress and strain localization from the latter may adversely affect SCC depending on the size and location of the flaw. Additionally, if one of the sources of defect is mis-heat treatment, the potential lowering of fracture toughness parameters due to precipitation of embrittling phases (μ-phase in Alloy 22), in combination with internal flaws and residual stresses, can cause mechanical fracture of the container. Therefore, internal flaws cannot be eliminated from consideration only on the basis of lack of cyclic loading. The poor weld joint design is eliminated as a source of defect because considerable testing is expected to be performed prior to actual WP fabrication. However, at present, there has been no trial fabrication of the current Alloy 22 WP design and, therefore, no experience in the proper joint design, especially for remote welding and post weld processes such as laser peening and induction annealing .

The low probability for the presence of surface intersecting weld flaws arises in part from an estimation of the probability of nondetection of flaws by ultrasonic methods. The probability estimates for UT inspection were derived from records of intergranular SCC of SS. These probability estimates need to be improved through focused UT investigations of various weldments of Alloy 22. Additionally, the inspectability of subsurface flaws of different orientations and morphologies needs to be considered. The inspectability of welds depends on a number of factors including grain size and orientation of defects. Estimation based on intergranular SCC of SSs may not yield a conservative bound on the probability of nondetection of flaws, especially subsurface flaws.

The only source of surface contamination considered appears to be postfabrication contamination (e.g., use of cleaning solvents, etc.). Prefabrication contamination is considered briefly in the AMR (CRWMS M&O, 2000l), but the consequence of this on WP corrosion is determined to be negligible. However, failures of SS and Ni-base alloy components can occur because of contamination (e.g., solvents, lubricants) prior to welding or thermal treatments. These defects can result in much more significant performance reduction than postfabrication surface contamination. Because, precipitation of primary carbides in Alloy 22 from carbonaceous materials cannot be easily dissolved by routine annealing operation, such defects can affect the performance even though they occur at a much earlier step in the fabrication of WP. These defects are not detectable by NDE techniques currently in use. Therefore, the probability of occurrence may have to be evaluated on the basis of human error probabilities.

The flaws that may arise from welding internal components to the container walls (e.g., thermal shunts, guides) are not evaluated. The defects that may arise from such internal welds include "heat-tint" effect (heat from internal welds may affect external surface microstructure) and generation of local residual stresses in the base metal. These defects may affect locally the structural integrity of the inner stainless steel container.

The consequence of initial defects on WP performance is evaluated only for SCC. However, depending on the type of defect and combination of defect sources (e.g., weld flaw and improper heat treatment), rapid mechanical failure may be possible and should be evaluated. Additionally, the effect of initial defect on disruptive failure (e.g., seismicity and rock fall) needs to be examined.

5.2.3 Status and Path to Resolution

This subissue is closed, pending additional information, DOE agreed to provide the necessary information to close the subissue at the time of submitting the LA. The path to resolution is based on DOE's presentation and the agreements reached in the NRC/DOE Technical Exchange and Management Meeting on CLST regarding this subissue. Any NRC concern not specifically covered in this section is dealt with a risk-informed approach (i.e., the concern may not be important in PA). The agreements summarized below are abstracted from the transcripts of the meeting.[5]

DOE agreed to provide information on the effect of the entire fabrication sequence on phase instability of Alloy 22, including the effect of welding thick sections, using multiple-weld passes and the proposed induction annealing process. DOE has stated that the aging studies will be expanded to include solution-annealed and induction-annealed Alloy 22 weld and base metal samples from the mock-ups, as well as laser peened thick, multipass welds. The information will be included in the revision of the AMR titled Aging and Phase Stability of Waste Package Outer Barrier (ANL-EBS-MD-00002) prior to LA. This AMR will include data on microstructural characterization, testing of tensile properties, and Charpy impact tests performed on aged (welded and nonwelded) samples of Alloy 22. Theoretical models, using thermodynamic principles of the process, will be used for the DOE to enhance confidence in the extrapolation of kinetic data on thermal aging to repository thermal conditions and time scale. In addition, aging at temperatures lower than 300 °C will be studied experimentally.

DOE agreed to provide information on the effect of rockfall and seismicity on mechanical failure. Rockfall evaluations will include the potential embrittlement of the WP closure weld material after stress annealing caused by aging and multiple rockfalls. The information will be included in the next revision of the AMR titled Design Analyses for UCF Waste Packages (ANL-UDC-MD-000001) to be completed prior to LA. Point loading rockfall analysis will be documented in the next revisions of the AMR titled Design Analysis for the Ex-Container Components (ANL-XCS-ME-000001) and in ANL-UDC-MD-00001. In the latter document, the technical basis for the mechanical integrity of the inner overpack closure weld will be provided. The DOE has stated that the mechanical analysis of WP failure addressing seismic excitation is consistent with the design basis earthquake covered in the SDS KTI.

DOE will provide information on the effect of initial defects in failure of closure welds. Definition and implementation of process qualifications and control (material procurement, inspection, NDE,

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[5]Schlueter, J., Letter (October 4) to S. Brocoum, U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Key Technical Issue: Container Life and Source Term (ML003760868). Washington, DC: U.S. Nuclear Regulatory Commission. 2000.

etc.) will be described in detail. Documentation will be provided for the fabrication processes, controls, and implementation of the phases that may affect the TSPA model assumptions (e.g., filler metal, composition range, etc.). Updates of the documentation on the fabrication processes and controls titled Waste Package Operations Fabrication Process Report (TDR-EBS-ND-000003) and Waste Package Operations FY-00 Closure Welds Technical Guidelines Document (TDP-EBS-ND-000005) will be available to the NRC in January 2001.

5.3 SUBISSUE 3: THE RATE AT WHICH RADIONUCLIDES IN SPENT NUCLEAR FUEL ARE RELEASED FROM THE ENGINEERED BARRIER SUBSYSTEM THROUGH THE OXIDATION AND DISSOLUTION OF SPENT FUEL

The DOE basecase design calls for emplacing 70,000 MTHM of waste, consisting of 63,000 MTHM of CSNF, 2,600 MTHM of DSNF, and 4,400 MTHM (equivalent) of vitrified HLW (CRWMS M&O, 1997). The DSNF will be placed in the same overpack as the HLW glass WF, called codisposal packages. There will be 7,860 CSNF WPs and 3,910 codisposal packages (CRWMS M&O, 2000c). The DSNF has been grouped into 12 categories, including the ceramic Pu WF for the purposes of PA (CRWMS M&O, 2000c). Most of the DSNF is metallic fuel in the form of U or U alloyed with Pu, Th, Al, C, or Si. Of the DSNF other than the U.S. Navy fuel, the N-reactor fuel from Hanford, which is metallic U, constitutes about 84 percent of these fuels in terms of MTHM. The radionuclide inventory of DSNF is small compared to that of CSNF, and most of the DOE's PAs conducted on these fuels to date has shown small dose contribution from these fuels in comparison to CSNF (Duguid, et al., 1997).

Eight major components are used by DOE to assess the performance of WFs in the repository (CRWMS M&O, 2000c,f), as shown in Table 3. The NRC CLST IRSR, Revision 2 (U.S. Nuclear Regulatory Commission, 1999c), addressed the performance of WFs in Subissue 3 pertaining to SNF (including CSNF and DSNF) and Subissue 4 pertaining to HLW glass. In Subissue 3, eight components were identified. While there are differences between the DOE and NRC classifications of the WF performance subissues, the components identified by NRC are being addressed by DOE in their PMR on WF as well as the supporting AMRs. The DOE component related to in-package chemistry is evaluated in detail in the NRC IRSR on the evolution of near-field environment. However, because of the intimate connection between in-package environment and radionuclide release, this component will be examined in this IRSR from the point of view of consistency in the assumed parameters for calculating in-package chemistry with parameters used for calculating CSNF dissolution rate. The NRC component related to dry-air oxidation of the CSNF has not been addressed by DOE in detail because of DOE design changes leading to lower anticipated fuel temperatures. The DOE component of HLW glass dissolution will be examined as part of Subissue 4 in this IRSR.

The following NRC model abstractions apply to this subissue:

- ENG3 Quantity and Chemistry of Water Contacting the WPs and WFs
- ENG4 Radionuclide Release Rates and Solubility Limits

Table 3. Relationship between the U.S. Department of Energy components of waste form process model report and the U.S. Nuclear Regulatory Commission components of spent nuclear fuel and high-level waste glass performance subissues

Components of U.S. Department of Energy Waste Form Process Model Report	Components of Nuclear Regulatory Commission Subissue 3 on Spent Nuclear Fuel	Components of Nuclear Regulatory Commission Subissue 4 on High-Level Waste Glass
Radionuclide inventory	Radionuclide inventory and distribution	High-level waste glass dissolution
In-package chemistry	Dry-air oxidation of the spent nuclear fuel	Effects of colloids and microbes
Commercial spent nuclear fuel degradation rate	Dissolution in aqueous environments	Radionuclide transport in the engineered barrier system
Commercial spent nuclear fuel cladding degradation	Cladding performance	—
U.S. Department of Energy owned spent nuclear fuel degradation rate	Secondary mineral formation and coprecipitation	—
High-level waste glass degradation rate	Formation of colloids	—
Radioisotope dissolved concentration (solubility)	Solubility of radionuclides	—
Radioisotope colloidal concentration	Conceptual models for release	—

5.3.1 Description of the U.S. Department of Energy Approach

The description of the DOE approach in the following sections is based on the WF Degradation PMR and supporting AMRs. In the NRC/DOE Technical Exchange and Management Meeting on CLST[6], DOE agreed to provide additional information through revised AMRs or other documents before or at the time of the LA, as described in detail in Section 5.3.3.

[6]NRC/DOE Technical Exchange and Management Meeting on the Key Technical Issue: Container Life and Source Term, Las Vegas, NV, September 12–13, 2000.

5.3.1.1 Radionuclide Inventory

Radionuclide inventory is used for two purposes: (i) in a radionuclide screening evaluation to determine which radionuclides should be tracked for the TSPA calculations and (ii) as input to the TSPA calculations to determine the fuel heat generation rates and the release rates of radionuclides. The DOE accounts for the radionuclide inventories in CSNF assemblies, DSNF canisters, and defense HLW (DHLW) canisters (CRWMS M&O, 2000c). Fuel assembly characteristics such as burnup, enrichment, and cooling time for CSNF are derived from a 1995 data submittal from the commercial utilities that supplied historical information about reactor assembly discharges through December 1995 and forecasts about future discharges. Based on these average fuel assembly radionuclide inventories, the DOE derived a representative WP for both CSNF WPs and codisposal WPs, which contains both DSNF and DHLW. This representative WP inventory was developed based on a weighted average of the radionuclide inventories for all potential WP loadings.

Radionuclide screening was performed to ensure all radionuclides that could contribute significantly to the dose were tracked in the TSPA. This screening was performed by summing the product of the inventory of a radionuclide in a representative WP and the inhalation or ingestion dose conversion factor (DCF) for all radionuclides. The radionuclides that made up the upper 95 percent of this sum were screened into the analysis. This screening process will be conducted at times between 100 and 10,000 years for the TSPA-SR analyses and up to 1,000,000 years for the final environmental impact statement analyses (CRWMS M&O, 2000ff). Also, the process was repeated for subgroups of radionuclides based on their solubility and transport properties. Radionuclides were divided into two solubility groups (soluble and insoluble) and three transport groups (highly sorbing, mildly sorbing, and nonsorbing). This categorization is performed to identify the important radionuclides for the nominal release scenario, IA scenario, and the human intrusion scenario.

5.3.1.2 In-Package Chemistry

Integral to the CSNF and DSNF dissolution rate calculations is the estimation of the in-package environment. To estimate the in-package environment, the assumption is made that the composition of water dripping into the WP is similar to J-13 water, and the drip rate ranges from 0.0015 m^3/yr to 0.15 m^3/yr (CRWMS M&O, 2000i). The dripping water is assumed to enter and exit the WP at the same rate and not interact to any significant degree with the WP walls as it enters the WP. However, the dripping water is assumed to react uniformly with the Type 316L SS inner overpack and the internal contents of the WP, including the borated SS neutron absorbers, A 516 steel baskets, aluminum alloy thermal shunts, and the fuel pellets. No interaction between the Zircaloy cladding and the internal environment is assumed, although sensitivity analyses include the percentage of fuel area exposed by breached cladding. The water is assumed to fill the void volume (estimated to be 4,511 L for CSNF WP), and the WP internal components are lumped into equivalent masses per unit volume for calculating the reaction products. EQ6 is used to calculate the time evolution of solution composition as a result of these interactions (CRWMS M&O, 2000i). The assumed ranges of dissolution rates for this calculation for some of these components are shown in Table 4, along with calculated current

Table 4. Rates of various reactions assumed for in-package chemistry (CRWMS M&O, 2000q)

Waste Package Component	U.S. Department of Energy Molar Dissolution Rate ($mol/cm^2 \cdot s^1$)	n	Current Density (A/cm^2)
Type 316 Stainless Steel	2.53×10^{-14} to 2.53×10^{-13}	2.24	5.7×10^{-9} to 5.7×10^{-8}
Type 316 Stainless Steel/B	1.169×10^{-14} to 1.169×10^{-13}	2.24	2.53×10^{-9} to 2.53×10^{-8}
A516 Steel	8.706×10^{-12} to 2.487×10^{-11}	2	1.7×10^{-6} to 4.8×10^{-6}
Al	2.28×10^{-13}	3	6.6×10^{-8}
Commercial Spent Nuclear Fuel	$4.42 \times 10^{-14} + 10^{-10.59-0.5\,pH}$	2	—

densities. The current densities were calculated from the assumed molar dissolution rates using Faraday's law as follows:

$$i\left(\frac{A}{cm^2}\right) = R\left(\frac{mol}{cm^2}\cdot s\right) \times n \times F \tag{10}$$

where, i is the current density, R is the molar reaction rate, n is the equivalent net charge transfer during the dissolution, and F is the Faraday's constant.

The dissolution rate used for CSNF (Table 4) was derived by fitting the dissolution rate data of Grambow (1989) at pH < 9 with a rate of 4.42×10^{-14} $mol/cm^2 \cdot s$ at higher pHs.

In this approach, the pH decrease inside the WP occurs because of the dissolution of SS components, specifically the chromium oxidation to soluble Cr(VI) species. The pH increases due to the dissolution of the SNF. Therefore, the pH change in the WP is abstracted (CRWMS M&O, 2000c,q) using a linear regression expression of the form

$$pH = a_n - b_n \log(f_{clad}) + c_n q_{seep} \tag{11}$$

where a_n, b_n, c_n , are constants depending upon the WP failure time, waste type, and assumed corrosion rate of WP components, f_{clad} is the area fraction of cladding failed, and q_{seep} is the assumed flux of water entering the WP. Because the pH in Eq. (11) is directly related to water flux, a limit was placed on the pH as a function of water flux, so that as the water flux exceeded a

limiting value dependent on the failure time and type of WP, the pH attained a value of 8.1 corresponding to that of J-13 water.

DOE recognizes some of the limitations of the in-package chemistry calculations in the WF PMR and the complexities in considering the geometrical effects (CRWMS M&O, 2000c). The assumption that the WP void volume is completely filled with water and the reactions occur between an equivalent lumped mass of WP components and this water without any feedback between corrosion and chemistry is cited as a conservative approach. DOE discounts the possibility of formation of NO_2 and nitric acid by radiolysis because of the buffering capacity of the corrosion products from the WP components and the possible outgassing of NO_2 from the breached WP. DOE believes that the neglect of evaporative effects is conservative because the higher amount of water will lead to greater leaching of radionuclides. However, it is recognized that neglecting the formation of saline solutions by evaporation may be nonconservative for the dissolution rate of the WF.

5.3.1.3 Commercial Spent Nuclear Fuel Dissolution Rate

The CSNF dissolution rates have been measured using a wide range of techniques, including flow-through experiments using SNF and UO_2 pellets, static tests in autoclaves, and unsaturated drip tests with SNF pellets contained in Zr holders (see Section 4.3.6). However, only the data from the flow-through tests are used to derive the dissolution rate model for PA (CRWMS M&O, 2000c,j). Two regression equations are used in DOE's latest abstraction of CSNF dissolution rate in the WF PMR (CRWMS M&O, 2000f).

For pH > 7

$$\text{Log(Rate)} = 4.69 - \frac{1085}{T} + 0.12\log_{10}[CO_3]_{Total} + 0.32\log_{10}[P_{O_2}] \qquad (12)$$

For pH ≤ 7

$$\text{Log(Rate)} = 7.13 - \frac{1085}{T} + 0.32\log_{10}[P_{O_2}] - 0.41\text{pH} \qquad (13)$$

where the rate is expressed in $mg/m^2 \cdot day$, T is the absolute temperature in K, carbonate concentration is in moles/liter, and oxygen partial pressure is in atmospheres. The abstracted equations are derived such that the rates from the two equations are equal at pH 7. The burnup in these tests ranged from 0 to 50 Mwd/KgU.

It must be noted that Eq. (12) is an empirical regression model that is only loosely based on irreversible thermodynamic reasoning (Stout and Leider, 1998a,b). The regression coefficient, adjusted R^2, for the high pH equation is 0.5014 (CRWMS M&O, 2000j), indicating the model does not represent a significant portion of the experimental data. A more elaborate model, with cross terms and a term involving burnup, was proposed by Stout and Leider (1998a,b) and exhibited a much better statistical fit to data (adjusted $R^2 = 0.8174$).

Equation (13) is derived by assuming that the dependence of dissolution rate on oxygen partial pressure and temperature is the same at pH values below 7 as it is above this pH. The term involving carbonate is neglected based on the reasoning that surface adsorption of carbonate ions is negligible below this pH. Additionally, one experimental data point at pH 3 and the calculated rate at pH 7 from Eq. (12) are used to derive the slope of the pH dependence for pH values between 3 and 7. The model is then compared to other rate measurements and found to predict higher rates than the experiments, thus justifying its use as a "bounding" model.

Unsaturated drip tests have been performed during the past 8 years. The tests involve SNF contained in Zircaloy holders exposed to dripping water or moist environment. The drip rates used, 0.0078 L/year to 0.078 L/year, are much lower than those assumed in the in-package calculations (1.5 to 150 L/year). The drip rates used should scale to surface area of reacting media exposed. Based on 1 cm^2 of fuel surface, the low end of the drip rate would correspond to about 8 cm/year of dripping. However, this scaling relationship is at present poorly understood—it may depend on the manner in which dripping contacts the fuel (Wronkiewicz, et al., 1992). The release rate of various radionuclides are monitored. The release rates of ^{99}Tc and ^{90}Sr are used to derive the intrinsic dissolution rate of the SNF (CRWMS M&O, 2000c,n). The dissolution rates measured in the high drip rate tests are close to that predicted by Eq. (12) if a surface roughness factor of 3 is assumed in the drip tests (CRWMS M&O, 2000j). This result is surprising because, unlike the flow-through tests used to derive Eq. (12), the drip tests encourage corrosion product formation and would be expected to yield lower dissolution rates. The low drip rate tests exhibited lower dissolution rates. The drip tests show that ^{237}Np and ^{239}Pu are retained in the corrosion product after an initial period of high release (CRWMS M&O, 2000c).

5.3.1.4 U.S. Department of Energy Spent Nuclear Fuel Dissolution Rate

The DSNF has more than 250 potential WF types for disposal. These types were grouped into 16 categories based on similar performance characteristics (CRWMS M&O, 1998b). Performance analyses of the first 13 categories indicated only categories 1, 4, 5, 6, 8, and 11 contributed significantly to dose, and the dose from a composite of 13 categories was about two orders of magnitude below that of the CSNF in the repository. Based on these analyses, the TSPA-VA analyses used a surrogate DSNF with a radionuclide inventory based on a weighted average of the inventories of categories 1, 4, 5, 6, 8, and 11. A conservative assumption was built into the surrogate model by using a dissolution rate based on the U metal fuel dissolution model. The metallic SNF dissolution rate is faster than the rate for the nonmetallic fuels.

For the TSPA-VA, the model for the degradation of metallic fuel was an Arrhenius kinetic equation using parameters derived from assessments of SNF and HLW (Rechard, 1995). The model is based on the equation

$$M = Ae^{-B/T}(t_2^c - t_1^c)D \cdot E \cdot SA \qquad (14)$$

where

M	— mass of layer corroded in a time step (kg)
A	— Arrhenius-type preexponential term (kg/m^{2}s)
B	— Arrhenius-type activation energy term (K)
T	— temperature (K)
t_2 and t^1	— time at the beginning and end of the time step in seconds
c	— time dependence term
E	— oxygen concentration dependence term
SA	— surface area of the layer (m^2)
D	— saturation dependence term, which is 0, 1, or $1-e^{-\alpha(Sat-TS)}$

where

α	— ln $(0.01)/(S_{99} - TS)$
Sat	— fracture water saturation
TS	— threshold fracture saturation below which wet corrosion does not occur
S_{99}	— fracture saturation where the wet corrosion rate is 99 percent of the corrosion rate at 100-percent saturation

When the temperature in the repository is below 100 °C, water was assumed to be present on the WF (wet oxidizing conditions), and humid-air conditions are assumed at all other times.

In the TSPA-SR, DOE will consider 12 groups of SNF (CRWMS M&O, 2000c). In the TSPA-SR methods and assumptions report (CRWMS M&O, 1999a), DOE notes there were little applicable experimental data to substantiate the parameter values selected for the TSPA-VA, and the TSPA-SR will use a degradation rate and a corresponding effective surface area that bounds the experimental data on N-Reactor fuel collected by the DOE during a range of conditions in the last few years. In the WF PMR, three types of dissolution models are proposed for each fuel type: (i) upper-limit models that assume complete dissolution of the fuel occurs at any time step after breach of the container and all radionuclides are available for instantaneous release; (ii) conservative models that use the higher end of the dissolution rate data or where no data are available consider a multiplier of data for a similar fuel, and (iii) best estimate models that are constructed from a reasonable database of the specific fuel type.

For the TSPA-SR, upper limit model for each fuel type is used, except for the U.S. Navy fuel, (CRWMS M&O, 2000c). Alternatively, the N-reactor fuel is used as the surrogate for all DSNF fuel and the conservative or best basis models for this fuel is used to represent all DSNF, including the U.S. Navy fuel. The best estimate dissolution rate for the N-reactor fuel is given by

$$\text{Rate}\left(\frac{\text{mg}}{\text{m}^2\text{day}}\right) = 1.75 \times 10^5 \left(\frac{D_{\text{matrix}}}{D_{\text{U-metal}}}\right) \tag{15}$$

where, D_{matrix} is the density of the SNF matrix and $D_{\text{U-metal}}$ is the density of the U metal.

The conservative model is 10 times the above value. The DSNF AMR was withdrawn by DOE and reissued recently. Therefore, an evaluation of this AMR is not included in this IRSR revision. A review of this AMR is necessary to fully understand the technical bases for the dissolution model used. While the U.S. Navy fuel is considered bound by either the CSNF or the N-reactor fuel, the dissolution rate data on this fuel are not publicly available. Therefore, the inclusion of this fuel in the DSNF bounding case using N-reactor fuel is tentative, pending further information. However, use of the upper limit model does not require further experimental data.

5.3.1.5 Radionuclide Solubility

For the TSPA-VA, and also for the TSPA-SR, the DOE approach to calculate bounds on the aqueous concentration of radionuclides in groundwater that reacted with the WF is to initially derive the concentrations from the WF dissolution model. Subsequently, a comparison is made between the WF dissolution-based aqueous radionuclide concentration and a value determined thermodynamically by the solubility limit for each radionuclide considered. If the solubility-limited value is lower for a given radionuclide than its concentration derived from the WF dissolution, the aqueous concentration is set to the solubility-limited value and the difference in mass is assumed to precipitate out of solution. The solubility-limited values place constraints on the aqueous concentration of the particular radionuclide element considered with each isotope of that element present in proportion to its isotopic abundance (CRWMS M&O, 1998b).

The concentration limit usually is the solubility limit of the solid phases that contains the radioisotopes (either solid phases with the radioisotope as the dominant element or solid phases with trace amounts of the radionuclide, as in coprecipitated species). For one radioelement (neptunium), the DOE claims that oversaturation and undersaturation experiments indicate lower concentrations in solution compared to literature values. The solid phases that form depend on the temperature, redox conditions, and chemical composition of the groundwater. Because of uncertainty in the precise values for these variables in the WP and near-field environment, there is a wide range of possible radionuclide concentration limits.

For the TSPA-VA, the distribution of each radioisotope transported was primarily based on an elicitation of experts both inside and outside the YMP conducted in 1993 (Wilson, et al., 1994; U.S. Department of Energy, 1998c). The assumptions behind the expert panel's development of the distributions are (i) the unsaturated zone water composition is bounded by the composition of J-13 well water and that of UE-25p#1, (ii) the solubility limits will be determined by the far-field groundwater environment, (iii) the environment is oxidizing, and (iv) future climate changes will cause groundwater compositional changes. Additional sources were used to further constrain distributions of solubility limits for the radionuclides used in the TSPA-VA analysis. Also, the solubility-limited concentration distribution for Np used in previous TSPA calculations was revised based on an analysis by Sassani and Siegmann (1998).

For the TSPA-SR, the dissolved concentration limits calculation builds upon three primary feeds: (i) estimates of in-package fluid chemistry (pH, Eh, ionic strength, and carbonate concentration), (ii) measured (and estimated) thermodynamic parameters describing the stabilities of aqueous species and solid radioisotope phases, and (iii) a determination of the likely solubility controlling

phases for the radionuclides of concern (CRWMS M&O, 2000c). The DOE approach to estimate in-package fluid chemistry is discussed in Section 5.3.3.1.1.1. For the TSPA-SR analysis, pure phases were chosen because, in general, they yield higher dissolved concentrations compared to coprecipitated phases. The specific phase selected for a particular radionuclide is based on information from geologic and experimental observations or crystallochemical arguments. Where no information can be gleaned from field or experimental observations, the most amorphous and hydrated form of the radionuclide believed to be the most soluble was selected. For U, schoepite was assumed to be the solubility controlling phase. For Np, Pu, Am, and Ni, the solubility controlling solids chosen were Np_2O_5 [or $Np(OH)_4$(am) under reducing conditions], $Pu(OH)_4$(am), $AmOHCO_3$, and NiO, respectively.

The amount of thermodynamic data available for the different radionuclides, the sensitivity of the solubilities to fluid chemistry, and the importance of the different radionuclides to total system performance is uneven. Thus, the DOE used three approaches to implement solubility limits within the TSPA-SR analysis: (i) multi-termed functions of chemistry for U, Np, and Am; (ii) distributions for Pu, Pa, Pb, and Ni; and (iii) constant bounding values for Tc, I, Th, Cs, Sr, Cl, C, Nb, Zr, Ra, and Sn. The concentration of U for the TSPA-SR analysis was calculated using an equation fit to EQ3NR-derived schoepite solubility as a function of pH, CO_2 fugacity, and temperature. The solubility of Np for the TSPA-SR analysis was calculated from a pH-dependent equation. A log-uniform distribution was assigned for Pu solubility, with a minimum of 1.0×10^{-9} and a maximum of 1.9×10^{-4} mol/L, based on EQ3NR calculations of $Pu(OH)_4$ solubility at pH 8 and a range of Eh and CO_2 fugacity. An equation with pH and CO_2 fugacity terms was used to calculate Am concentrations for the TSPA-SR analysis, and the solubilities of Ac, Cm, and Sm were assumed identical to that of Am. The solubilities of Tc, C, Cl, I, and Cs were set to 1.0 mol/L, which lets the waste inventory control their release, because no solubility limiting solids are predicted to form for these radioelements. The solubility of Sr was also set to 1.0 mol/L to simplify the analysis. A log-uniform distribution was proposed for Ni solubility with a minimum of 1.4×10^{-6} and a maximum of 3.1 mol/L. However, the solubility of NiO (assumed to be the solid phase determining the solubility) is expected to be orders of magnitude lower than this value. The value noted in the PMR is probably a calculation or typographic error. For Pb solubility, a log-uniform distribution was recommended for the TSPA-SR with a minimum of 1.0E-10 and a maximum of 1.0×10^{-5} mol/L. In the case of Pa solubility, a log-uniform distribution was recommended, with a minimum of 1.0E-10, a maximum of 1.0×10^{-5}, and a mean of 3.2E-8 mol/L. Constant values of 1.0×10^{-7}, 2.3×10^{-6}, 5.0×10^{-8}, 1.0×10^{-5}, and 6.8×10^{-10} mol/L, respectively, for the solubilities of Ni, Ra, Sn, Th, and Zr were recommended (CRWMS M&O, 2000c).

The DOE recognizes that inherent limitations in the database lead to uncertainties in calculated solubilities. However, these limitations are claimed to lead to only a factor of two uncertainty when the ionic strength exceeds about 0.7 M. The DOE claims this uncertainty is small relative to other uncertainties within the system. Also, the DOE made improvements in its calculation of dissolved concentration limits compared to the approach taken for the TSPA-VA in response to concerns expressed by the TSPA peer review panel. For example, the thermodynamic data for Np were thoroughly reviewed, and a regression model was developed such that the solubility limit could be coupled to the estimated in-package chemical environment (CRWMS M&O, 2000n).

Also, formation of U secondary phases that could potentially incorporate Np and reduce Np solubility was not incorporated into the DOE abstraction of dissolved concentration limits because experiments studying this mechanism were not conclusive. The distributions of Pu, Th, and Ni were carefully reevaluated taking into account expected in-package chemical conditions. Also, solubility limits for other key radionuclides (Tc, I, C, Nb, Zr, Pa, Pb, Ra, Sn, Cs, and Cl) were reevaluated and fixed at bounding values. According to the DOE, the solubility values determined by informal expert elicitation conducted in 1993 (Wilson, et al., 1994) were used only to corroborate the newly evaluated distributions and fixed values (CRWMS M&O, 2000c).

5.3.1.6 Colloidal Release

The discussion of colloidal release from HLW glass under Subissue 4 (Section 5.4) provides details on the DOE colloid source term abstraction, which is presented in a preliminary version of AMR F0115 (CRWMS M&O, 2000k). For HLW glass, the abstraction includes both reversible and irreversible radionuclide attachment to colloids. In contrast, the abstraction for SNF WFs includes only reversible attachment (CRWMS M&O, 2000c), due to limited laboratory evidence for generation of WF colloids during SNF corrosion (CRWMS M&O, 2000p). In every other respect, the discussion in Subissue 4 (Section 5.4) is relevant to SNF WFs, and the reader is directed there for a complete discussion.

5.3.1.7 Degradation of Zircaloy Cladding in Commercial Spent Nuclear Fuel

DOE has developed a model to evaluate cladding degradation as part of the WF degradation model (CRWMS M&O, 2000c) to determine the rate at which the CSNF is exposed to in-package environment. This model represents a significant improvement with respect to that presented in the TSPA-VA (U.S. Department of Energy, 1998c). The degradation of the CSNF cladding is assumed to occur in two stages. The first stage corresponds to rod failure as a result of perforation of the cladding. The second stage is due to the progressive exposure of the SNF matrix as a result of splitting (unzipping) the cladding due to oxidation of the irradiated UO_2 pellets either by air and moisture or by an aqueous environment.

Cladding perforation may occur prior to or after WP emplacement. The initial condition of the cladding and the percentage of rods perforated are evaluated taking into account data obtained from reactor operation, pool storage, dry storage, and transportation, including fuel handling (CRWMS M&O, 2000t). A distribution of initially perforated Zircaloy fuel rods expressed as a complementary cumulative distribution function was developed from the available data. All the CSNF cladded with SS instead of Zircaloy (assumed to be ~1.1 percent of the total) was assumed to be initially perforated (CRWMS M&O, 2000t).

DOE used an empirical creep model developed by Matsuo (1987) to define the creep damage in Zr cladding upon disposal. DOE computed the creep strain as a function of initial rod stress for cladding in dry storage alone and dry storage with transportation, using an assumed temperature history profile that is representative of dry storage, and transportation conditions (CRWMS M&O, 2000t). DOE concluded that little creep occurs for rod stresses less than 80 MPa. It is assumed that most of the creep occurs during the dry storage whereas only a small amount of creep

occurs during transportation. The amount of creep strain accumulated is expected to be less than 1 percent at initial stresses less than 90 MPa (at 27 °C). A creep failure strain of 3.3 percent was established based on experimental data of tensile and creep tests. This creep failure strain led to a prediction of approximately 0.24 percent for rod failure by creep in dry storage and transportation, compared with an actual failure rate of 0.45 percent (CRWMS M&O, 2000t).

Cladding perforation after WP emplacement is assumed caused by creep, SCC, mechanical failure due to seismic events, and localized corrosion. To evaluate the possibility of creep and SCC under disposal conditions, the temperature history of the cladding during storage and transportation and the evolution of temperature after WP emplacement were estimated, as well as distribution of internal pressure and corresponding hoop stresses (CRWMS M&O, 2000t). The Murty's creep-versus-strain correlation was selected on the basis of experimental data for unirradiated cladding to evaluate creep rupture because it is claimed Murty's creep is more adequate for modeling cobble creep, a type of creep important at low stress and temperature. The approach is considered conservative because irradiated cladding has a creep rate significantly lower than that of the unirradiated material. Nevertheless, the criterion for creep failure strain was developed based on data for irradiated cladding and is conservative with respect to other creep failure criteria. On the basis of the distribution of hoop stresses, an abstraction is developed to provide the fraction of rods that failed by creep as a function of the peak WP surface temperature as a controlling variable.

SCC was also considered in the distribution of hoop stresses. The causative species for SCC is considered to be iodine, above a certain critical concentration, as a fission product found free in the pellet-cladding gap. Although the iodine concentration is asserted to be negligible, conservatively it is assumed to be above the critical value. A critical stress level of 180 MPa is selected as a threshold stress for SCC to occur, which is a relatively high value to be attained by more than a few rods.

Local corrosion is also considered as a process leading to the perforation of the CSNF cladding. Fluoride is assumed to be the anionic species promoting accelerated corrosion on a relatively small area of cladding (about 10 mm of rod length). The fraction of fuel cladding surface on different fuel rods inside the same WP is proportional to the volume of water entering the WP in a flow-through scenario. This approach is considered to be a bounding analysis because it is implicitly assumed a 100-percent efficiency in the chemical reaction of fluoride with Zircaloy.

The DOE analysis of delayed hydride cracking is based on a fracture mechanics approach in which the cladding stress and crack depth were used to compute the mode I stress intensity factor of pre-existing cracks in the cladding (CRWMS M&O, 2000t). The stress intensity factor, K_I, was taken to be the driving force for delayed hydride cracking and compared against the threshold stress intensity factor, K_{IH}. Failure by delayed hydride cracking is considered not to occur when K_I is lower than K_{IH} but it can occur when K_I is higher than K_{IH}. An extensive review of literature data by the DOE (CRWMS M&O, 2000t) indicated that the minimum reported value of K_{IH} for Zr cladding is 5 MPa$\sqrt{m}$. Delayed hydride cracking of existing cracks in cladding was analyzed by the DOE using distributed stresses and crack sizes (CRWMS M&O, 2000t). It was concluded that delayed hydride cracking can be ruled out as a possible mechanism for cladding

failure of SNF in the repository because the computed mean K_I value was too low (0.0016 to 2.7 MPa·m$^{1/2}$ range).

Failure of cladding by hydrogen or hydride embrittlement, delayed hydride cracking, and hydride reorientation were screened out by DOE as possible events in the repository (CRWMS M&O, 2000dd). DOE considered that stresses and temperatures of the cladding are too low for hydride orientation to occur and that the cladding material would maintain sufficient strength even if hydride reorientation did occur such that cladding failure would be unlikely.

The remaining process leading to perforation of the cladding is mechanical failure due to seismic events when frequency is of the order of 1×10^{-6}/yr. This type of event perforates the cladding and initiates unzipping. It is considered that rockfall will not lead to mechanical failure of the cladding with the argument that collapse of the WP takes hundreds of thousands of years to occur.

After cladding perforation, the inventory of radionuclides in the gap and in the grain boundaries of the irradiated fuel pellets is considered to experience fast release. The gap inventory of iodine and cesium is predicted to be release in proportion to the fission gas release fractions, while that in the grain boundaries is estimated from released experiments using intact and defective (i.e., with slits and holes) fuel rod samples. Cumulative distribution function for the fast release fraction of the radionuclides is used in the model abstraction.

The time to unzip a fuel rod under dry and wet conditions is estimated as a function of WP temperature. For weight unzipping, time is also a function of the in-package chemistry, that for this purpose is defined in pH, partial pressure of O_2, and CO_3^{2-} concentration. Although it is considered that the criteria are conservative and include the consideration of uncertainties, it is argued the criteria are not so conservative as in previous TSPAs.

5.3.2 Staff Evaluation of the U.S. Department of Energy

5.3.2.1 Radionuclide Inventory

Acceptance Criteria

- Total System Performance Assessment adequately incorporates important design features, physical phenomena, and couplings and uses consistent and appropriate assumptions throughout the radionuclide release rates and solubility limits abstraction process.

- The Total System Performance Assessment abstraction on radionuclide release rates and solubility limits provides sufficient, consistent design information on WPs and engineered barrier systems. For example, inventory calculations and selected radionuclides are based on the detailed information provided on the distribution (both spatially and by compositional phase) of the radionuclide inventory within the various types of HLW.

NRC Staff Evaluation

Nine radionuclides were selected for detailed analyses in the TSPA-VA based on their high solubility, low-sorption affinity (including potential for colloid transport), large inventory, high DCF, and long half-life. However, there was no transparent methodology in the selection of these radionuclides similar to the one described in the Inventory Abstraction AMR for the TSPA-SR. This clear description of the screening process used to identify important radionuclides is an improvement in the transparency of the TSPA. Also, consideration of important radionuclides for the human intrusion and igneous event scenarios in the inventory abstraction AMR is an improvement in the comprehensiveness of the analysis.

The TSPA-VA accounted for the effect of chain decay on the important radionuclides in the following manner. For important radionuclides having parents with shorter half-lives not modeled in the TSPA, the TSPA-VA assumed that the entire inventory of the parent had decayed to the daughter radionuclide and added this quantity to the initial quantity of the radionuclide. For important radionuclides having parents with longer half-lives not modeled in the TSPA, the TSPA-VA assumed that the daughter was in secular equilibrium with the parent at all times. Although this methodology appears reasonable, it is not clear how radionuclides further up the decay chain, such as Cm-245, which decays to Pu-241, which is the parent of Am-241, will be accounted for in the inventory of important radionuclides. Also, it is not clear if this method or another method will be used in the TSPA-SR to account for chain decay leading to the buildup of important radionuclides.

Finally, the TSPA-VA included analyses to determine if the radionuclides screened from the calculations would have a significant effect on the results of the analysis. It is not clear if the TSPA-SR will include a similar analysis.

Because the technical documents describing the calculations of inventories for the different waste types are not available, no evaluation can be made on the methods, computer codes, and data sources used to derive the inventories of radionuclides in the WPs. The approach appears to account for all waste types that will be emplaced in the repository and seems complete in this regard.

There are several concerns about the methodology used for screening radionuclides. First, the product of the inventory and the inhalation and ingestion DCFs for the radionuclide are not directly related to the risk that the radionuclide poses to the critical group, even when the solubility and transport properties in the geosphere of the radionuclide are accounted for. Processes that affect transport in the biosphere, such as uptake by plants and bioaccumulation, are not accounted for using this methodology. Also, the direct exposure pathway is not accounted for by this approach. Thus, radionuclides for which ground shine constitutes a significant exposure pathway, such as Nb-94 and Sn-126, could be inappropriately screened using this methodology.

Second, the grouping of radionuclides based on solubility and transport properties appears to be too broad. Dividing the radionuclides into only two groups of solubility classes and three groups of transport classes can lead to the grouping of radionuclides that do not really behave similarly

under repository conditions and the masking of potentially important radionuclides. For example, ^{79}Se, which has been screened from the analysis, is grouped in the soluble and moderately sorbing transport group. This group also contains elements such as Np and U, which have significantly larger DCFs than Se. However, Se is more soluble than Np and U by several orders of magnitude and also is transported much more quickly than Np and U (U.S. Department of Energy, 1998c). Thus, Se could pose a much greater risk to the critical group than Np or U, especially at early times, but be screened from the analysis. Also, there does not seem to be any proposed methodology to investigate the effect of certain radionuclides such as Se-79 that have been identified in previous DOE and NRC TSPAs as important, but have not been identified as important using the proposed methodology.

Finally, the inventory abstraction AMR does not indicate how radionuclides not considered important to performance in themselves, but that generate daughter products important to performance, will be accounted for.

DOE should consider a method to determine the importance of radionuclides that incorporates the effects of biosphere transport and all exposure pathways to ensure that no important radionuclides are screened. One possible method to account for these factors would be to use the product of the average biosphere DCF and the inventory as the screening criteria rather than the product of the inhalation and ingestion DCFs from FGR-11 (Eckerman, et al., 1988) and the inventory. These biosphere DCFs would be the dose to an average member of the critical group from a unit concentration of radionuclide in the groundwater or on the ground surface, as could be derived from the GENII-S code (Napier, et al., 1988) and would incorporate biosphere transport and all significant pathways to exposure of the critical group.

DOE should consider segregating the radionuclides into smaller groups to determine the importance of radionuclides on performance. Radionuclides with several orders of magnitude difference in solubility or retardation in the unsaturated or saturated zones should not be grouped together as a relatively mobile radionuclide with a smaller DCF could be hidden by a less mobile radionuclide, which may not be transported quickly enough to affect the critical group during the compliance period.

DOE should include analyses in the TSPA-SR to determine whether radionuclides screened from the analysis could have a significant effect on performance, particularly for those radionuclides that have been identified as important to performance in other TSPAs. Alternatively, DOE could include all radionuclides that are present in the waste at repository closure to ensure that all significant radionuclides are included in the TSPA.

5.3.2.2 In-Package Chemistry

Acceptance Criteria

- Sufficient technical bases and justification are provided for Total System Performance Assessment assumptions and approximations for modeling coupled thermal-hydrologic-mechanical-chemical effects on seepage and flow, the WP chemical environment, and

the chemical environment for radionuclide release. The effects of distribution of flow on the amount of water contacting the WPs and waste forms are consistently addressed in all relevant abstractions.

- The DOE reasonably accounts for the range of environmental conditions expected inside breached WPs and in the engineered barrier environment surrounding the WP. For example, DOE should provide a description and sufficient technical bases for its abstraction of changes in hydrologic properties in the near field due to coupled thermal-hydrologic-mechanical-chemical processes.

- Sufficient data have been collected on the characteristics of the natural system and engineered materials to establish initial and boundary conditions for conceptual models and simulations of thermal-hydrologic-chemical coupled processes. For example, sufficient data should be provided on design features such as the type, quantity, and reactivity of materials that may affect radionuclide release for this abstraction.

- The corrosion and radionuclide release testing program for HLW WFs intended for disposal provides consistent, sufficient, and suitable data for the in-package and in-drift chemistry used in the abstraction of radionuclide release rates and solubility limits. For expected environmental conditions, DOE provides sufficient justification for the use of test results not specifically collected from the Yucca Mountain site for engineered barrier components such as HLW WFs, drip shield and backfill.

- Alternative modeling approaches of FEP are consistent with available data and current scientific understanding and consider the results and limitations appropriately in the abstraction.

NRC Staff Evaluation

DOE described the general design features associated with the EDA II design of the WP in the WF degradation PMR (CRWMS M&O, 2000c). The quantities of the various WP components assumed in their calculations are identified in the associated AMR (CRWMS M&O, 2000i) that at this time is not approved by DOE. The couplings to other models, such as the drift-scale thermohydrology models, are described briefly in the PMR. The assumptions regarding the flux of water entering the WP, chemistry of water, void volume in the WP, and reactions with various WP components are delineated clearly. The analysis method (EQ3/6) and code modifications are described in the AMR (CRWMS M&O, 2000i).

As shown in Table 4, the dissolution rate assumed for Type 316 SS and the borated SS is one order of magnitude lower than measured experimentally. Additionally, the lower dissolution rate assumed for the borated SS compared to Type 316 SS is counterintuitive. The presence of boron, in the form of second-phase particles of borides, would be expected to result in a higher corrosion rate, especially in local zones around the boride particles. Better technical bases for these assumptions need to be provided.

The in-package chemistry and the dissolution rate of SNF are influenced by the flux of water entering the WP and its chemical composition. However, the quantity of water assumed to drip into the WP for calculating the in-package chemistry is 2 to 3 orders of magnitude greater than the drip rate of water used in experimental studies conducted at ANL. The drip rate used may scale with the surface area or mass of fuel. However, this scaling relationship is poorly understood at present and may depend on how the water spreads across the SNF surface exposed. While the ANL test results are not used for TSPA model abstraction, and the rate of fuel dissolution is not used in calculating the in-package chemistry, the ANL test results are used to confirm model abstractions and increase the confidence in the assumptions used for WF degradation models. The chemical composition of the water, in particular the concentration of anions such as Cl^- and F^-, is important in the localized corrosion and SCC of the cladding.

The rate of dissolution of CSNF (Table 4) used to calculate the in-package environment is significantly different than the rate of dissolution used for calculating radionuclide release [Eqs. (11) and (14)]. However, Eq. (14) is proposed as a conservative upper bound for acidic dissolution because its predicted dissolution rate was higher than that reported by Grambow and others (CRWMS M&O, 2000j).

Radiolysis could have complex effects on the release of radionuclides from SNF (Shoesmith and Sunder, 1992; Christensen, et al., 1994; Christensen and Bjergrakke, 1987). In aqueous solution, radiolysis produces oxidizing species such as hydrogen peroxide (H_2O_2), hydroxyl radical (OH), and perhydroxyl radical (HO_2), and reducing species such as hydrated electron (e^-), hydrogen atom (H), and hydrogen molecule (H_2) (Spinks and Woods, 1990). In an air-water-vapor system, nitrogen fixation products (nitrogen acids, nitrogen oxides, and ammonia) would also be formed in addition to the radiolytic products formed in the aqueous system (Burns, et al., 1982; Reed and Van Konynenburg, 1987; Willis and Boyd, 1976).

In DOE's analyses (CRWMS M&O, 2000c), gamma radiolysis effect was neglected on the basis that the radiation level in the WP would not be significant after about 1,000 years and the probability of breach is quite low before 1,000 years. For the dissolution of (UO_2) SNF, the effects of gamma and alpha radiation have been extensively studied in aqueous solutions (Shoesmith, et al., 1985; Shoesmith and Sunder, 1992; Christensen, 1991; Christensen, et al., 1994; Christensen and Bjergrakke, 1987). Shoesmith, et al. (1997) conducted experiments in aerated noncomplexing solutions and in aerated carbonate solutions under gamma irradiation conditions. They concluded that the effect of gamma irradiation becomes insignificant below ~1 to ~10 Gy/h. In a more recent review, Shoesmith (1999) predicted that the gamma radiolysis effect on fuel dissolution rate will be negligible after a few hundred years on the basis that the gamma would decay to an insignificant level (below 1 ~ 10 Gy/h).

Sunder, et al. (1997) conducted experiments on the oxidation of UO_2 SNF in aqueous solution by the products of alpha radiolysis of water. They predicted that the corrosion of SNF, supported solely by the alpha radiolysis of water, could be significant for periods of ~2000 years for the enriched PWR SNF. Corbel, et al. (2000) also found that the release of U in aerated water is strongly enhanced by alpha irradiation. Shoesmith (1999), however, recently predicted that the alpha radiolysis will have no significant effect on fuel corrosion and can be ignored. This is

because the conditions at YM will be perpetually aerated and the oxidizing products produced by the alpha radiolysis may not have significant impact on the redox conditions. On the other hand, Shoesmith (1999) did caution that the influence of alpha radiolysis in tight wet cracks in the fuel remains to be determined.

The unsaturated drip tests with SNF (CRWMS M&O, 2000n; Stout and Leider, 1998a,b; Finch, et al., 1999) may have indicated the effects of radiation on the dissolution rate of U fuel in the moist-air system by the fact that the overall leaching rate of radionuclides is higher with the higher burnup fuel than with the lower burnup fuel. However, the conditions for the unsaturated tests were not designed to study the effect of irradiation; the parameters related to radiation effects, such as dose rate, air-to-water volume ratio, and air partial pressure were not controlled. After the failure of the WP, the effect of alpha, gamma, and beta irradiation on the dissolution of U fuel in humid air may still be significant. DOE needs to assess the effect of alpha, gamma and beta radiation on SNF in the humid-air environment after the failure of the WP as a confirmative measure.

DOE assumed that the outer overpack, Alloy 22, does not react with the dripping water and, therefore, does not affect the in-package chemistry. The other WP components are assumed to dissolve uniformly such that they can be lumped into a single mass for purposes of chemical calculations. The Cr in the SS is assumed to dissolve in its hexavalent form. While this assumption is conservative, lumping all the components into a single mass for estimating the chemistry may lead to highly nonconservative estimates of pH values. For example, the lowest pH in the EQ-6 calculations is approximately 3.6 (CRWMS M&O, 2000i). This assumption, while it simplifies calculations of in-package chemistry, needs further justification.

At issue is the spatial variation in chemistry that is likely to occur in the WP and likely to result in local pH values considerably more acidic than calculated based on a volume averaged mass. The pH in crevices and other tight spaces differs from bulk pH values because the dissolution reactions become spatially separated from the reduction reactions. Alternative models that consider the electrochemical reactions coupled to transport processes should be considered. For example, Cavanaugh, et al. (1983) reported that the pH values in corroding cavities of SS range from 0 to 2, with the pH increasing with increasing Mo and decreasing Cr concentration. The pH in crevices of Al alloys can be either acidic (pH 4) or alkaline (pH 9) depending on the initial pH and surface condition (Holroyd, et al., 1987). Therefore, the pH generated by localized dissolution of Al would be most likely influenced by the pH resulting from the corrosion of other components. Because the internal geometry of the WP will have many tightly packed regions, local pH may affect the dissolution rate of fuel locally and, hence, the local release rate of highly soluble radionuclides such as ^{99}Tc.

The abstractions for in-package environment are derived from the detailed process level model that used the EQ3/6 code. The predictions of this code have not been verified by empirical observations. DOE recognized the difficulties in modeling the detailed effects of geometry and corrosion reactions on the in-package chemistry. Because the corrosion reactions of metallic materials and SNF are electrochemical in nature, a lumped-mass chemical reaction approach, such as that embodied in EQ-6 code, may not be adequate. Detailed reactive transport models

that incorporate electrochemical reactions, while more appropriate for this case than the EQ3/6 code, can be difficult to implement in a system that consists of multiple materials and geometries. Experiments to simulate certain aspects of WP geometry and materials may aid in gaining confidence in the model abstractions.

Based on the information, NRC considers the component pertinent to the DSNF closed. This is because of the small effect on dose even assuming an upper-limit model. NRC considers the CSNF dissolution rate component to be closed pending additional information outlined next.

DOE recognized the difficulties in conducting detailed modeling of the in-package chemistry due to the complexities in materials and geometry. However, the lumped-mass calculation performed using EQ6 may not provide a conservative bound for the in-package chemistry. Local acidification may result from spatially separated anodic and cathodic regions that may enhance the dissolution rate of fuel and the solubility of radionuclides. Additionally, better technical bases are needed for the dissolution rates of various components used in in-package chemistry calculations.

Because of the complexity of interactions of the incoming water with WP components, experimental confirmation of model predictions may be necessary. While there will be issues regarding the ability of experiments to adequately represent all the complexities in a WP, experiments may increase confidence in model abstractions.

5.3.2.3 Commercial Spent Nuclear Fuel Dissolution Rate

Acceptance Criteria

- Total System Performance Assessment adequately incorporates important design features, physical phenomena, and couplings and uses consistent and appropriate assumptions throughout the radionuclide release rates and solubility limits abstraction process.

- The DOE reasonably accounts for the range of environmental conditions expected inside breached WPs and in the engineered barrier environment surrounding the WP. For example, DOE should provide a description and sufficient technical bases for its abstraction of changes in hydrologic properties in the near field due to coupled thermal-hydrologic-mechanical-chemical processes.

- Technical bases for inclusion of any thermal-hydrologic-mechanical-chemical couplings and FEP in the radionuclide release rates and solubility limits model abstraction are adequate. For example, technical bases may include activities such as independent modeling, laboratory or field data, or sensitivity studies.

- In considering alternative conceptual models for radionuclide release rates and solubility limits, DOE uses appropriate models, tests, and analyses that are sensitive to the processes modeled for both natural and engineering systems. Conceptual model

uncertainties are adequately defined and documented and effects on conclusions regarding performance are properly assessed. For example, in modeling flow and radionuclide release from the drifts, DOE represents significant discrete features such as fault zones separately, or demonstrates that their inclusion in the equivalent continuum model produces a conservative effect on calculated performance.

- The models implemented in this Total System Performance Assessment abstraction provide results consistent with output from detailed process-level models and/or empirical observations (laboratory and field testings and/or natural analogs).

NRC Staff Evaluation

A key hypothesis of the TSPA-VA (CRWMS M&O, 1997) and in the preliminary calculations of TSPA-SR was that the SNF intrinsic dissolution rate determined the aqueous release of highly soluble radionuclides and the rate of SNF alteration to form secondary minerals and colloids. The product of the intrinsic dissolution rate and the wetted surface area provided the source term for radionuclide transport through the unsaturated zone. Whereas the intrinsic dissolution rates derived from flow-through tests were used by DOE as input to the release of radionuclides in the TSPA-VA (CRWMS M&O, 1997), the drip test results from ANL were used to estimate the retention of certain highly soluble radionuclides (e.g., Cs) in the secondary minerals. The rate of secondary mineral formation was assumed to be proportional to the intrinsic dissolution rate of the SNF. In the TSPA-VA, the chemistry of the water reacting with the SNF was not assumed to be affected by reaction with WP components.

The abstraction for CSNF dissolution rate considers the pH, total carbonate, oxygen partial pressure, and temperature. A significant improvement in the TSPA-SR modeling of WF dissolution is the consideration of in-package chemistry alteration by reaction with WP components. The detailed design features of WPs are considered in developing the abstractions of in-package chemistry, which are then used to calculate the CSNF dissolution rate and radionuclide solubility. As mentioned, the in-package chemistry calculations should be supported by empirical observations and more detailed process-level models. The abstractions do not explicitly consider the interactions between various WP internal components and SNF. SNF because of its hyperstoichiometry, is a p-type semiconductor and, hence, capable of sustaining electrochemical reactions. This means that galvanic interactions between cladding and fuel, and basket materials and fuel and others need to be evaluated.

The CSNF degradation component considers the in-package chemistry abstraction and temperature to calculate the dissolution rate. The flux of water entering the WP does not directly affect the dissolution rate, but affects the in-package chemistry through the abstracted model [Eq. (12)]. The fuel burnup is also not considered directly in the abstracted model, although a variety of burnups was used in the flow-through tests. The abstracted model for CSNF dissolution was consistent with models proposed by the expert elicitation panel. The unsaturated drip test data are not used in the dissolution rate model abstraction, but the high drip rate data were indicated to be consistent with the flow-through data. This is surprising because the drip tests have an ill-defined hydrodynamics and cannot be said to be free of transport limited

reactions, unlike the flow through tests. It is possible that the drip test results are influenced by (i) the method of dissolution rate calculation, which uses ^{99}Tc concentration; (ii) periodic sloughing off of secondary minerals which may accelerate dissolution; and (iii) galvanic interactions with Zr casing, that may increase the corrosion potential of the SNF. The secondary minerals observed in the drip tests have been correlated to the minerals found in the natural analog site at Peña Blanca (Pearcy, et al., 1994).

The CSNF dissolution rate abstraction in the TSPA-SR considers the effect of various WP internal components through the in-package chemistry abstraction. However, the multiple linear regression model used for dissolution rate in the TSPA-SR [Eqs. (13) and (14)] are more simplified than the expression used in the TSPA-VA, although both were based on high flow rate data. Possibly because some of the factors, such as burnup, are ignored in the TSPA-SR abstraction, the statistical fit of the abstractions used is poor (adjusted $R^2 = 0.5014$) for the alkaline environments. The statistical significance of the abstraction for the acid environment is difficult to estimate because it is based on only two data points, one of which is a calculated value. Because the in-package environment can be acidic, at least locally, SNF dissolution rate model in acidic environment should be improved.

The dissolution rates used in the model abstraction, which are considered to be bounding values, appear to be consistent with those measured in the high drip rate tests. However, the drip rate, even in the high drip rate tests, is 2 to 3 orders of magnitude lower than the drip rates used in the in-package chemistry calculations. The scaling relationship between the drip rates used in small-scale experiments and actual SNF surface exposed is not well understood (Wronkiewicz, et al., 1992). The drip rates used in the in-package chemistry calculations are in general agreement with the bounding calculations of flow through the DS (CRWMS M&O, 2000c). Because drip rate can have an important effect on the measured dissolution rates, the model may not represent a bounding value of the dissolution rate. Additionally, the model is based on tests that do not consider the electrochemical interactions between cladding and fuel.

In the DOE modeling of CSNF dissolution, an alternative conceptual model, using an electrochemical approach (Shoesmith, 1999), is considered. It is shown that the calculated dissolution rate is consistent with the dissolution rates measured in electrochemical tests. The linear regression model developed in the abstraction is loosely based on irreversible thermodynamics. However, the model does not explicitly consider the effect of potential on the dissolution rate. In an electrochemical model, the corrosion potential of the CSNF will be dictated by the anodic and cathodic reactions occurring not only on the SNF surface but also on the surface of cladding in contact with the fuel. The corrosion potential will be determined by summing the anodic and cathodic currents to zero (zero charge condition). This corrosion potential will then determine the dissolution rate through a Butler-Volmer or a Tafel relationship (Shoesmith, 1999). The purely chemical models are incapable of considering the electrochemical coupling between Zircaloy cladding and the SNF. Therefore, an electrochemical model should be explored further.

The model abstraction used for CSNF dissolution rate in the TSPA-SR is based on experimental measurements. The flow-through experiments used to derive the model are considered to be

bounding because the dissolution process is not limited by transport of species, corrosion products, or back reactions. However, the flow-through tests does not adequately simulate the geometries and material interactions that can occur in the WP. The flow-through experiments also does not correspond to natural analogs because of the lack of secondary minerals in the former. However, it is expected that the secondary minerals would lower the dissolution rate.

The technical bases for the dissolution rate model abstraction should be strengthened, especially in the acidic regime. The interactions between SNF and cladding or other WP components need to be considered to verify if the abstracted model, based on flow-through experiments, are conservative.

The effect of alpha radiolysis in humid environments should be explored to determine if the formation of oxidizing, acidic environments can lead to higher corrosion rates than predicted by the model based on flow-through experiments.

5.3.2.4 Radionuclide Solubility

Acceptance Criteria

- Where DOE uses data supplemented by models to support abstraction of solubility limits, the anticipated range of proportions and compositions of phases under the various physicochemical conditions expected are supported by experimental data (U.S. Nuclear Regulatory Commission, 1984).

- Parameter values, assumed ranges, probability distributions, and bounding assumptions used in the abstractions of radionuclide release rates and solubility limits in theTSPA are technically defensible and reasonable based on data from the YM region, laboratory tests, and natural analogs. For example, parameter values, assumed ranges, probability distributions and bounding assumptions adequately reflect the range of environmental conditions expected inside breached WPs.

- Uncertainty is adequately represented in parameter development for conceptual models, process models, and alternative conceptual models considered in developing theTSPA abstraction of radionuclide release rates and solubility limits, either through sensitivity analyses or use of bounding analyses.

- The models implemented in this TSPA abstraction provide results consistent with output from detailed process-level models and/or empirical observations (laboratory and field testings and/or natural analogs).

NRC Staff Evaluation

In its review of the DOE TSPA-VA, staff commented that the solubility limits need to be reevaluated by the DOE as the water chemistry inside the WP becomes better known (U.S. Nuclear Regulatory Commission, 1999c; 2000b). For the TSPA-SR, the DOE plans to

reevaluate the radioisotope solubility limits. The distribution of concentration limits will be based on a range of chemical conditions that takes into account the design of the EBS, fluid flow rates, and thermal history of the repository. Information presented in the DOE TSPA-SR methods and assumptions report (CRWMS M&O, 1999a) indicates that an in-drift geochemical environment model is being developed to determine the changes in water chemistry resulting from the interaction of EBS materials with water seeping into the drift and to provide this information to TSPA analyses. Specifically, an in-package chemistry submodel is being developed that will provide a quantitative description of the combined effects of important chemical interactions that can occur between aqueous seepage entering the WP and materials in the package, including WP internals, corrosion products, and WF. Staff agrees the DOE should use the range of water chemistries calculated from the in-package chemistry model to determine the distribution of solubility limits for the important radionuclides.

The DOE has stated in the TSPA-SR methods and assumptions report that the lower range of solubility-limit probability distribution function for Np may be revised to incorporate the observation that ^{237}Np concentrations in SNF experiments are much lower than would be predicted through pure phase equilibrium calculations if the experimental evidence is sufficiently defensible. Staff previously noted (U.S. Nuclear Regulatory Commission, 1999c) that the DOE needs to provide experimental confirmation of the solid Np compounds assumed to be in equilibrium with the dissolved Np species in these experiments. The updated thermodynamic data for calculating the solubility of various Np compounds is provided in the Pure Phase Solubility Limits AMR (CRWMS M&O, 2000n).

Radionuclide-bearing solid-phase solubility depends on the chemical environment, which, in turn, can be affected to varying degrees by numerous FEP. Staff review of the FEP database (U.S. Department of Energy, 1999) indicated that 50 are relevant to the DOE abstraction of dissolved radionuclide concentration limits. In the absence of the DOE AMRs on FEP for near-field environment (N0080) and in WF FEP screening (F0185), it is not clear which FEP the DOE has considered in its abstraction and analysis of radionuclide concentration limits. Staff will review the AMRs pertinent to solubility and to dissolved concentration limits to determine which FEP were included in the DOE abstraction of solubility limits, and if those FEP have been incorporated adequately. For those FEP that have not been included in the abstraction and analyses, the DOE will need to provide adequate justification for their exclusion.

As planned, the DOE should incorporate the results from ongoing SNF corrosion tests in deciding whether to include irreversible radionuclide attachment in the colloid abstraction for SNF. These tests should employ methods similar to, or more rigorous than, those that helped identify radionuclide-bearing, WF-generated colloids in HLW glass tests. If the DOE does not alter the abstraction, it should provide a technical argument that exclusion of irreversible attachment will not neglect a potential means for increasing radionuclide concentrations. Additional information is also required regarding Np solubility and uncertainties in the thermodynamic data, as well as the effect of coprecipitation.

5.3.2.5 Colloidal Release

Acceptance Criteria

The DOE colloid source term abstraction was assessed with respect to the five generic AC (U.S. Nuclear Regulatory Commission, 2000a).

NRC Staff Evaluation

The overall staff evaluation of the DOE colloid source term abstraction is discussed in Section 5.4. With respect to SNF WFs, an additional comment is necessary. The WF degradation PMR acknowledges that the assumption of only reversible attachment of radionuclides on colloids during SNF corrosion is "potentially nonconservative and remains to be verified when results from ongoing tests become available" (CRWMS M&O, 2000c). Exclusion of irreversible attachment can potentially result in an underestimate of the concentration of colloid-associated radionuclides released from SNF. This assumption is not yet sufficiently supported with respect to potential effects on repository performance.

5.3.2.6 Degradation of Zircaloy Cladding on Commercial Spent Nuclear Fuel

Acceptance Criteria

- Important design features such as WP design and material selection, backfill, drip shield, ground support, thermal loading strategy, and degradation processes, are adequate to determine the initial and boundary conditions for calculations of the quantity and chemistry of water contacting WPs and WFs.

- The expected range of environmental conditions within the WP emplacement drifts, inside of breached WPs, and contacting the WFs and their evolution with time are identified. These ranges may be developed to include: (i) the effects of the drip shield and backfill on the quantity and chemistry of water (e.g., the potential for condensate formation and dripping from the underside of the shield), (ii) conditions that promote corrosion of engineered barriers and degradation of WFs, (iii) irregular wet and dry cycles, (iv) gamma-radiolysis, and (v) size and distribution of penetrations of WPs.

- Sufficient information to formulate the conceptual approach(es) for analyzing water contact with the drip shield, WP, and WFs is provided.

- The DOE reasonably accounts for the range of environmental conditions expected inside breached WPs and in the engineered barrier environment surrounding the WP. For example, DOE should provide a description and sufficient technical bases for its abstraction of changes in hydrologic properties in the near field due to coupled thermal-hydrologic-mechanical-chemical processes.

- Sufficient data have been collected on the characteristics of the natural system and engineered materials to establish initial and boundary conditions for conceptual models and simulations of thermal-hydrologic-chemical coupled processes. For example, sufficient data should be provided on design features such as the type, quantity, and reactivity of materials that may affect radionuclide release for this abstraction.

- The corrosion and radionuclide release testing program for HLW WFs intended for disposal provides consistent, sufficient, and suitable data for the in-package and in-drift chemistry used in the abstraction of radionuclide release rates and solubility limits. For expected environmental conditions, DOE provides sufficient justification for the use of test results not specifically collected from the Yucca Mountain site for engineered barrier components such as HLW WFs, drip shield and backfill.

- The models implemented in this TSPA abstraction provide results consistent with output from detailed process-level models and/or empirical observations (laboratory and field testings and/or natural analogs).

NRC Staff Evaluation

DOE considers most of the forms of degradation that may affect the integrity of CSNF cladding under disposal conditions, as included in the AC. The cladding and SNF degradation rate and the solubility of radionuclides depend on the abstraction of in-package chemistry. DOE needs to establish better technical bases for the abstracted in-package chemistry.

In the analysis of both localized corrosion and SCC of cladding, the effect of chloride anions is not considered. In the case of localized corrosion, chloride is known to induce pitting corrosion as discussed in Section 4.3.2.8 and confirmed by recent studies (Greene, et al., 2000). The requirement is to reach a potential above the repassivation potential that can be attained easily in the presence of radiolysis products such as H_2O_2 or other oxidizing species. The same electrochemical and environmental conditions promote SCC in the presence of sufficiently high hoop stresses. A detailed discussion has been provided in one of the AMRs (CRWMS M&O, 2000u) questioning the occurrence of these corrosion processes induced by chloride under repository conditions.

In the WF PMR (CRWMS M&O, 2000c), the role of fluoride as a specie promoting accelerated corrosion in local areas is emphasized. However, the analysis of the flow and volume of water contacting the fuel rods to evaluate the local attack by fluoride is limited and requires additional justification. There are inconsistencies regarding the evaluation of the in-package pH because a low pH is assumed for the attack by fluoride whereas it is not taken into account the concentration in solution of Fe^{3+} ions that may promote the oxidizing conditions for the pitting in chloride solutions.

The possibility of SCC induced by iodine as discussed in the WF PMR (CRWMS M&O, 2000c) does not appear so important because it is limited essentially by the availability of iodine. The phenomenon as such has been postulated as the cause of pellet cladding interaction failure

under reactor operating conditions following steep power ramps, but it does not seem plausible under disposal conditions.

There is agreement with the approach adopted by the DOE to consider the potential for creep failure in dry storage and transportation that concurs with the DOE findings regarding the percentage of rod failure by creep, based on the representative temperature history profile.

In the assessment of hydride reorientation and delayed hydride cracking (CRWMS M&O, 2000t), the stress distribution reported for cladding is that corresponding to 27°C, which appeared to be the basis that led to the conclusion that the stress and temperature in the cladding were too low to cause hydride reorientation. There is a concern that the proper cladding stress might not have been used in the analysis. For hydride reorientation, the relevant stress to consider is the cladding hoop stress at temperatures just below the solvus temperature, which is in the range of 260-300 °C depending on the hydrogen content (Northwood and Kosasih, 1983). The peak cladding temperature for the design basis WP was estimated to be 325 °C (CRWMS M&O, 2000ee). This peak temperature is above the solvus temperature of hydrogen in Zircaloy-2 and Zircaloy-4. Consequently, some of the circumferential hydrides in Zircaloy cladding would dissolve into the matrix and subsequently reorient and reprecipitate as radial hydrides when they cool slowly below the solvus temperature in the repository. The DOE analysis of delayed hydride cracking was based on properties of Zircaloys that contain circumferential hydrides, which would not be applicable if hydride reorientation does occur. The prediction of the lack of potential for delayed hydride cracking based on a K_{IH} of 5 MPA·m$^{1/2}$ might not be conservative if hydride reorientation occurs in the cladding. Thus, it is important to consider the distribution of cladding stresses and temperatures and their evolution upon disposal in the repository.

The DOE analyses of delayed hydride cracking relied solely on a large crack fracture mechanics approach. No consideration was given to crack initiation at large hydrides. DOE discounted the importance of this failure event on the basis that this failure process can only occur for Zircaloy-4 cladding of PWR fuel assemblies with a burnup exceeding 55 MWd/KgU (CRWMS M&O, 2000ee). However, the percentage of PWR assemblies with burnup exceeding 55 MWd/KgU is about 15 percent (CRWMS M&O, 2000t). The possible failure rate of these high burnup fuel rods has not been considered.

This component of the subissue is closed, pending additional information because the models for cladding degradation have been improved substantially. The main limitations for the resolution of this component are related to the definition of the in-package chemistry, including Cl^- and F^- concentrations and pH (assuming realistic gradients in concentrations and redox conditions), as well as calculations of cladding temperatures, including the uncertainties related to spatial and temporal variations. These two aspects may have a significant influence in the distributions of failure times for cladding, in particular for high burnup of SNF.

5.3.3 Status and Path to Resolution

This subissue is closed, pending additional information. The path to resolution is based on the DOE's presentation and agreements reached in the NRC/DOE Technical Exchange and

Management Meeting on CLST regarding this subissue. Any NRC concern not specifically covered in this section is dealt with a risk-informed approach (i.e., the concern may not be important in PA). The agreements summarized below are abstracted from the transcripts of the meeting.[7]

DOE has stated that in the revision to the Summary of In-Package Chemistry for Waste Forms, AMR (ANL-EBS-MD-000050), to be available in January 2001, specific NRC questions regarding radiolysis, chemistry of incoming water, localized corrosion, corrosion products, and transient effects will be addressed. A sensitivity study on differing dissolution rates of components will also be included, as well as a more detailed calculation of the in-package chemistry effects of radiolysis, the effects of engineered materials on the chemistry of water used for input to in-package abstractions, and the applicability of abstractions for incoming water, taking into account the revised AMR on Environment on the Surfaces of the Drip Shield and Waste Package. DOE stated the current planning provides for the analysis of additional in-package chemistry model support. This analysis will determine which parts of the model are amenable to additional support by testing and which parts are more amenable to sensitivity analysis or use of analogues. Based on these results, if testing is determined to be appropriate, test plans will be written in FY2001 and made available to the NRC.

Regarding the failure rate of Zircaloy cladding, DOE agreed to provide additional technical bases for the failure rate and how the rate is affected by localized corrosion. DOE stated that the technical basis for local corrosion conditions will be included through an additional discussion of local chemistry in the revised Summary of In-package Chemistry for Waste Forms AMR (ANL-EBS-MD-000050). DOE stated that Current Clad Degradation Summary Abstraction AMR (ANL-WIS-MD-000007) and Clad Degradation–Local Corrosion of Zr and Its Alloys Under Repository Conditions AMR (ANL-EBS-MD-000012) contain the overall technical basis. DOE agreed to provide data to address chloride-induced localized corrosion and SCC under the environment predicted by in-package chemistry modeling. DOE stated that the technical bases for the models used for localized corrosion and SCC will be expanded in future revisions of the Clad Degradation Summary Abstraction AMR (ANL-WIS-MD-000007), to be available by LA.

DOE agreed to provide the technical basis for the critical stress relevant to the environment in which external SCC of Zircaloy cladding takes place. DOE stated that critical stress from SCC experiments under more aggressive conditions will be cited in the Revision of the Cladding Degradation Summary Abstraction AMR (ANL-WIS-MD-000007), which will be available in January 2001.

DOE agreed to provide updated documentation on the distribution of cladding temperature and hoop stresses, parameters that are critically important to evaluate the propensity to hydride reorientation and embrittlement. DOE stated that the stresses are documented in the Initial Cladding Conditions AMR (ANL-EBS-MD-000048), whereas a supporting document (CAL-UDC-

[7]Schlueter, J. Letter (October 4) to S. Brocoum, U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Key Technical Issue: Container Life and Source Term (ML003760868). Washington, DC: U.S. Nuclear Regulatory Commission. 2000.

ME-000001) contains the WP internal temperatures. WP surface temperatures were provided within the TSPA model (ANL-EBS-HS-000003, Rev. 00, ICN 01 and ANL-EBS-MD-000049). DOE indicated that it will provide updated versions of these documents in January 2001.

DOE agreed to provide analysis of the rockfall and vibratory loading effects on the mechanical failure of cladding, as appropriate. DOE stated that the vibratory effects are documented in Sanders, et al. (1992) SAND 90-2406, A Method for Determining the Spent-Fuel Contribution To Transport Cask Containment Requirements. This issue will be discussed in the DOE/NRC SDS KTI technical exchange. The analysis of the rockfall effects on the mechanical failure of cladding will be addressed if updated rockfall analyses, considered in subissues 1 and 2, demonstrate that the rock can penetrate the drip shield and damage the WP.

5.4 SUBISSUE 4: THE RATE AT WHICH RADIONUCLIDES IN HIGH-LEVEL WASTE GLASS ARE RELEASED FROM THE ENGINEERED BARRIER SUBSYSTEM

This section discusses the status of resolution with respect to the adequacy of the DOE consideration of the effects of degradation of HLW glass on repository performance, taking into account the rate of degradation and its effect on the rate of radionuclide releases from the EBS. The following model abstractions apply to this subissue:

- ENG3 Quantity and Chemistry of Water Contacting the WPs and WFs
- ENG4 Radionuclide Release Rates and Solubility Limits

5.4.1 U.S. Department of Energy Approach

The description of the DOE approach in the following sections is based on the WF Degradation PMR and supporting AMRs. In the NRC/DOE Technical Exchange and Management Meeting on CLST[8], DOE agreed to provide additional information through revised AMRs or other documents to or at the time of the LA, as described in detail in Section 5.4.3.

5.4.1.1 Glass Dissolution

The basic form of the rate expression adopted by DOE (CRWMS M&O, 2000c) to describe the dissolution of waste glass immersed in water is given by a form of transition state rate law as

$$\text{Rate} = S\left\{k_0 \bullet 10^{\eta \cdot \text{pH}} \bullet \exp\left(\frac{-E_a}{RT}\right) \bullet \left[1 - \frac{Q}{K}\right]\right\} \tag{16}$$

where

S — surface area of glass immersed in water, in units of area

[8]NRC/DOE Technical Exchange and Management Meeting on the Key Technical Issue: Container Life and Source Term, Las Vegas, NV, September 12–13, 2000.

k_o — intrinsic dissolution rate, which depends only on glass composition, in units of mass/(area•time)
η — pH dependence coefficient
E_a — effective activation energy, in units of kJ/mol
R — gas constant, which is 8.314 J/(mol•K)
T — absolute temperature in K
Q — concentration of dissolved silica in the solution, in units of mass/volume
K — a quasi-thermodynamic fitting parameter for glass equal to the apparent silica saturation value for the glass, in units of mass/volume

Equation (16) contains two main factors. The first factor is the forward rate, $k_o \bullet 10^{\eta \bullet pH} \bullet \exp(-E_a/RT)$, which represents the dissolution rate in the absence of concentration effects of dissolved silica (and other aqueous species), and the other factor is the reaction affinity term $1-(Q/K)$, which quantifies such effects. Because of the complexity in defining parameters and associated uncertainties, a simpler bounding approach was adopted that combined $1-(Q/K)$ with k_o, and the following abstraction was developed for aqueous degradation of HLW.

$$\text{Rate} = S\left\{k_{eff} \bullet 10^{h \bullet pH} \bullet \exp\left(\frac{-E_a}{RT}\right)\right\} \tag{17}$$

where

$$k_{eff} = k_o \bullet (1 - Q / K)$$

This reduces the abstracted model to an equation involving four parameters (η, E_a, S, and k_{eff}) and two variables (pH and T). The forward rate was measured in flow-through experimental conditions under which the affinity term can be maintained close to 1 due to the absence of concentration effects from the products of the glass dissolution. Test results indicated that the rate dependence on pH and temperature was independent of the glass composition, within the range of the glass compositions tested, and, therefore, the same values were used for all waste glasses. The pH dependence of log rate exhibited a V-shaped curve. The value of k_{eff} was determined through experimental observations. Several options were evaluated to conservatively bound the three stages of glass corrosion. Based on this evaluation, data from the PCT-A test were used to obtain bounding values for k_{eff}. The exposed surface area was estimated based on 20 times the surface area of the glass log and assuming all the surface available corrodes at the same rate when exposed to water. In addition, it assumes the surface area remains constant during the corrosion process.

Because of the discontinuity in the pH dependance of the log rate at intermediate pHs, separate rate expressions were obtained for the acid range and the alkaline range, as shown by Eqs. (18) and (19).

For the low pH range ($pH < pH_m$)

$$\frac{\text{Rate}}{S}(\text{gm}\cdot\text{m}^2/\text{day}) = 10^{(9\pm1)} \bullet 10^{(-0.6\pm0.1)\bullet pH} \bullet \exp\left(\frac{-58\pm10}{RT}\right) \tag{18}$$

For the high pH range ($pH \geq pH_m$)

$$\frac{\text{Rate}}{S}(\text{gm}\cdot\text{m}^2/\text{day}) = 10^{(6.9\pm0.5)} \bullet 10^{(0.4\pm0.1)\bullet pH} \bullet \exp\left(\frac{-80\pm10}{RT}\right) \tag{19}$$

where pH_m, the pH at which minimum dissolution rate occurs, is given by the following expression

$$pH_m = 2.1 + \frac{1149}{T} \tag{20}$$

where T is in K.

5.4.1.2 Colloidal Release

Colloidal radionuclide release from WFs is addressed in two AMRs—an AMR report describing the abstraction to be incorporated in DOE's TSPA, supported by a data AMR. This colloid release abstraction is limited to defining colloid-associated concentrations of certain radionuclides in water leaving the WP. No retardation in the WP is assumed, and transport outside the WP is not within the scope of the release model. For HLW glass, the abstraction allows for both reversible and irreversible radionuclide attachment to colloids. The abstraction AMR is discussed in detail, followed by brief comments on the supporting data AMR. The staff evaluation of this abstraction applies also to treatment of SNF WFs, with the exception that irreversible attachment was not included for SNF sources by DOE (see Sections 5.3.16 and 5.3.2.5 for comments specific to SNF colloid release).

DOE's abstraction of colloidal radionuclide release, as reported in a preliminary version of AMR F0115 (CRWMS M&O, 2000k), uses empirical data on release and colloid stability to formulate a dependence of colloidal radionuclide release on in-package ionic strength and pH. The report uses literature and YMP data to support its construction of an algorithm for calculating colloid-associated radionuclide concentrations in solutions leaving the WP. No credit is taken for colloid retardation within the WP. Direct inputs for conceptual models and parameters were obtained from YM P laboratory studies, as well as from a small number of literature sources. The abstraction takes output from in-package geochemical models and uses pH, ionic strength, and dissolved radionuclide concentration to calculate colloid concentrations, irreversibly colloid-bound radionuclide concentrations, and reversible colloid binding of radionuclides. The results are combined to provide a total colloid-associated source term for a given radionuclide; presently, the abstraction is applied only to Pu and Am, though the Am abstraction is incomplete. The abstraction classifies colloids as WF, groundwater (preexisting), or iron oxyhydroxide (from corrosion) colloids.

The following key inputs are used in the colloid release abstraction (CRWMS M&O, 2000k):

- solution ionic strength, pH, and radionuclide concentration from separate TSPA in-package geochemical calculations
- effect of ionic strength on water concentration of WF colloidal plutonium, including a maximum colloidal Pu concentration of 6×10^{-8} mol/L at ionic strength < 0.01 mol/L and a minimum of 1×10^{-11} mol/L at ionic strength > 0.05 mol/L; from data in an AMR (CRWMS M&O, 2000p)
- maximum stability limits for WF colloids as a function of pH, ranging from ionic strength of 0.01 mol/L at pH 2 to ionic strength of 0.05 mol/L at pH ≥ 6; based on montmorillonite data from Tombacz, et al. (1990) and on an AMR (CRWMS M&O, 2000p)
- maximum stability limits for iron oxyhydroxide colloids as a function of pH, ranging from ionic strength of 0.05 mol/L at pH < 6 and > 11 to a minimum ionic strength of 0.01 mol/L at pH 8–9; from Liang and Morgan (1990)
- relationship between ionic strength and mass of groundwater colloids, ranging between a minimum of 3×10^{-6} mg/L and a maximum of 3×10^{-2} mg/L; from the TSPA-VA technical basis document (CRWMS M&O, 1998b)
- range of distribution coefficients for reversible sorption onto colloids using literature and YMP laboratory data.

The order of calculation is as follows:

1. water concentration of radionuclide irreversibly sorbed to WF colloids, using ionic strength and pH,
2. mass concentration of WF colloids, using experimental relationship between concentrations of colloids and radionuclide irreversibly sorbed to them,
3. radionuclide reversibly sorbed to WF colloids, using distribution coefficient,
4. mass concentration of iron oxyhydroxide colloids, using ionic strength and pH,
5. radionuclide reversibly sorbed to iron oxyhydroxide colloids, using distribution coefficient,
6. mass concentration of groundwater colloids, using ionic strength,
7. radionuclide reversibly sorbed to groundwater colloids, using distribution coefficient, and
8. summed colloidal radionuclide concentration and summed colloid mass concentration output to exterior of WP.

AMR F0105 (CRWMS M&O, 2000o) describes literature data and YMP laboratory studies on colloid stability and colloid sorption of radionuclides, providing direct input to the abstraction AMR (CRWMS M&O, 2000k) in the form of a range of sorption coefficients, or K_ds, to be used in modeling reversible attachment of Pu to colloids. The K_ds were based on batch colloid sorption experiments at Los Alamos National Laboratory (LANL). This report has not yet been received in final form and is expected to be substantially revised.

This AMR includes an extensive discussion on literature relevant to reversible binding of radionuclides to colloids, including a discussion of kinetics, followed by a report on previously unavailable laboratory data on Pu and Am attachment to mineral colloids. The experiments were designed to observe adsorption and desorption rates, as well as the effect of colloid concentration. Dependence on pH and ionic strength of sorption onto colloids was not addressed. The key output to the abstraction AMR was a distribution of K_d values for Pu to be used in modeling reversible attachment. This approach appears valid, as long as sufficient uncertainty is applied to the K_d range to account for deviations of repository conditions from those in the laboratory. As mentioned previously, discussion of uncertainty applied to parameter ranges needs better attention in the abstraction AMR.

AMR F0110 (CRWMS M&O, 2000p) contains literature and previous ANL data from static- and drip-corrosion tests on HLW glass and SNF supporting a model of irreversible Pu colloid attachment used in the colloid source term abstraction AMR (CRWMS M&O, 2000k). The direct inputs to the adopted abstraction—all based on ANL work—are (i) a relationship between colloidal Pu concentration and ionic strength based on static HLW glass corrosion tests, (ii) effect of ionic strength on colloid stability, and (iii) a direct relationship between colloidal Pu concentration and colloid concentration. The adopted abstraction uses data only from the HLW glass tests, but SNF results were included in the development of a model in the ANL AMR that was used in the abstraction AMR as an alternative model.

5.4.2 Staff Evaluation of the U.S. Department of Energy Approach

5.4.2.1 Glass Dissolution

Acceptance Criteria

- The Total System Performance Assessment abstraction on radionuclide release rates and solubility limits provides sufficient, consistent design information on WPs and engineered barrier systems. For example, inventory calculations and selected radionuclides are based on the detailed information provided on the distribution (both spatially and by compositional phase) of the radionuclide inventory within the various types of HLW.

- The DOE reasonably accounts for the range of environmental conditions expected inside breached WPs and in the engineered barrier environment surrounding the WP. For example, DOE should provide a description and sufficient technical bases for its

abstraction of changes in hydrologic properties in the near field due to coupled thermal-hydrologic-mechanical-chemical processes.

- Technical bases for inclusion of any thermal-hydrologic-mechanical-chemical couplings and FEP in the radionuclide release rates and solubility limits model abstraction are adequate. For example, technical bases may include activities such as independent modeling, laboratory or field data, or sensitivity studies.

- Uncertainty is adequately represented in parameter development for conceptual models, process models, and alternative conceptual models considered in developing the Total System Performance Assessment abstraction of radionuclide release rates and solubility limits, either through sensitivity analyses or use of bounding analyses.

- DOE uses an appropriate range of time-history of temperature, humidity, and dripping to constrain the probability for microbial effects, such as production of organic by-products that act as complexing ligands for actinides and microbial-enhanced dissolution of the HLW glass form.

- The models implemented in this Total System Performance Assessment abstraction provide results consistent with output from detailed process-level models and/or empirical observations (laboratory and field testings and/or natural analogs).

NRC Staff Evaluation

The abstraction presented in the WF PMR (CRWMS M&O, 2000c) differs from that provided in the VA because it excludes the K_{long} term, which accounts for the long-term dissolution rate when Q/K reaches unity, in the rate expression by introducing a fixed value for the term 1-(Q/K). This eliminates the need of the term K_{long} and provides a more conservative estimate. In the model presented in the VA, the term 1-(Q/K) approaches zero as silica dissolution occurs.

Based on the review of the DOE abstraction of HLW glass degradation presented in the WF degradation PMR (CRWMS M&O, 2000c) and the AMR on degradation of HLW glass (CRWMS M&O, 2000v), the following comments are provided:

1. The coefficients for the effect of pH as a variable were obtained using Si dissolution rate data from a single-pass flow-through test in buffer solutions ranging from pH 1 to 13 conducted by Knauss, et al. (1990). It is not evident from the AMR (CRWMS M&O, 2000v) whether the release rate data used in the calculation represent release rates after initial exposure or after 7, 14, or 28 days of exposure time. This difference is critical to ensure that coefficients for all parameters used in the abstracted equation are determined on the same basis. A parameter such as k_{eff} is based on 7-day release rate data. In addition, it is assumed in the AMR (page 9, bullet #1) that B release rate can be used to provide an upper bound for the radionuclide release rate. The analysis for determining the coefficients for the pH dependence violates this assumption. While the B release rate was

Table 5. Independent verification of dissolution rate data

pH	Dissolution Rate (CRWMS M&O, 2000c)	Verification
7	3.6E–6	3.8E–05
8	9.1E–6	9.6E–05
9	2.3E–5	2.4E–04

used for calculating k_{eff}, the coefficients for the pH dependence were determined using the Si release rate.

2. The dissolution rates calculated on page 3-53 of the PMR (reproduced in Table 5) could not be reproduced with the Eqs. 3.6-4 and 3.6-5 of the PMR [or Eqs. (10), (19), and (20) of this report]. This inconsistency should be corrected.

3. The pH coefficients were determined using buffered solutions prepared with deionized water. The analysis ignores the presence of corrosion products from the dissolution of WP internal components such as FeOOH, $FeCl_2$, and $FeCl_3$ that could influence glass corrosion processes and, hence, the activation energy and the coefficients for the pH

   dependence. The β-FeOOH (akaganeite) can occlude significant concentration of chloride within its lattice structure.

4. The work of Advocat, et al. (1991), cited in the AMR for the effect of pH on release rate, indicates the presence of K ions on the surface of the corroded glass. Because the glass had no K , the presence of K ions is attributed to the ion exchange from KOH or KH_2PO_4 used for adjusting the pH of the solutions. The K ion, by virtue of its larger size, could lower the release rate from glass by retarding the migration of H ions in the glass matrix. Such comparisons could lead to erroneous conclusions.

5. DOE assumed that the release rate is independent of glass composition. At best, one can state that the intrinsic dissolution rate, k_o, can be represented as a bounding value of a distribution due to the expected variation in glass compositions. In addition, the coefficients for pH and E_a are assumed to be independent of glass composition. Again, pH and E_a values should bound the variability expected from glass compositions. This analysis is acceptable as long as it captures the expected variability in glass composition.

6. Long-term corrosion studies of HLW glasses indicate formation of secondary phases on the exposed surface of the HLW glasses. This process is dependent on the external environment. Long-term PCTs in J-13 water show formation of clay, Ca-phosphate, and (Th, U, Ca) titanate as secondary phases (Bates, 1998a), whereas the vapor hydration tests show accumulation of clay, zeolites, Ca-silicates, weeksite, and K-feldspar as secondary phases (Bates, 1998a). Formation of different phases under diverse test

conditions is attributed to varying solution chemistries. The formation of secondary phases may also be influenced by the corroding container materials. Secondary minerals play an important role in radionuclide release because they can incorporate low-solubility radionuclides, such as Pu and Am, and control their solubility limits. These minerals may also act to block the reactive surface area of the primary phase. The proposed abstraction model based on the available data, accounts for the release of radionuclides from the alteration phases.

7. Many studies and reviews have been reported on the effects of γ- and α-radiation on the dissolution or alteration of glass waste in the moist-air systems (Burns, et al., 1982; Wronkiewicz, et al., 1994, 1997). Wronkiewicz, et al. (1997) reported that although both γ- and α-radiation have no adverse effect on the dissolution of nuclear glass WF immersed in water in contact with air, the radiation exposure of the glass WF to humid air has resulted in a four to tenfold increase of alteration layer thickness relative to samples reacted without radiation exposure. Wronkiewicz suggested that the increases for the irradiated humid-air experiments appear to result from condensation of radiolytic acids into the thin film of water contacting the glass surface. The radiolytic acids increased the rate of ion exchange between the glass and the thin film of condensate, resulting in accelerated corrosion rates for the glass. This finding should be considered in DOE's model in the evaluation of the dissolution of glass WF because after the failure of the WP, the glass WF may be exposed to a thin film of water under dripping conditions, and the radiation dose rate from the long lasting alpha emitters in the glass WF still may be high enough to produce a significant effect. On the other hand, the radiolysis-induced nitric acid is a stable product under the repository conditions and, therefore, it may accumulate on the surface of the glass WF and produce acidic water condensation film even if the radiation field may be low after the failure of the WP.

The status of this component of Subissue 4 is closed, pending additional information. The following information is needed:

1. The coefficients for the pH parameter should be determined using B release rate, and the test duration used for estimating release rate should be compatible with durations used for other parameters.

2. DOE should correct the inconsistency between the dissolution rates calculated on page 3-53 of the PMR (reproduced in Table 1) and the Eqs. 3.6-4 and 3.6-5 of the PMR or Eqs. (19) and (20) of this report.

3. The effect of WP corrosion components such as FeOOH, $FeCl_2$, and $FeCl_3$ that could influence corrosion mechanisms and, hence, coefficients for pH and activation energy should be evaluated. DOE stated in the VA technical basis document, dissolution rates of glass strongly decrease in the presence of dissolved Mg, Pb, and Zn, but are strongly enhanced under some conditions by Fe. The potential effect of dissolved Fe is particularly important because corrosion of the SS inner barrier of the EDA-II design could provide significant quantities of dissolved Fe. The DOE should demonstrate that the

abstraction model used for HLW glass captures the range of chemical compositions of water (e.g. formation of nitric acid induced by water/air radiolysis) and WP corrosion products.

4. DOE should ensure that glasses with similar leaching solutions are used for comparison because cations in buffer solutions may change the release rates.

5.4.2.2 Colloidal Release

Acceptance Criteria

The DOE colloid source term abstraction was assessed with respect to the five generic AC (U.S. Nuclear Regulatory Commission, 2000a).

NRC Staff Comments

With respect to the approach to reversible attachment of radionuclides to colloids, the modeling approach presented in the colloid release abstraction (CRWMS M&O, 2000k) does not represent a significant departure from the approach adopted in the TSPA-VA (CRWMS M&O, 1998b). The AMR abstraction is, however, an improvement. The TSPA-VA abstraction—applied only to Pu—used modeled in-package ionic strength to constrain colloid concentration, then applied a K_d to calculated dissolved concentrations. The relationship between colloid concentration and ionic strength was based on groundwater data. Different classes of colloids were assigned different K_ds, but it is not clear from the technical basis document (CRWMS M&O, 1998b) how their individual colloid concentrations were calculated. The abstraction AMR (CRWMS M&O, 2000k) used the groundwater ionic strength relationship only for groundwater colloids and used laboratory and literature data for the ionic strength effect on concentrations of colloids derived from engineered materials and waste. In all cases, pH dependence of colloid concentration was incorporated into the ionic strength relationship. In addition, more recent K_d data from LANL were applied. The new abstraction, therefore, represents a marked refinement because model parameters were more specific to colloid type and repository conditions.

The new approach to modeling irreversible colloid attachment, in contrast, differs fundamentally from the VA approach. In the TSPA-VA (CRWMS M&O, 1998b), the flux of irreversibly attached Pu was calculated as simply a fraction of the reversible flux; the fraction was based on Nevada Test Site observation of Pu transport and was given a log-uniform distribution covering six orders of magnitude. The AMR (CRWMS M&O, 2000k), in contrast, uses direct measurements of colloid-associated Pu from laboratory experiments on WFs to derive model expressions for concentrations of both colloids and irreversibly-bound colloidal radionuclides. Clearly, the AMR abstraction of colloidal release modeling represents an appropriate enhancement of the TSPA-VA approach.

The staff agrees with the general approach to modeling colloid release as described in the AMR (CRWMS M&O, 2000k). The abstraction attempts to quantify the effects of possibly changing in-package chemical conditions on colloidal radionuclide release using limited, site-specific data

supplemented by literature review. The colloid-release model is well integrated into the TSPA by (i) drawing input from in-package chemical models and (ii) providing output to models of in-drift radionuclide concentrations. Uncertainty is addressed in part by considering alternative conceptual models [such as a kinetic approach proposed in AMR F0110 (CRWMS M&O, 2000p)].

However, the abstraction AMR does not provide sufficient justification that the abstraction is unlikely to neglect effects that could increase the colloidal radionuclide concentration. For example, the corrosion test results discussed in AMR F0110 (CRWMS M&O, 2000p) were conducted at 90 °C and the colloid sorption tests in AMR F0105 (CRWMS M&O, 2000o) at room temperature, but the abstraction AMR did not discuss possible temperature effects. In addition, the abstraction AMR did not critically assess the potential effects on colloid behavior of chemical parameters other than ionic strength and pH [e.g., oxidation potential and alkalinity (U.S. Nuclear Regulatory Commission, 2000c)]. Notably, the abstraction adopted a maximum concentration of Pu irreversibly attached to colloids of 6×10^{-8} mol/L, based on results of 15 ANL HLW glass experiments (CRWMS M&O, 2000p). The literature on this topic is admittedly sparse, but the AMR did not make a strong case that this value is likely to bound Pu concentrations under particular repository conditions. Another category of THC effect is water-flow rate. While it may be acceptable that the abstraction does not incorporate effects of flow rate on colloid release, the DOE must provide a technical basis that this omission will not significantly underestimate release. In summary, the abstraction AMR (CRWMS M&O, 2000k) does not explicitly address a sufficient range of possible coupled and uncoupled effects on colloid stability and radionuclide attachment to ensure that the abstraction is adequate for the range of possible repository conditions.

In addition, no technical basis was provided for the inclusion of colloidal effects only on Pu and Am release. The exclusion of a colloidal release component for other radionuclides needs to be supported.

Areas in which stronger technical bases may be needed in AMR F0110 (CRWMS M&O, 2000p) in supporting the adopted abstraction include (i) demonstrating that test samples were sufficiently representative of the range of WFs expected in the proposed repository, (ii) accounting for deviation of repository physical and chemical conditions from those in the laboratory, and (iii) demonstrating that the effects of water chemical parameters other than pH and ionic strength may be neglected in characterizing colloid behavior.

To address these comments, the DOE should either conduct additional analyses or incorporate critical assessments of the effects on colloidal radionuclide release beyond the scope of available experimental work. Parameters that may need to be so addressed include temperature, oxidation potential, major cation and anion concentrations, and in-package hydrologic conditions.

In addition, the DOE should more explicitly evaluate if the experimental results are adopted in a manner that is conservative with respect to ionic strength and pH effects (e.g., on colloidal Pu concentration).

Finally, the DOE should extend the colloidal release abstraction to other radionuclides or provide a technical basis for exclusion of important radionuclides.

5.4.3 Status and Path to Resolution

This subissue is closed, pending additional information. The path to resolution is based on DOE's presentation and the agreements reached in the NRC/DOE Technical Exchange and Management Meeting on CLST regarding this subissue. Any NRC concern not specifically covered in this section is dealt with a risk-informed approach (i.e., the concern may not be important in PA). The agreements summarized below are abstracted from the transcripts of the meeting.[9]

As presented in Section 5.3.3. DOE has agreed to provide revised documentation on in-package water chemistry modeling for wasteforms in an AMR to be issued in January 2001 (ANL-EBS-MD-000050). In this AMR, the evaluation of the chemical form and concentration of iron corrosion products will be included. This assessment will be critical to determine if dissolution of glass is likely to be accelerated, as discussed in Section 5.4.2.

In the revision of the AMR titled Defense High-Level Waste Glass Degradation (ANL-EBS-MD-000016), available in January 2001, DOE will address specific NRC questions regarding (a) the inconsistency of the rates in the acidic pH region (pH < 4) for the dissolution of HLW glass, (b) the technical basis for use of Si in the calculation of radionuclide release from glass, and (c) clarification of the definition of long-term rates for glass dissolution. DOE stated that the response to these questions will elaborate a justification for the terms in the equation and the level of uncertainty considered, as well as a demonstration of the validity of the model for the expected pH range.

5.5 SUBISSUE 5: THE EFFECTS OF IN-PACKAGE CRITICALITY ON WASTE PACKAGE AND ENGINEERED BARRIER SUBSYSTEM PERFORMANCE

In January 1999, DOE submitted its Disposal Criticality Analysis Methodology Topical Report, YMR/TR-004Q, Revision 0 (U.S. Department of Energy, 1998e), for staff review and approval. This report provides a description of the DOE methodology for demonstrating postclosure criticality control for the proposed YM repository and, correspondingly, protection of public health and safety. The methodology is risk-informed and, as such, focuses on probabilistic evaluations of the various processes and events that may result in configurations with a potential for criticality. The report also discusses the potential consequences of criticality and the related impacts to total repository system performance. A Safety Evaluation Report (SER) documenting the staff assessment of the topical report (TR) has been issued (U.S. Nuclear Regulatory Commission, 2000b).

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[9]Schlueter, J. Letter (October 4) to S. Brocoum, U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Key Technical Issue: Container Life and Source Term (ML003760868). Washington, DC: U.S. Nuclear Regulatory Commission. 2000.

DOE plans to apply the methodology presented in the TR "to the different WFs: commercial SNF (including BWR, PWR, and mixed oxide SNF); DOE SNF (including naval SNF); immobilized Pu; and vitrified HLW glass" (U.S. Department of Energy, 1998e). Specific application of the methodology to U.S. Navy fuel has been addressed in an addendum submitted to the NRC by the Naval Nuclear Propulsion Program (NNPP), and DSNF will be included in a series of addenda to the TR, to be submitted for NRC review and approval. Given the confidential nature of the NNPP fuels, the status of criticality issue resolution for the U.S. Navy fuel will not be discussed in this document. The addendum for DSNF has not been submitted to the NRC at this point. Therefore, no discussion of criticality of DSNF can be presented at this time.

The scope of the TR includes a range of possible postclosure criticality locations (in-package, near-field, and far-field) over time. The following sections provide the status of the in-package criticality issues, which have been identified as a result of the staff review of the DOE TR. The issues are discussed in specific technical area with respect to the AC. The following discussions are derived from the SER (U.S. Nuclear Regulatory Commission, 2000b) where technical issues are covered in more detail.

As part of the recent prelicensing consultation, the NRC and the DOE participated in a Technical Exchange and Management Meeting on subissues related to criticality[10] This Technical Exchange meeting was one in a series of meetings related to the NRC KTI and sufficiency review and the DOE site recommendation decision. The purpose of the Technical Exchange was to assure that sufficient information will be available on the criticality subissue to enable the NRC to docket a proposed LA. Part of the sufficiency issue is data and analyses that were not within the scope of Topical Report, Revision 0, and the SER issued by the staff. Therefore, in this revision of CLST IRSR, in addition to the methodology, data and analyses associated with the in-package criticality subissue are also discussed.

During the Technical Exchange, the DOE identified sections in the Topical Report, Revision 01 (to be issued in January 2001), which addresses the Open Items related to methodology included in the SER. With respect to data and analyses, the DOE identified various reports that are in the process of being issued or are to be issued. With the identification of this additional information, the in-package criticality subissue was considered closed, pending the staff review and acceptance of the information to be provided by the DOE. The following sections provide the DOE's proposed approach for each component of the criticality subissue and the staff assessment of the approach.

[10]NRC/DOE Technical Exchange and Management Meeting on Subissues Related to Criticality, Las Vegas, NV. October 23–24, 2000.

5.5.1 Criticality Design Criteria

5.5.1.1 U.S. Department of Energy Approach

The design criteria proposed by the DOE for the in-package criticality scenario pertain mainly to CSNF. DOE presented a set of design criteria with respect to critical limit (CL), probability, criticality consequence, and repository performance.

In the criticality TR (U.S. Department of Energy, 1998e), the DOE requested acceptance of the following design criteria:

> The CL criterion discussed in Section 3.4: the calculated k_{eff} for systems (configurations) for postclosure will be less than the CL. The CL is the value of k_{eff} at which the system is considered potentially critical as characterized by statistical tolerance limits.
>
> The probability criterion discussed in Section 3.5: a criticality frequency of 10^{-4} per year for the entire repository will not be exceeded in any of the first 10,000 years for all combinations of WPs and WFs. This criterion is intended to ensure that the expected number of criticalities is less than one during the regulatory period of the repository (10,000 years). It is used to define a WP criticality control design requirement in support of defense-in-depth with respect to the repository criticality performance objective in item 4 (item 4 being the performance objectives criterion).
>
> The criticality consequence criterion discussed in Section 3.6: the expected radionuclide increase from any criticality event will be less than 10 percent of the radiologically significant radionuclide inventory (curies present at time of criticality) that is available for release and transport to the accessible environment. This criterion is intended to ensure that the average radionuclide increment from any single criticality is much less than the uncertainty of the performance assessment dose estimation, and is also used to define a WP criticality control design requirement in support of defense-in-depth with respect to the Repository Performance Objective in item 4.
>
> The repository performance objectives criterion discussed in Section 3.7: the ability to satisfy dose rate performance objectives will not be compromised by the radionuclide increment due to criticality events (if any).

5.5.1.2 NRC Staff Evaluation

The staff evaluation of the DOE's approach and positions has been conducted based on the following AC.

- DOE includes degradation of the in-package criticality control system as FEP in the TSPA. DOE uses sound technical bases for selecting the design criteria that mitigate degradation of the criticality control system or any potential impact of the in-package criticality on repository performance; identifies all FEP that may increase the reactivity of the system inside the WP; identifies all the configuration classes and configurations that have potential for nuclear criticality; and includes changes in radionuclide inventory and thermal conditions in their abstraction of EB degradation.

The detailed staff evaluation of the DOE proposed design criteria is provided in the SER (U.S. Nuclear Regulatory Commission, 2000b). The following paragraphs provide a summary of staff evaluation of each of the above four design criteria proposed by the DOE.

With respect to the CL, subject to its appropriate implementation in the LA, the staff agrees with the concept of establishing a k_{eff} limit that would include all the appropriate biases and associated uncertainties for each in-package configuration.

With regard to the criticality probability criterion, as long as the probability criterion described in Sections 1.2.A.2 and 3.5 of the TR is used only for deciding among different design options for the criticality control systems in WPs, the staff has no objection. However, the staff stresses that only the probability defined in the proposed 10 CFR 63.114(d) can be used for screening the criticality events for the purposes of PA.

With respect to the criticality consequence design criterion, the staff agrees that a 10-percent increase in radionuclide inventory from internal steady-state criticality can be used as a consequence criterion for deciding to perform a TSPA analysis or to bypass it during the design process, provided that

1. The consequences of a 10-percent radionuclide increase and associated heat production are determined.

2. The heat impact and other degradation impacts of steady-state criticalities are included in a TSPA analysis.

Furthermore, if the DOE is selecting a criterion for one of the consequences of criticality, it is not clear why criteria for other types of criticalities are not established. Other types of criticalities include internal transient and external steady state. Therefore, the following item has been identified with respect to criticality consequence design criteria.

The consequence criteria for transient and external criticalities are not addressed in the TR. The DOE must specify, whether if it intends to perform full consequence analyses for transient and external criticality events and include them in the TSPA or use some type of criteria for the purpose of criticality control design selection. In the October 2000 Technical Exchange, DOE identified Topical Report, Rev. 01 (to be issued in January 2001), as the document addressing the above Open Item.

With regard to the performance objective design criterion, the staff agree that the ability to satisfy the dose rate performance objectives must not be compromised by the radionuclide increase caused by criticality events. However, in its overall evaluation, the DOE must

1. Consider all aspects of criticality events including, but not limited to, increase in radionuclide inventory, waste heat output, and degradation of EBS.

2. Define what is considered an insignificant impact.

3. Include all the probability-consequence products from postclosure criticality into a TSPA, as indicated by Figure 1-1 and Section 3.6.3, last sentence in the TR.

In the October 2000 Technical Exchange, DOE stated that all probability/consequence pairs will be evaluated for inclusion in at least one TSPA sensitivity analysis. Furthermore, with respect to verification of SNF burnup, which is an indirect verification of CL, the DOE has stated that it will address it during the preclosure discussion.

Based on the information provided by the DOE in October 2000, the staff consider this component to be closed, pending the review and acceptance of the Topical Report, Rev. 01, to be issued in January 2001 and further discussion of burnup verification measurement during the preclosure discussions.

5.5.2 In-Package Criticality Scenarios

5.5.2.1 U.S. Department of Energy Approach

The DOE proposed a master scenario list (MSL) that consists of a standard set of degradation scenarios that must be considered part of the criticality analysis of any WF disposed of in the repository. The development of degradation scenarios is based on a combination of FEP within the proposed YM repository that result in degraded configurations to be evaluated for criticality. Groups of similar degraded configurations are combined into configuration classes to reduce the calculational burden while ensuring that a comprehensive set of configurations is considered. These configuration classes consist of configurations with similar material compositions and geometries that differ because of parameters, such as U enrichment and burnup or water infiltration rate that vary in a given range.

The internal scenarios are combinations of FEP that may result in critical configurations inside the WP and are determined based on several discriminators. The top-level discriminator is whether the location of the initial WP penetration is at the top or bottom of the package, which determines if water can accumulate inside the package. The second level discriminator is the rate of degradation of the WP internal structures as compared with the degradation of the WF. Lower-level discriminators include items such as the transport characteristics of the FM and structural materials. These scenarios can result in the set of configuration classes identified in the TR (U.S. Department of Energy, 1998e).

In the October 23–24, 2000, Technical Exchange, DOE provided discussions with respect to seismicity and igneous activity and faulting. With respect to seismically and volcanically induced criticality, DOE stated that both issues have been addressed in the Topical Report, Rev. 01, to be issued in January 2001. For the igneous-activity-induced criticality, DOE also cited the Disruptive Events Process Model Report, TDR-NBS-MD-000002, Rev. 00, (CRWMS M&O, 2000z) and Probability of Criticality Before 10,000 Years, CAL-EBS-NU-000014, Rev. 00, (CRWMS M&O, 2000aa).

With respect to the impact of faulting on WP integrity and a possible criticality event afterward, the DOE indicated in the Technical Exchange that the FEP for faulting (1.2.02.03.00, Fault Movement Shears Waste Container) have been screened out based on low probability. Therefore, faulting has not been included in the Topical Report, Rev. 01, configuration classes. The DOE cited Fault Displacement Effects on Transport in the Unsaturated Zone, ANL-NBS-HS000020; Disruptive Events FEP AMR, ANL-WIS-MD-000005; and FEP Database, 1.2.02.03.00.

5.5.2.2 NRC Staff Evaluation

The staff evaluation of the DOE approach and positions have been conducted based on the following AC.

- DOE includes degradation of in-package criticality control system as FEP in the TSPA. DOE uses sound technical bases for selecting the design criteria that mitigate degradation of the criticality control system or any potential impact of the in-package on repository performance; identifies all FEP that may increase the reactivity of the systems inside the WP; identifies all the configuration classes and configurations that have potential for nuclear criticality; and includes changes in radionuclide inventory and thermal conditions in their abstraction of EB degradation.

The NRC staff found that grouping sets of similar configurations into configuration classes is a reasonable way to reduce the calculational burden but still provide reasonable assurance that the probability of criticality will not be significantly underestimated. The NRC staff found that the MSL and the additional analyses conducted for seismic events, as stated in the response to Request for Additional Information (RAI) 3-1, will adequately identify scenarios that may significantly impact the potential for, or consequences of, a criticality event within the WP, based on the FEP associated with the YM repository. The NRC staff found that all FEP important to the criticality evaluation inside the WP can be incorporated in the proposed methodology if the additional steps accounting for seismic events are performed.

The in-package criticality scenario component is considered closed, pending the NRC review and acceptance of Topical Report, Rev. 01, revised, Disruptive Events Process Model Report, TDR-NBS-MD-000002, Rev. 00 (CRWMS M&O, 2000z), and Probability of Criticality before 10,000 Years, CAL-EBS-NU-000014 (CRWMS M&O, 2000aa), with respect to seismic and igneous-induced criticality. With respect to impact of faulting, the NRC acceptance is pending

the review of the revised Disruptive FEP AMR, which was agreed on in the Structural Deformation and Seismicity (SDS) KTI Technical Exchange.

5.5.3 In-Package Criticality Configurations

5.5.3.1 U.S. Department of Energy Approach

In its response[11] to the RAI,[12] the DOE requested approval of the methodology, modeling, and validation of the method for generating a comprehensive set of internal configurations. The method is described both in the RAI response and in the TR (U.S. Department of Energy, 1998e).

Methodology

The proposed methodology to determine internal configurations is to use the appropriate range of configuration parameters to further specify the identified configuration classes for each combination of WF and WP. This methodology will be accomplished by performing a geochemical analysis for each configuration class to identify the chemical composition of the corrosion products remaining in the WP and by determining the physical properties of the remaining corrosion products. This end result will be a specific and detailed range of configurations that must be considered in the parametric criticality evaluation of each configuration class.

The geochemical processes will be used to track the location of important fissionable, neutron-moderating, and neutron-absorbing materials and will be specified using the following steps:

1. Identify specific corrosion rates for all internal components, the range of drip rates of water onto a WP under a dripping fracture, and the range of dripping-water chemistry parameters.

2. Estimate the location of potentially reacting materials to determine if a reaction is possible.

3. Perform probabilistic flow-through model geochemical calculations for the representative parameter range for each configuration class.

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[11]Brocoum, S., U.S. Department of Energy Responses to the U.S. Nuclear Regulatory Commission Request for Additional Information on the U.S. Department of Energy Topical Report on Disposal Criticality Analysis Methodology, Letter (November 19) to C.W. Reamer, U.S. Nuclear Regulatory Commission. Washington, DC, U.S. Department of Energy, 1999.

[12]Reamer, C.W., U.S. Nuclear Regulatory Commission Request for Additional Information on the U.S.Department of Energy Topical Report on Disposal Criticality Analysis Methodology, Letter (August 18) to S. Brocoum, U.S. Department of Energy, Washington, DC, U.S. Nuclear Regulatory Commission, 1999.

4. Determine concentrations of fissionable materials and neutron absorbers in solution and in solids and insoluble corrosion products within the package.

5. Determine if clay has formed from chemical alteration of glass WFs or from the silica and alumina in the water, and determine the amounts of undegraded material and solid degradation products present.

6. Determine the range of hydration of degradation products possible if the package is not flooded.

7. Quantify the amounts of undegraded material and solid degradation products present for each configuration class.

8. Evaluate the potential for adsorption of soluble FM or of neutron-absorbing material on corrosion products.

At appropriate intervals in the progress of the geochemical process, physical processes will be evaluated. These physical processes include possible locations for solids; the density and physical stability of corrosion products; the thermal and structural behaviors of the internal structures and the WF; and the effects of external events on the internal components, WF, or the location of the corrosion products.

The DOE indicated[13] it will evaluate the probability of occurrence of all configurations identified as potentially autocatalytic in published articles. This evaluation will provide additional confidence that all realistic potentially high-consequence criticality events have been considered.

Modeling Approach

The determination of internal criticality configurations depends on the degradation rate of WP barrier materials, internal components, and WFs determined from the quantity of water contacting the material and the chemistry of the dripping water.

Individual corrosion models are developed based on data from the DOE material testing program for each of the materials that make up the WP and WF. WP degradation models will be the models used in the TSPA that output a distribution of breach times at various locations on the WP for a given set of environmental conditions. The degradation rates used in the criticality evaluation also will be consistent with the WF corrosion models used for TSPA.

The geochemistry within the WP will be calculated using a commercial software code such as EQ3/6 (Wolery, 1992). The software will be qualified under an appropriate QA program. A series of runs of the geochemistry code will be used to simulate water dripping into and leaking

[13]Brocoum, S., U.S. Department of Energy ...Methodology. Letter (November 19) to C.W. Reamer, U.S. Nuclear Regulatory Commission, Washington, DC, U.S. Department of Energy, 1999.

out of a WP. The DOE stated[14] that a modification to the EQ6 (Wolery and Daveler, 1992) portion of the code, called the solid-centered-flow-through code, will be used to model water inflow and outflow and track the time step adjustment.

The configuration generator code will be used to track the concentrations of neutronically significant isotopes and chemical species that can affect the solubility of the neutronically significant elements. This code uses time-dependent, first-order differential equations to represent the chemical transformations of elements or compounds that have coefficients determined by fitting data from detailed calculations of a geochemistry code such as EQ3/6 (Wolery, 1992). The code will provide bookkeeping for the transport between sites of the application of a detailed geochemistry code and, in some situations, provide more rapid calculation where the detailed geochemistry code results can be used to develop heuristic models for the most significant ions for a few solution parameters.

At each time step, the configuration generator code will calculate the increase in the quantity of water in the WP; the amount of each element dissolved in this water, the amount of each element lost because of the removal of water from the WP, the pH of the water, the solubility of materials in the water inside the WP, and the precipitation or dissolution of the species being tracked, based on solubility. Uncertainties in parameters to be used in these equations will be represented using the Monte Carlo technique. These uncertain parameters will be assigned distributions of possible values. Many realizations will be conducted by sampling a single value from the distributions of values assigned to all the uncertain parameters and by calculating the results for each realization.

Validation Approach

The DOE proposes to not validate models that have been validated and used in the TSPA because the model validation will be evaluated during the LA review process for the repository. The degradation rates of internal components not modeled and validated in the TSPA will be developed from material test data and will be validated based on information and data provided as part of the disposal criticality analysis supporting the LA.

The geochemical code modified to track the water movement of, and used to determine the chemical environment inside, the WP will be compared against analytical solutions and against results obtained by chaining several thousand individual EQ6 runs, with adjustment of the water mass between runs. Additionally, the geochemical code will be validated by comparison with the other geochemistry-transport codes. Validation of specific computer codes is beyond the scope of this review, so no finding will be made as to the acceptability of the use of the EQ3/6 code for the repository environment.

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[14]Brocoum, S., U.S. Department of Energy ...Methodology. Letter (November 19) to C.W. Reamer, U.S. Nuclear Regulatory Commission, Washington, DC, U.S. Department of Energy, 1999.

Model Implementation, Data, and Analyses

In the October 23–24, 2000, Technical Exchange, the DOE identified a number of reports as the basis for closing the criticality configuration component. With respect to model implementation and analyses, the issues that were raised in CLST IRSR, Rev. 2, DOE cited a number of documents. Specifically, with respect to the quantity of corrosion products assumed in the WP, the DOE identified the following documents:

- Criticality Analysis Methodology Topical Report, Rev. 01 (January 2001)
- Probability of Criticality Before 10,000 Years (November 2000)
- Updated Calculation of Probability of Criticality for EDA II Waste Package Design, CAL–UDC–MD–0000001, Rev. 00 (CRWMS M&O, 1999c)
- Probability of Criticality for MOX SNF,. CAL–EBS–NU–000007, Rev 00 (CRWMS M&O, 1999d)
- Waste Package Related Impacts of Plutonium Disposition Waste Forms in a Geologic Repository, TDR–EBS–MD–000003, Rev 01 (CRWMS M&O, 2000bb), for application to the Pu-ceramic-containing WP

With respect to alternative forms of corrosion products, the DOE identified the following documents:

- EQ6 Calculation for Chemical Degradation of Shippingport LWBR (Th/U oxide) Spent Nuclear Fuel Waste Packages, CAL–EDC–MD000008, Rev 00
- EQ6 Calculation for Chemical Degradation of Pu-Ceramic Waste Packages: Effects of Updated Materials Composition and Rates, CAL–EDC–MD–000003, Rev 00 (CRWMS M&O, 2000cc)

The DOE also presented a table that contained the primary and secondary FEP and the corresponding configuration classes listed in the Topical Report.

With respect to data, the DOE stated that the geochemical models validation reports, which would contain the range of configuration parameter values, will be available during FY2001. The remaining geochemistry validation reports will be available during FY2002.

5.5.3.2 NRC Staff Evaluation

The staff evaluation of the DOE approach and positions has been conducted based on the following AC.

- DOE includes degradation of in-package criticality control system as FEP in the TSPA. DOE uses sound technical bases for selecting the design criteria that mitigate degradation of the criticality control system or any potential impact of the in-package on repository performance; identifies all FEP that may increase the reactivity of the system inside the WP; identifies all the configuration classes and configurations that have potential for nuclear criticality; and includes changes in radionuclide inventory and thermal conditions in their abstraction of EB degradation.

Methodology

The NRC staff reviewed the methodology the DOE will use to identify critical configurations against the previous acceptance criterion. The methodology uses models to develop the configurations of interest, but acceptance of these computer codes will be assessed during LA. Modeling verification and validation of these computer codes will be evaluated when the DOE submits the appropriate validation reports.

The NRC staff found that, provided the DOE evaluates the probability of occurrence of all configurations identified as potentially autocatalytic in published articles, as stated in the RAI response,[15] the proposed methodology is sufficient to provide reasonable assurance that the analysis has been performed on a comprehensive set of internal configurations and that no configuration that could increase substantially the calculation of the probability or consequence of a criticality event has been omitted from the analysis.

Modeling Approach

The NRC staff reviewed the methodology that the DOE will use to identify critical configurations against the previous acceptance criterion to ensure that the proposed methodology, including the degradation models, geochemistry codes, differential equations used to track locations of materials, and the coefficients that will be used with these differential equations, will identify the configurations that have potential for nuclear criticality. The methodology uses models to develop the configurations of interest, but the assessment of these computer codes will be performed after the LA submittal.

The NRC staff found that using corrosion models consistent with those used in the TSPA for the LA for YM was acceptable for determining breach times of the WP and degradation rates of the WF and other components inside the WP. These models will be reviewed in detail during the review of the PA. The DOE only needs to demonstrate that these models do not contain any assumptions that are conservative for PA calculations but nonconservative for the criticality analysis. The NRC staff found the use of a steady-state geochemistry code with modifications to track the quantity of water in the WP is acceptable to calculate the loss of fissionable elements and neutron absorbers and the composition of degradation products precipitating in the WP, as long as the code is properly validated and verified. Additionally, NRC staff found the

[15]Brocoum, S., U.S. Department of Energy ...Methodology, Letter (November 19) to C.W. Reamer, U.S. Nuclear Regulatory Commission, Washington, DC, U.S. Department of Energy, 1999.

use of differential equations is acceptable to track the concentration of fissionable and neutron-absorbing materials, as long as the coefficients for these equations are developed based on sufficient and appropriate data. NRC staff found the abstraction of the results from a steady-state geochemistry code is acceptable to develop the coefficients for these equations.

Validation Approach

The NRC staff reviewed the proposed methodology that the DOE will use to validate and verify the computer codes used to identify critical configurations against the AC. The methodology was reviewed to ensure that the approach to model validation and verification for the degradation models and geochemical codes will provide confidence that the codes will provide a reasonable representation of the configuration classes and configurations that may occur in the repository with a potential for nuclear criticality. Modeling verification and validation of these computer codes will be evaluated when the DOE submits the appropriate validation reports as part of the LA.

The NRC staff found that the proposal to not validate models that have been validated and used in the TSPA is acceptable, as long as the model is used for the same purpose for which it was used in the TSPA and no assumptions were made, in the TSPA modeling that were conservative for purposes of PA that could be nonconservative for criticality analyses. The NRC staff will review the corrosion data supplied by the DOE and used as input in the model calculations during the review of the DOE TSPA. The proposed methodology of validating and verifying the geochemistry code used to determine the chemical environment inside the WP by comparing (i) results of the code to analytical solutions, (ii) results obtained by chaining several thousand individual code runs, and (iii) results obtained using other geochemistry-transport computer codes is acceptable to the NRC staff. The acceptability of the EQ3/6 to model conditions expected in the repository has not been evaluated in this review, however. Additionally, the NRC staff found that the proposed methodology for validation of the configuration generator code by comparing the results of the code with appropriate hand calculations is acceptable. In the LA, the DOE will have to provide verification that all computer codes used in the analysis are being implemented correctly and demonstrate that using these computer codes does not underestimate the probability of a criticality event for all WFs that will be disposed of in the repository. The NRC staff will review the corrosion models, as well as the corrosion data provided by the DOE and used as input in the model calculations, to assure these are acceptable and that an appropriate correspondence exists between the TSPA calculations and those used in the criticality analysis.

Model Implementation, Data, and Analyses

The staff's assessment of the model implementation, data, and analyses for criticality configurations component is pending the DOE providing the reports identified in the October 23–24, 2000, Technical Exchange and the staff review of these reports. At the time of writing this revision of CLST IRSR, volumes of reports have been received by the staff. The staff have not had opportunities to locate, review, and assess the report that was identified by the DOE at the Technical Exchange. Furthermore, the Topical Report Revision 01 is not scheduled

to be released until January 2001, and the validation reports are scheduled to be issued in FY2001.

The staff considers the criticality configuration component of the criticality subissue, with respect to model implementation, data, and analyses, to be closed, pending the review and acceptance of the documents released and to be released by the DOE.

5.5.4 Criticality Analysis

5.5.4.1 U.S. Department of Energy Approach

With regard to criticality evaluation, the DOE requested[16] approval of a criticality evaluation process and a specific approach to regression for k_{eff} calculations. The following sections provide a summary of the DOE proposed methodology, modeling, and validation approaches.

Methodology

Section 3.4 of the TR describes the methodology for calculating the k_{eff} for a given internal or external configuration. The DOE-proposed methodology for determining the values of k_{eff} for both internal and external configurations is depicted in Figure 3-3 of Enclosure 2 in the responses to the RAI. The following sections provide a summary of the DOE proposed methodology for material composition, criticality evaluations, and regression analysis.

Results from the degradation analyses—which would include results from corrosion, geochemistry, and configuration generation models, along with some isotopic inventories at a given time-step—will be provided as the material and geometry input for k_{eff} calculations. In its methodology, DOE proposed to take "... credit for the reduced reactivity associated with the net depletion of fissionable isotopes and the creation of neutron-absorbing isotopes during the period since nuclear fuel was first inserted into a commercial reactor." This is referred to as burnup credit. The DOE requested approval of a specific set of radionuclides for the purpose of criticality analyses. However, as indicated in the DOE's revised requests, through the response to RAI 3-13 and Enclosure 2, DOE is not seeking approval of a set of specific isotopes at this time. DOE is requesting approval for the use of the burnup credit concept in disposal criticality. The initial isotopic inventory (i.e., isotopic inventory at time of emplacement in a repository) will be established through validated isotopic models that simulate reactor operating history and the impact on the isotopic inventory for CSNF and U.S. Navy SNF. For other WFs, such as DSNF, the DOE is not seeking credit for the previous operating history. The changes in isotopic inventory from decay and degradation processes will be taken into consideration.

The results from degradation and isotopic analyses and Monte Carlo-based computer codes will be used to determine the k_{eff} for a range of both internal and external configurations. In its response to RAI 1-8, the DOE indicates that the k_{eff} evaluation for the full range means

[16]Brocoum, S., U.S. Department of Energy ...Methodology, Letter (November 19) to C.W. Reamer, U.S. Nuclear Regulatory Commission, Washington, DC, U.S. Department of Energy, 1999.

evaluation using the "... bounding values for certain key parameters and the range of values for other parameters." The k_{eff} value for a specific configuration shall be compared with the corresponding CL. The CLs shall be established as described in Section 3.2 of the TR. In addition, the CLs shall be modified based on the range of applicability of benchmark experiments. As indicated in Figure 3-3 of Enclosure 2 of the RAI responses, the modification of CL is based on extending its range of applicability through adding additional data points from critical experiments or taking a penalty for the lack of critical experiment. The range of applicability shall be discussed further in Section 3.5.3 of the TR. If the k_{eff} for any of the bounding configurations exceeds the corresponding CL-margin value, the DOE has proposed to develop a regression equation, for k_{eff}, for that configuration class which is a function of a specified set of parameters (e.g., fissionable material, absorbers, moderator, and degradation products). A comparison of k_{eff} values with the corresponding CL values, modified for the range of applicability, will be performed to identify specifically those configurations with k_{eff} values exceeding the corresponding CL values. Depending on the probability of the configurations with k_{eff} values exceeding the CL values, design modifications or consequence analyses will be performed.

The DOE also proposed a methodology for developing a regression equation, from a set of k_{eff} values, which will be used for determining k_{eff} for a range of internal or external configurations, within a configuration class.

The DOE proposed first to identify those configuration parameters that impact the k_{eff} values. The DOE has identified a partial list of parameter types such as WF isotopic inventory, amount of fissile material, and geometry. Once all the configuration parameters are determined, a look-up table or a linear regression equation is developed, which provides the values of k_{eff} as a function of the configuration parameters. This equation or look-up table will be used to determine further the specific configuration in a configuration class that showed the k_{eff} value to be higher than the corresponding CL, using the bounding configuration parameter values. In addition, this regression equation or look-up table will be used in calculating the probability of criticality during a period of the postclosure.

Modeling Approach

The following paragraphs provide a summary of DOE approaches to modeling the isotopic, criticality, and k_{eff} regression analyses. Part of the DOE request, stated in Section 3.5 of the TR, is the use of a model to predict the isotopic inventory in the WF at the time of emplacement

dimensional, discrete-ordinates code that produces a weighted cross-sectional library and spectral data. COUPLE uses these data to update an ORIGEN-S data library for selected nuclides. ORIGEN-S is a point-depletion and decay code that calculates the time-dependent isotopic concentrations using a matrix, exponential-expansion technique. ORIGEN-S computes the isotopic concentrations (actinides and fission products) for all specified operating histories. ORIGEN-S uses a point-depletion model. Therefore, spacial effects are not specifically modeled.

ORIGEN-S is also used in calculating radioactive decay and the buildup of daughter isotopes after the fuel has been discharged from reactor cores. Therefore, the DOE also proposes to use ORIGEN-S to calculate postclosure isotopic concentrations. No other changes, other than decay in the isotopic inventory, are assumed during the postclosure period in an intact SNF assembly.

With respect to criticality modeling, the DOE proposes to use the MCNP4B computer code with a set of cross-section data to calculate the k_{eff} values for different WP configuration classes. MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron transport, having the capability to calculate k_{eff} for systems containing fissionable material. The Monte Carlo approach simulates the behavior of individual particles within a system. The Monte Carlo method, as applied to neutrons in an MCNP criticality calculation, is based on following a number of individual neutrons through transport, including interactions such as scattering, fission, absorption, and leakage. The average behavior of a sample set of neutrons is used to estimate the average behavior of the system with regard to the number of neutrons in successive generations (i.e., effective neutron multiplication factor, k_{eff}).

DOE proposes to select a cross-sectional library based on the following criteria (CRWMS M&O, 1998d):

- Nuclear data file/B-V-based (ENDF/B-V) cross-sectional libraries were selected for use when available, with the exceptions of H-2, B-11, Zr (natural), Ag-107, Ag-109, Eu-151, and Eu-153;

- Either ENDF/B-VI, T-2, or LLNL-based cross-sectional libraries were selected for use when ENDF/B-V-based libraries are not available or selected; and

- ENDF/B-VI, T-2, or LLNL-based cross-sectional libraries were selected based on number of energy points included in the main energy grid, date of evaluation, and availability of certain data.

DOE proposes to use a multivariate regression approach in calculating the k_{eff} values for the range of configurations that exists in a configuration class. For a selective number of configurations, detailed calculations using a Monte Carlo-based code such as MCNP4B are performed, and, subsequently, regression analysis is used to predict the intermediate k_{eff} values.

The effect on correction factors of various amounts of boron remaining in solution for 21 partially and fully degraded PWR basket configurations is taken into account.

In responses to the RAI, the DOE indicated that look-up tables may be used because there are "... enough cases of k_{eff} calculation (over 2000 for the various WFs and various degradation parameters) ...".

Validation Approach

The following paragraphs provide the DOE approach regarding validation of neutronics models. The DOE presented its revised requests in Enclosure 2 of the responses to the RAI.

In the responses to the RAIs,[17] DOE indicated it is not seeking approval of the method for validation of the isotopic model, but is only requesting acceptance of the method for confirmation of the bounding-applications model.

The three requirements that DOE listed in the TR are

1. Reactor operating histories and conditions must be selected together with axial burnup profiles such that the isotopic concentrations used to represent CSNF assemblies in WP design shall produce values for k_{eff} that are conservative in comparison to any other expected combination of reactor history, conditions, or profiles.

2. These bounding reactor parameters will be used to predict isotopic concentrations that, when compared to best estimate isotopic predictions of the measured radiochemical assay data or the measured radiochemical data itself, must produce values for k_{eff} that are conservative.

3. The values for the isotopic concentrations representing CSNF must produce conservative values for k_{eff} for all postclosure time periods for which criticality analyses are performed.

Aside from isotopic-model validation, a set of reactor operating parameters is needed to run a depletion code. Because the SNF assemblies have been irradiated in a variety of reactor-core operating conditions, the DOE needs to determine a set of reactor core conditions that, when used in a depletion computer code, would result in a bounding isotopic inventory with respect to criticality. DOE proposes to use Requirement A to determine the values for parameters such as moderator density, fuel temperature, soluble boron, burnable poisons, control rod histories, and burnup profiles. In Section 4.1.3.1.4 of the TR, the DOE attempts to describe how these bounding parameter values will be determined, using Commercial Reactor Criticals (CRC), radiochemical assays, and other means.

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[17]Brocoum, S., U.S. Department of Energy... Methodology, Letter (November 19) to C.W. Reamer, U.S. Nuclear Regulatory Commission, Washington, DC, U.S. Department of Energy, 1999.

In its explanation of Requirement A in the TR, the DOE states "The second requirement addresses the problem of using integral experiment (CRC) exclusively for validating the isotopic model and imposes the additional use of radiochemical assay data for commercial SNF." In its response to RAI 4-5 (c), the DOE states that "DOE is not currently requesting review and acceptance of the method to be used for validation of the isotopic depletion model and establishment of the isotopic code bias. Furthermore, in responses to other RAIs, DOE has indicated that the isotopic validation method will be demonstrated in the validation reports." Attachment A of the RAI responses lists the types of data and analyses that will be used in performing isotopic validation.

The third requirement addresses changes to the initial isotopic concentration values, as a function of time, for postclosure. The only changes to the isotopic inventory in intact SNF assemblies in a flooded WP during the postclosure considered by the DOE is caused by decay. Therefore, DOE proposes a method in quantifying the uncertainties associated with the half-life and branching fractions. The method consists of performing many depletion calculations for a given fuel burnup, enrichment, and postclosure period. The half-life and branching fractions for each isotope are allowed to vary randomly in their uncertainty ranges. Then, the isotopic concentrations from each set of depletion calculations are used in a criticality calculation to predict the k_{eff} for that set of isotopic concentrations. When a sufficient number of calculations are performed, a distribution of k_{eff} values is obtained about a mean value. The mean value for k_{eff} for each of these sets will also be compared with the k_{eff} value from a single criticality calculation for each set. Based on these comparisons, any potential bias in the k_{eff} associated with this method for evaluating uncertainties is estimated from the difference between the mean k_{eff} values and the k_{eff} values at nominal conditions.

With respect to the approach for validating the model that calculates the k_{eff} of an internal configuration, DOE requested approval of a specific criticality model validation process (U.S. Department of Energy, 1998e). DOE proposed to use laboratory critical experiments (LCE) and CRCs for estimating the bias and uncertainties associated with k_{eff} values calculated by MCNP4B. These biases and uncertainties are used in establishing CLs for a range of configurations and WFs according to the aforementioned formulas. Attachment A of the RAI responses also describes the types of data and analyses to be used in preparing a validation report for WPs with CSNF covering the range of internal configurations. At this point, DOE has examined 338 LCE and 45 CRC statepoints to establish the biases and uncertainties associated with the MCNP4B k_{eff} values.

The approach for validation of the model for calculating k_{eff}, using the LCE and CRC, is mainly discussed in Section 4.1.3.2 and its associated subsections. As stated in Section 4.1.3.2 of the TR, a CL is estimated such that a calculated k_{eff} below this limit is subcritical.

Depending on the trend or lack of it in the bias and uncertainties associated with k_c, the DOE has defined three types of CLs. As depicted in Figure 4-1 in the TR, the type of CL is based on the regression results of k_c.

The determined CL based on the lower uniform tolerance band (CL_{LUTB}) method, is described in Section 4.1.3.2.1 of the TR. DOE proposes to use the method described in Section 4.1.2 of Lichtenwalter, et al. (1997).

The CL, using the normal distribution tolerance limit (CL_{NDTL}) method, is for estimating a CL based on a set of benchmark critical experiments for which normally distributed k_Cs do not exhibit any trends with respect to any parameters.

The third type of CL is the CL determined using the distribution free tolerance limit (CL_{DFTL}) approach. This approach is used when the calculated k_{eff} for the critical benchmarks does not exhibit trends for any of the parameters and does not pass the normality test.

Part of the DOE request for a validation process for the criticality model, is the acceptance of

> ... the general approach presented in Subsection 4.1.3.3 for establishing the range of applicability of the critical limit values ....

In Subsection 4.1.3.3 of the TR, DOE presents its approach to identifying and extending the range of applicability of the critical benchmarks with respect to the internal configurations. DOE proposes to identify the range of applicability using parameters that represent material, geometry, and the neutron spectrum of the benchmark experiments and the WPs. DOE suggested using the Guidelines for Experiment Selection and Areas of Applicability discussed in NUREG–6361 (Lichtenwalter, et al., 1997). The specific parameters and their ranges of applicability will be determined and documented in the criticality model validation report.

In cases where a specific configuration is beyond the range of the applicable critical benchmark, the DOE proposes to extend the range of applicability by either including new data in the critical benchmark data set or by using the established trend to extend the range of applicability to include the calculated data and add additional margin in establishing the CL. In response to RAI 4-22, the DOE presented several approaches on how to quantify the additional margin if the method of adding margins is selected. However, the DOE has stated in the response that "... the approach to establishing additional margin when extrapolation is made beyond the range of applicability will depend on the nature of the bias and the applicable experiments used to establish the bias. Thus, the approach is dependent upon the WF and its configuration, as well as various aspects of the applicable experiments. The specific approach is, therefore, an application issue for which acceptance is not being sought." DOE indicated that the methodology and justification of the specific approach in the appropriate model validation report will be documented and submitted to the NRC as part of the LA.

Model Implementation, Data, and Analyses

In the October 23-24, 2000, Technical Exchange, the DOE cited reports that would show examples of model implementation, data, and analyses for criticality. These reports are:

- Updated Calculation of Probability of Criticality for EDA II Waste Package Design, CAL–UDC–MD–0000001, Rev. 00 (CRWMS M&O, 1999c)

- Probability of Criticality for MOX SNF, CAL–EBS–NU–000007, Rev. 00 (CRWMS M&O, 1999d)

- Waste Package Related Impacts of Plutonium Disposition Waste Forms in a Geologic Repository, TDR–EBS–MD–000003, Rev. 01 (CRWMS M&O, 2000bb), for application to the Pu-ceramic-containing WP

5.5.4.2 NRC Staff Evaluation

The staff evaluation of the DOE approach and positions has been conducted based on the following AC.

- DOE includes degradation of in-package criticality control system as FEP in the TSPA. DOE uses sound technical bases for selecting the design criteria that mitigate degradation of the criticality control system or any potential impact of the in-package on repository performance; Identifies all FEP that may increase the reactivity of the system inside the WP; identifies all the configuration classes and configurations that have potential for nuclear criticality; and includes changes in radionuclide inventory and thermal conditions in their abstraction of EB degradation.

To calculate the radionuclide inventory and thermal conditions, DOE must first develop capabilities for calculating the critical conditions accurately. The following sections present the NRC staff evaluation of the DOE proposed approach for determining the critical conditions required for generating radionuclide source term and thermal heat. The following paragraphs present the results of staff evaluations with respect to methodology for material composition, k_{eff} evaluation, and regression analysis.

Methodology

The staff agrees that the configurations resulting from corrosion, geochemistry, and configuration generation models can be used if the validity and accuracy of these models can be established, as discussed in Section 3.4 of the TR. With respect to the isotopic inventory assumption, the staff accepts the approach of taking into account the reduced reactivity of the SNF due to its irradiation in reactor cores. The extent to which DOE can take credit for the burnup of fuel depends on the level of information to be provided in the LA with respect to predicting the isotopic inventory and k_{eff} accurately. In addition, the irradiation history must be appropriately modeled (e.g., local conditions in the reactor core, presence of neutron-absorbing materials, and axial and radial nonuniform burnup distribution), identifying, quantifying, and including all the uncertainties through model validation as discussed in Section 3.5.1.3. The staff does not approve inclusion of any reactivity-reducing isotopes in the criticality analyses at this point because of the absence of validation reports.

With respect to postclosure isotopic inventory in configurations with intact SNF assemblies, DOE proposes to take into account the changes in isotopic inventory caused only by decay. The staff believes that the DOE must consider changes in the isotopic inventory, especially the fission products with high solubility, because of the presence of cracks and pin-hole leaks in the cladding, if the DOE is planning to take credit for cladding.

In its examination of the DOE proposed methodology for performing k_{eff} analysis as depicted in Figure 3-3 of Enclosure 2 in the RAI responses, the staff finds the initial parametric k_{eff} analysis to be the crucial step. If the DOE is relying on this parametric k_{eff} analysis to determine which configuration classes have the potential for criticality, the analysis must not be too coarse—overlook configuration classes with configurations having potential for criticality. Therefore, staff acceptance of that portion of methodology related to the initial criticality evaluation for the range of parameters and parameter values of the configurations in each configuration class, (depicted in Figure 3-3 of the TR), is contingent on DOE performing fine parametric criticality evaluations.

Furthermore, the criticality margin depicted in Figure 3-3 of the TR should also be used when comparing k_{eff} values from regression analyses with CL values. In addition, DOE must present an approach for developing the criticality margin.

The range of applicability portion of Figure 3-3 is evaluated in the Validation Section, and the regression model portion is discussed in the next section.

With respect to regression analysis, DOE must identify all the parameters that would affect the k_{eff} values, and incorporate them in the look-up table or regression equation. Furthermore, limitation of the regression or look-table model must be examined for the expected range of configuration parameter values. The data points used in developing the regression equation or the look-up table must be finely partitioned. Therefore, the staff agrees with the approach recommended by the DOE, provided that all configuration and WF parameters affecting k_{eff} are identified and in the case of the look-up table, the interpolation must be within a small interval.

Additional information should be provided to close this component of Subissue 5 as follows:

1. The DOE must include the effects of radionuclide migration from intact fuel assemblies though pin-holes and cracks in the cladding.

2. The DOE must include a criticality margin when comparing k_{eff} values from regression analyses to CL values.

3. The DOE must present an approach for developing the criticality margin.

In the October 23–24, 2000 Technical Exchange, the DOE stated that the above Open Items have been addressed in the Disposal Criticality Analysis Methodology Topical Report, Rev. 01. Therefore, the staff consider the above Open Items closed, pending the review and acceptance of the applicable parts of the Topical Report, Rev. 01.

Modeling Approach

The following paragraphs provide the staff evaluation of the DOE proposed modeling approach for isotopic, criticality, and regression modelings.

The staff evaluated the modeling approach used in the functional modules of SAS2H in SCALE-4.3 and its appropriateness for predicting the initial and postclosure isotopic inventory to be used for criticality analysis.

With regard to using a one-dimensional type model, the staff has concerns about the approach not taking into account the fuel geometry and spacial effect that would impact the neutron spectrum and, consequently, the isotopic inventory. These effects become more pronounced in BWR fuel assemblies with much more variation in the neutron spectrum, across the radial and axial regions, because of varying enrichment and absorbers. DOE has not presented any arguments on how a point-depletion approach can appropriately estimate the isotopic inventory across fuel assemblies with varying neutron spectra.

In addition, the modeling approach must include, at the minimum, the effect of changes in the following parameters on the isotopic inventory.

- Dissolved boron in reactor core,
- Moderator density,
- Fuel pellet temperature,
- Presence of burnable absorbers, power shaping, and control rods,
- Axial and radial neutron leakage in reactor core resulting in axial and radial nonuniform burnup, and
- Void coefficient and any other features specific to BWR irradiation.

As indicated in the Methodology Section, in addition to the decay for the postclosure period, the effects of isotope leaching from the fuel rods—especially some nuclides such as ^{99}Tc with high solubility—shall be quantified as a function of time, in assuming a selected set of isotopes present in the fuel assemblies.

The staff evaluated the DOE approach with regard to criticality modeling and the selecting of a nuclear cross-sectional library. The staff agrees with the selection of a Monte Carlo-based-type modeling, such as MCNP4B, for calculating the k_{eff}s of different WF in different internal and external configurations. However, the applicability, appropriateness, and validity of modeling these configurations using a Monte Carlo-based code, such as MCNP4B, has to be demonstrated in the LA.

With regard to selection of an appropriate cross-sectional library, the staff has no objection to the criteria used by the DOE in selecting a set of cross-sectional libraries. However, examination of the reference material indicated that the cross-sectional data for the majority of the nuclides are at room temperature. If a cross-sectional set at higher temperatures is needed (e.g., critical benchmarks at elevated temperatures), additional cross-sectional data at the

relevant temperatures must be used, or the impact of temperature on cross sections for each relevant nuclide and, subsequently, on k_{eff}, must be quantified.

With regard to using the regression-modeling technique, the staff emphasizes those conditions listed in the regression methodology. Furthermore, use of the third-order no-interaction model appears to be an assumption that may not be true. Different assumptions can be made in building a multi-parameter regression model. One of these assumptions is if the modeler assumes there should be reacting parameter terms, that model the influence of the independent parameters on each other within the multi-parameter regression model. The appropriate models must also be verified through comparison with specific data points calculated using detailed models for the range of expected configurations.

In addition, the staff is not satisfied that equations such as C-3 and C-4 in Topical Report can accurately predict the impact of boron in the solution on the k_{eff} of the WP. Using a correction factor may not simulate the behavior of k_{eff} appropriately. DOE needs to provide the technical basis for the proposed approach.

Provided the following conditions are met and open items closed, the staff can accept the DOE proposed multi-parameter regression technique.

1. Validity of the assumptions and the models is established;

2. k_{eff} values for the selective number of configurations are based on the initial principal isotopic inventory, calculated using the limiting reactor-operating conditions and the appropriate biases and uncertainties, as defined in the isotopic validation section;

3. Regression is performed based on the full range of parameter values; and

4. Validation of the regression approach covering the compliance period is provided.

Additional information should be provided to close this component of Subissue 5 as follows:

1. The DOE must demonstrate the adequacy of using one-dimensional calculations to capture three-dimensional neutron spectrum effects in their point-depletion calculation or use two- and three-dimensional calculations for determining the neutron spectra during the depletion cycles used in the depletion analyses.

2. The DOE needs to use cross-sectional data corresponding to the temperature for the WP or critical benchmarks.

3. The DOE must include the cross dependency of configuration parameters for k_{eff} regression equations.

4. The DOE must provide the technical basis for the correction factors developed for boron remaining in the solution.

In the October 23–24, 2000, Technical Exchange, the DOE stated that the above Open Items have been addressed in the Disposal Criticality Analysis Methodology Topical Report, Rev. 01. Therefore, the staff consider the above Open Items closed, pending the review and acceptance of the applicable parts of the Topical Report, Rev. 01.

With respect to item 4, the DOE stated that "no reactivity credit will be taken for neutron absorber in solution." Therefore, the staff consider this open item closed, pending its confirmation during the review of the LA.

Validation Approach

The following paragraphs provide the staff evaluation of the validation approaches for isotopic, criticality, and regression models proposed by the DOE.

With respect to isotopic model validation approach, the staff agrees with Requirement A, but finds the explanation of the requirement provided in Section 4.1.3.1.4, which attempts to discuss how the requirement can be met, vague and unacceptable. The staff finds the responses to RAI 4-4 and 4-5 not to the point and confusing. It is not clear whether the DOE is proposing and asking for acceptance of a method on how to determine the bounding parameters or is leaving the subject to be discussed in the Validation Report.

The staff is not clear whether Requirement B is proposing to establish the biases and uncertainties of the isotopic model, or simply confirm the bounding reactor parameter values. From the responses, it appears that the DOE is not proposing and requesting approval of an isotopic validation method. In addition, Attachment A of the RAI responses does not present a complete approach for establishing isotopic bias and uncertainties. If Requirement B is simply established to confirm that the bounding reactor parameter values are indeed bounding, the staff does not see its necessity, once the isotopic model biases, uncertainties, and applicability are established. Therefore, the staff does not see the real purpose of Requirement B and finds no acceptable method for establishing isotopic depletion model bias and the associated uncertainty.

The staff accepts the proposed methodology for quantifying the uncertainty associated with isotopic decay and branching ratios associated with a depletion code. As stated in the Modeling Approach Section, the effect of the gradual loss of isotopic inventory, from intact assemblies, through the fuel rods with cracks and pin holes, must be considered. Therefore, the validation of such analysis must be considered also.

The staff evaluation of the DOE approach for criticality validation was performed using Regulatory Guide 3.71 (U.S. Nuclear Regulatory Commission, 1998), ANSI/ANS–8.17, and NUREG/CR–6361 (Lichtenwalter, et al., 1997). The approach prescribed by ANSI/ANS–8.17 for establishing an allowable neutron multiplication factor would be acceptable to the staff.

The approach indicates that parameters, against which k_c exhibits significant trends, must be included as the independent parameters in calculating CL. There may be more than one parameter. This approach is different than what the DOE proposed. The DOE proposed in

Section 4.1.3.2.1 of the TR "The parameter chosen to trend CL is the one that exhibits the best correlation." In other words, DOE proposed to use only one parameter, which exhibits the most trend.

Furthermore, when the value for k_c exceeds 1.0, the parameter value will be kept at the value of 1.0. This would prevent taking credit for positive bias.

The additional margin caused by extending the range of applicability in the absence of experimental data shall be included as part of Δk_c, as indicated by the definition of Δk_c in item (c).

The biases and uncertainties established for the principal isotopes representing the isotopic inventory of an SNF assembly (i.e., identified in a previous section as one of the open items) and the uncertainties from decay and branching ratios, described in the previous section, shall be included as part of Δk_c, in item (d), or an adjustment to the isotopic inventory, for calculating k_s.

In response to RAI 4-9, DOE indicated that a criticality margin (shown in Figure 3-3 of Enclosure 2 of the RAI responses as k_{eff} < CL - Margin) will be used in screening the general configuration classes. As stated earlier, this margin must be also included in the second screening after regression analysis shown in Figure 3-3 of Enclosure 2 in the RAI responses. The staff accepts the DOE inclusion of a margin in the screening step to compensate for other uncertainties not included in CL, provided this margin is also included in the screening of the configurations. This is margin in addition to the margin when the range of applicability is exceeded.

In a nontrending situation, the staff agrees with the approach presented by the DOE for the statistical uncertainty portion of Δk_c using the NDTL and DFTL in Sections 4.1.3.2.2 and 4.1.3.2.3 of the TR. However, an additional margin in the case of extending the applicability of the benchmarks beyond their range must be included in the CLs.

With respect to the range of applicability, the approach in demonstrating the applicability of the LCE and CRC for validating the MCNP4B for the range of configurations expected to exist within the WP must be similar, with some modifications for repository application, to the approach described in NUREG/CR–6361. In a systematic fashion, all LCE and CRC must be correlated to the specific WP configuration class for which the computer codes biases and uncertainties are calculated. A table similar to Tables 4.1 and 4.3, of NUREG/CR–6361, shall be constructed to include the LCE and CRC categories applicable to the different WP configuration classes. LCE and CRC shall be identified for each WP configuration class, with respect to parameters that would fall within the material, geometry, and neutron spectrum. Material, geometry, and neutron spectrum are the three areas within which trends and range of applicability are identified [i.e., area of applicability (AOA)]. The parameters within each AOA will be identified, and for those parameters exhibiting a trend, their range of applicability to the WP configurations must be established. Some of the parameters that cover these three areas are identified in NUREG/CR–6361.

With respect to extending the range of applicability, the staff agrees that either adding new data in the critical benchmark data set or using the established trend, with additional margin, would be appropriate. However, DOE has not proposed any methodology for quantifying the additional margin. Therefore, the staff requires where the extension of the range of applicability is large, that, at the minimum, the DOE proposed method of using the established trend should be

(i) subjected to a study of the bias and potentially compensating biases associated with individual changes in materials, geometries, or neutron spectra. This will allow changes that can affect the extension to be independently validated. In practice this can be accomplished in a stepwise approach; that is, benchmarking for the validation should be chosen (where possible) such that the selected experiments differ from previous experiments by the addition of one new parameter so the effect of only the new parameter on the bias can be observed.

(ii) supplemented by alternative calculational methods to provide an independent estimate of the bias (or biases) in the extended area (or areas) of applicability.

DOE has not presented any specific methodology or approach for validating the regression technique discussed in the TR. However, the staff requires that, for the proposed regression or look-up table to be acceptable, the range of its applicability to the configuration classes has to be established and validated.

The staff considers the regression or look-up table to be a simplified or abstracted model. Therefore, the applicable AC from the five criteria listed in the Total System Performance Assessment and Integration (TSPAI), with regard to model abstraction, were used as the basis of the staff evaluation for the look-up table or k_{eff} regression equation.

As DOE indicated in its response to RAI 3-16(d), the coefficient of some of the parameters in the regression equation for WFs with a relatively high Pu concentration exhibited some inaccuracies. Therefore, it is important for the DOE to examine the validity of the proposed regression equations or look-up table over the expected range of WP configurations.

With regard to uncertainty and variability AC, the DOE must account for the additional uncertainties introduced by the regression approach or the interpolation used in a look-up table. Furthermore, the addition of the uncertainties to the k_{eff} statistical uncertainties and uncertainties in the configuration parameter values must be included.

The following information should be provided by the DOE in order to close this component of Subissue 5.

1. The DOE is required to develop an acceptable methodology for establishing bias and uncertainties for the isotopic depletion model.

2. The DOE needs to establish the bias and associated uncertainty regarding the analysis or model keeping track of the isotopic inventory loss through cracks or pin-holes within intact SNF assemblies.

3. The DOE must address the types of criticality uncertainties and biases, are based on ANSI/ANS–8.17, presented by the staff in this SER.

4. The DOE must include a multi-parameter approach in its bias-trending analysis.

5. The DOE is required to include the isotopic bias and uncertainties as part of Δk_c if not included as isotopic correction factors.

6. The DOE must present a validation methodology or work scope for external criticality models.

7. The DOE should subject the method used for extending the trend to the procedures defined in ANSI/ANS–8.1–1998, C4(a) and C4(b).

8. The DOE must verify the regression equation or look-up table for all ranges of configuration and WF parameters affecting k_{eff}.

9. The DOE is required to include all uncertainties and variabilities introduced by the regression equation or the look-up table.

In the October 23–24, 2000, Technical Exchange, the DOE stated that the above Open Items have been addressed in the Disposal Criticality Analysis Methodology Topical Report, Rev. 01. Furthermore, the DOE provided a list of validation reports that included criticality validation reports for BWR, PWR, external, DOE SNF, and immobilized Pu. Therefore, the staff considers the above Open Items closed, pending the review and acceptance of the applicable parts of the Topical Report, Rev. 01, and the pertinent validation reports.

Model Implementation, Data, and Analyses

The reports that the DOE identified in the October 23–24, 2000, Technical Exchange as examples of model implementation, data, and analysis with respect to the criticality analysis component of the criticality subissue will be reviewed by the staff. Therefore, the closure of the criticality analysis component with respect to model implementation, data, and analysis will be dependent on the staff review and acceptance of the reports that the DOE identified in the Technical Exchange.

5.5.5 Criticality Probability

5.5.5.1 U.S. Department of Energy Approach

The DOE has requested[18] an approval of the methodology for determining the probability of critical configurations as summarized next.

Methodology

The probability of a critical configuration is determined by first identifying the configuration classes that have k_{eff}s exceeding the CLs in portions of their parameter ranges. This screening uses a multivariate regression for k_{eff} as a function of WF burnup, enrichment, and cooling times. These regressions will be developed using a commercial neutron transport code such as MCNP (Oak Ridge National Laboratory, 1997) for representative values of these parameters and will be based on the upper 95th percent confidence level of the regression such that configuration classes are not likely to be improperly screened because of uncertainty in the regression.

The scenario and configuration parameters are assigned probability distributions based on their uncertainty, and the Monte Carlo technique is used to estimate criticality probability. The Monte Carlo technique consists of a random selection of parameter values from the parameter distributions and determination of whether the selected parameter values satisfy the requirements for criticality. This process of selecting parameter values and determining if the associated configuration yields a criticality event is repeated many times to yield an estimate of the probability of a critical configuration. Correlations among sampled parameters will be accounted for by using appropriate conditional probability distributions for sampling parameters that depend on previously sampled parameters.[19] The criticality analysis will use the WAPDEG-generated probability distributions for the time of WP breach and duration of the bathtub (i.e., the pooling of water within this WP) associated with the most recent TSPA.

Modeling Approach

Because the potential of a criticality event occurring changes through time as the rate of infiltration to the drift changes, WPs fail, and materials within the WP are redistributed, the neutron multiplication factor must be calculated for many time steps to ensure that the criticality potential of a realization has been evaluated properly. The DOE calculation of the probability of occurrence of an internal criticality will consist of the following steps, as illustrated in Figure 4-8a of the DOE TR:

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[18]Reamer, C.W., U.S. Nuclear Regulatory Commission...Methodology, Letter (August 18) to S. Brocoum, U.S. Department of Energy, Washington, DC, U.S. Nuclear Regulatory Commission, 1999.

[19]Brocoum, S., U.S. Department of Energy... Methodology, Letter (November 19) to C.W. Reamer, U.S. Nuclear Regulatory Commission, Washington, DC, U.S. Department of Energy, 1999.

1. Sample from the distribution of infiltration to the drift from the most recent version of the TSPA.

2. Sample from the distribution of failure times determined by the TSPA programs WAPDEG and RIP, from the drip rate sampled in Step 1. WAPDEG is the code that calculates the failure times and conditions for WP degradation; RIP is the executive driver for the DOE's TSPA program. According to the response to RAI 4-25, these failure times will be based on corrosion rates determined by testing programs at LLNL and the University of Virginia.

3. Sample the height of WP penetration to determine the water level in the package.

4. Sample the WF characteristics, including enrichment, burnup, and cooling time, and determine if this fuel has the potential to yield a criticality event by comparing these characteristics to the bonding characteristics needed to achieve criticality (i.e., the CL derived previously). The realization is ended if the fuel cannot yield a criticality event inside the WP.

5. Sample the degradation rates of the WF and the internal components of the WP, accounting for correlations as appropriate.

6. Calculate the amounts of neutronically significant material remaining in the WP, using the degradation state of the WF and the internal components as inputs to the configuration generator code or the detailed calculations of a geochemistry code such as EQ3/6 (Wolery, 1992).

7. Test if the k_{eff} of the configuration analyzed exceeds the CL. The realization is ended if k_{eff} exceeds the CL.

8. Check if the ending condition has been reached and if not, increment the time and return to step 6. The ending condition is typically a time limit or the time at which a hole develops in the bottom of the WP, water is released, and criticality within the WP is no longer possible.

The probability of criticality will be calculated as the number of realizations that produced a critical configuration of FM divided by the total number of realizations. This process will be repeated for a sufficient number of realizations to yield a sufficiently small uncertainty in the probability of criticality. DOE indicated that preliminary estimates of the number of realizations required to drive the uncertainty to an acceptably small number are about 10^8.[20]

[20]Brocoum, S., U.S. Department of Energy... Methodology, Letter (November 19) to C.W. Reamer, U.S. Nuclear Regulatory Commission, Washington, DC, U.S. Department of Energy, 1999.

Similar to the calculation of the probability of an internal criticality, calculation of the probability of occurrence of an external criticality will be conducted with a Monte Carlo calculation and will consist of the following steps.

1. Sample the flow rate, concentration of FMs, and pH of the water flowing out of the WP.

2. Sample the external path leading to an external criticality location, the transport parameters, and the accumulation parameters. Parameters sampled to determine the location of accumulation include the groundwater flow rate, rock porosity, and the fracture density. Parameters sampled to determine the transport and accumulation properties of materials will include adsorption coefficients and will be consistent with the TSPA.

3. Calculate the amounts of fissionable material removed from the flow in the external environment. Geochemical analyses will be used to identify the portions of the external environment that can remove fissionable material from the flow and determine the chemical environment in these locations.

4. Evaluate the k_{eff} of configurations with a significant accumulation of FM. If the k_{eff} of the maximum concentration of FM exceeds the CL, it is recorded, and a new realization is started.

The probability of criticality will be calculated as the number of realizations that produced a critical configuration of FM divided by the total number of realizations. This process will be repeated for a sufficient number of realizations to yield a sufficiently small uncertainty in the probability of criticality. The ranges and distributions of most of the parameters sampled will be provided by the inputs into and results of the most recent TSPA.

Validation Approach

DOE proposes to validate the code that incorporates this Monte Carlo methodology using hand calculations and a commercial mathematical equation solver code to verify that the Monte Carlo code is properly sampling from the input parameter distributions and calculating the probability correctly. One example of the type of hand calculation that could be used in this validation process is fixing the value of sampled parameters to ensure that the code reproduces results that can be verified using an equation solver code.

Model Implementation, Data, and Analyses

In the October 23–24, 2000, Technical Exchange, the DOE identified some of the published reports as examples of model implementation, data, and analysis with respect to probability component of the criticality subissue.

- Probability of Criticality Before 10,000 Years (CRWMS M&O, 2000aa)

- Probability of a PWR Uncanistered Fuel Waste Package Postclosure Criticality (CRWMS M&O, 1999e)
- Probability of Criticality for MOX SNF (CRWMS M&O, 1999d)

5.5.5.2 NRC Staff Evaluation

The staff evaluation of the DOE approach and positions has been conducted based on the following AC.

- DOE includes the degradation of in-package criticality control system as FEP in the TSPA. DOE uses sound technical bases for selecting the design criteria that mitigate degradation of the criticality control system or any potential impact of the in-package on repository performance; identifies all FEP that may increase the reactivity of the system inside the WP; identifies all the configuration classes and configurations that have potential for nuclear criticality; and includes changes in radionuclide inventory and thermal conditions in their abstraction of EB degradation.

Methodology

The staff reviewed the proposed methodology to determine the probability of occurrence of a criticality event against the AC in the IRSRs. The methodology was reviewed to ensure it will be sufficient to provide reasonable assurance the DOE has developed a technically defensible, transparent, and traceable method to assign probability values to criticality scenario classes, scenarios, configuration classes, and configurations and has adequately addressed the uncertainty in data caused by both temporal and spatial variations in conditions affecting potential nuclear criticality.

The staff found the proposed methodology to use the Monte Carlo technique to account for uncertainty in data to determine the probability of critical configurations is acceptable. The staff found this technique will allow the DOE to provide reasonable assurance that the probability of postclosure criticality at the repository will not be underestimated. Acceptance is contingent on DOE incorporating the steps stated in the response to RAI 3-16 if there is a problem using a regression to represent a parameter. The staff found the use of the WAPDEG-generated probability distributions, for the time of WP breach and duration of the "bathtub" inside the WP, associated with the most recent TSPA, is acceptable, provided the DOE should demonstrate that no assumptions were made in the WAPDEG modeling that would be conservative for TSPA calculations but nonconservative for criticality calculations. The acceptability of the methodology to generate the regression equation used to determine k_{eff} has been evaluated in Section 5.5.4. The acceptability of the methodology to determine the risk from criticality has been evaluated in Section 5.5.6.

Modeling Approach

The modeling approach was reviewed to ensure that DOE has developed a technically defensible, transparent, and traceable method to assign probability values to criticality scenario

classes, scenarios, configuration classes, and configurations and has adequately addressed the uncertainty in data because of both temporal and spatial variations in conditions affecting potential nuclear criticality.

The staff found the use of the Monte Carlo technique an acceptable method to determine the probability of critical conditions occurring based on configurations defined by multiple uncertain parameters. The staff considered the use of data from the most recent TSPA in the criticality evaluation an acceptable source of input for the probability calculation as long as correlations among parameters are accounted for in the sampling scheme and the ranges from the TSPA are not conservative estimates for the calculation of dose but are nonconservative for criticality calculations. For example, the TSPA may use an unrealistically low value for the K_d of Pu in the unsaturated zone to be conservative. This value for the K_d of Pu may not be appropriate in the criticality calculations because a higher K_d could lead to a greater accumulation of Pu and a higher potential for criticality.

Validation Approach

The staff reviewed the proposed approach—to validate the models to be used to determine the probability of occurrence of a criticality event—against the AC in the IRSRs. The validation approach was reviewed to ensure DOE has developed a technically defensible, transparent, and traceable method for assigning probability values to criticality scenario classes, scenarios, configuration classes, and configurations.

The staff found the methodology acceptable using hand calculations and a commercial mathematical equation solver code, to verify the Monte Carlo code is properly sampling from the input parameter distributions and calculating the probability correctly, provided a sufficient number of these calculations is conducted to demonstrate that the code is performing the calculations properly across the range of the sampled parameters. In the LA, the DOE will have to provide verification that these computer codes are being implemented correctly and demonstrate that the use of these computer codes does not underestimate the probability of a criticality event for all WFs that will be disposed in the repository.

Because no open items have been identified with respect to the DOE approach in calculating the criticality probability, this area of the criticality subissue is considered closed at this time.

Model Implementation, Data, and Analyses

The reports that the DOE identified in the October 23–24, 2000, Technical Exchange as examples of model implementation, data, and analysis with respect to the probability component of the criticality subissue will be reviewed by the staff. Therefore, the closure of the criticality probability component with respect to model implementation, data, and analysis will be dependent on the staff review and acceptance of the reports that the DOE identified in the Technical Exchange.

5.5.6 Criticality Consequence

5.5.6.1 U.S. Department of Energy Approach

As part of the responses to the RAI,[21] the DOE stated that

> DOE requests acceptance of the following aspects of the consequence evaluation method for a steady-state criticality: (1) Determination of temperature such that the evaporation rate over the WP pond surface equals the volumetric drip rate into the WP (Section 4.4.1.1, page 4-45); (2) Use of the drip rate probability distribution as a function of time (which comes primarily from the climate-and mountain-scale hydrology model) (Section 4.4.1.1 as augmented in the response to RAI 3-23); and (3) Determination of radionuclide increment from depletion code (ORIGEN-S) as a function of power, integrated over the duration of the criticality (Section 4.4.1.1 as augmented in the response to RAI 4-51). Acceptance of this item is requested in Section 1.2, Part F of the TR. It should be noted that acceptance of the ORIGEN-S code will not be sought until the corresponding validation report is complete and referenced in the License Application. The use of this code in the TR, the responses to the RAIs, and supporting documentation, is intended only to provide background for understanding of the methodology.

As indicated by the request, the DOE is seeking approval of only specific aspects of criticality consequence analysis at this point. DOE is specifically requesting the review and approval of the methodology, modeling, and validation approaches for radionuclide buildup from a steady-state criticality configuration. DOE has not requested staff review of other aspects of criticality consequences, such as effect of heat from steady-state criticality on the material degradation, methodology, modeling, and validation approaches for the consequence of in-package transient criticalities and external criticalities. Therefore, the staff has not reviewed these aspects of disposal criticalities, and no approval is granted at this time.

Methodology

In Section 3.6 of the TR, the DOE stated that "... when the k_{eff} of the configuration analyzed exceeds the CL, and the probability of occurrence of that configuration is below the WP probability criterion, currently derived in Section 3.5 as approximately 10^{-4} per WP in 10,000 years, a consequence analysis is performed."

In Section 3.6.2 of the TR, DOE proposed an approach for examining the consequences of an internal or external steady-state criticality with respect to only radionuclide buildup.

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[21] Brocoum, S., U.S. Department of Energy... Methodology, Letter (November 19) to C.W. Reamer, U.S. Nuclear Regulatory Commission, Washington, DC, U.S. Department of Energy, 1999.

The proposed approach consists of first estimating the power and duration of a critical configuration. The power level is determined by the reactivity feedback (the influence of temperature on k_{eff}, the heat removal, and the rate of replenishment of the moderator). The criticality duration is most strongly determined by environmental parameters—particularly the drip rate into the WP for internal criticality—or percolation rate into the region of accumulation for external criticality.

The next step is to compute the total burnup for this power level and duration, using a point-depletion analysis to estimate the increment in radionuclide inventory caused by the criticality event.

Modeling Approach

In its approach for modeling the consequences of a steady-state critical configuration, the DOE assumes that a critical configuration is reached when the WP is flooded with water and slowly loses boron and iron from the package interior. Once a WP reaches the CL, continued small positive reactivity insertions will cause the power output of the WP to slowly rise. Subsequently, the temperature will increase and the evaporative water loss will increase. If the power exceeds a certain limit, the rate at which water is consequentially removed from the WP will exceed the rate of input, and the resulting water-level drop will provide a negative reactivity insertion, driving the WP back toward a subcritical condition. Conversely, if sufficient power is produced, the water level will be maintained, and the exchange process will continue to remove dissolved boron, thus providing a continued source of positive reactivity insertions until the point of equilibrium is achieved. The maximum steady-state power can then be estimated by determining the power required to maintain the bulk WP water temperature, taking into account the heat loss through radiation, conduction, and convection at the point where water is removed at the same rate that it drips into the WP.

Because the exact steady-state critical configuration cannot be predicted with respect to the amount of rubble covering the WP, DOE has proposed to use the average value between the rate of heat-loss by radiation versus conduction mode. DOE proposed to determine the values for the heat-loss terms by the use of specific equations.[22]

The DOE assumes the temperature increase is the value needed to evaporate only the amount of the incoming water, no more, for the WP to stay at a steady-state critical condition. With this assumption, the temperature at which the drip rate is equal to the evaporation rate can be calculated.

DOE requested acceptance under the first item for the specific equations, with respect to incremental radionuclide buildup as the result of a steady-state critical configuration.

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[22]Brocoum, S., U.S. Department of Energy... Methodology, Letter (November 19) to C.W. Reamer, U.S. Nuclear Regulatory Commission, Washington, DC, U.S. Department of Energy, 1999.

Validation Approach

In Enclosure 2 of the responses to the RAI, DOE requested acceptance of only a "... validation process for the steady-state consequence model" at this time. As part of the acceptance requested by the DOE in Enclosure 2 of the RAI responses,

> DOE seeks acceptance of the validation process for the steady-state criticality consequence model, specifically that computer code can be written to perform the numerical integration of power over time and distribution of drip rates, as well as calculating the heat loss according to well-known physics formulae. This process is described in Section 4.4.1.4 of the TR, as modified by the responses to RAIs 3-23 and 4-51. The resulting program will be checked by hand calculation. It is assumed that no validation is required for the use of well-known physics formulae. DOE plans to validate the use of ORIGEN-S to compute the radionuclide increment from steady-state criticality with available data.

In its discussion of model validation for steady-state criticality in Section 4.4.3.1 of the TR, DOE states "The methodology is validated by conservatism inherent in the methodology, which serves to define a range of configuration parameters to provide an upper bound on the increase in the radionuclide inventory." DOE points to the following assumptions, used to determine the criticality power level and its duration, as examples for inherent conservatism.

- The criticality duration extends through the period of high infiltration rate; and
- The maximum credible water infiltration rate is maintained in the wet part of a climatological cycle.

However, the DOE appears to have moved away from the conservatism argument, for validation purposes, because of the change in the modeling approach. DOE proposed to use a drip-rate probability distribution based on infiltration rates of a mountain-scale hydrology model, as opposed to some high infiltration rate. This approach would also eliminate the uncertainty associated with power calculation. Therefore, with regard to the validation of the part of the model that would calculate the power, DOE argues that using well-known physics formulae for heat loss, combined with verification of the power calculation module of the model using some hand calculations, would provide adequate validation. With respect to the radionuclide production model, the DOE indicates the model will be validated using available data.

Model Implementation, Data, and Analyses

In the October 23–24, 2000, Technical Exchange, the DOE identified reports that provide some of the data needed to support the DOE's assumptions. The reports identified by the DOE in addressing loss of isotopes through pinholes and cracks in the cladding are

- Results from NNWSI Series 3 Spent Fuel Dissolution Tests (Wilson, 1990a, pp. 3.41, 3.50)

- Cladding Credit (Ahn, 1998)

5.5.6.2 NRC Staff Evaluation

The staff evaluation of the DOE approach and positions has been conducted based on the following AC.

- DOE includes degradation of in-package criticality control system as FEP in the TSPA. DOE uses sound technical bases for selecting the design criteria that mitigate degradation of criticality control system or any potential impact of the in-package on repository performance; identifies all FEP that may increase the reactivity of the system inside the WP; identifies all the configuration classes and configurations that have potential for nuclear criticality; and includes changes in radionuclide inventory and thermal conditions in their abstraction of EB degradation.

Methodology

The staff evaluated the DOE proposed approach of estimating the steady-state criticality consequence for internal and external criticality, regarding only an increase in radionuclide inventory. The staff accepts the approach of using the quantity of water dripping on the WP as the factor determining the power level and, consequently, the incremental increase in radionuclide inventory. However, the approach for other types of critical configurations that may involve moderators other than water, especially for external criticality, must be considered. In addition, the loss of soluble neutron-absorbing isotopes from the SNF matrix through pin holes and cracks in the cladding must be considered also for contribution to the steady-state criticality. Furthermore, other types of steady-state criticality consequences, such as the heat impact of criticality on the material corrosion rate, must be considered also.

Furthermore, the staff agrees that the power can be used as an input to a depletion analysis for determining the incremental increase in the isotopic inventory. However, the modeling and the associated validation must be appropriately performed.

DOE has not considered the consequences of transient criticality. Seismically-induced and autocatalytic criticalities are the types of transient criticalities that must be considered by the DOE.

In summary, the following items should be considered in order to close the criticality consequence component of Subissue 5 with respect to the methodology.

1. In developing the methodology for steady-state criticality consequences, the DOE must consider other types of moderators, especially with respect to external criticality.

2. The DOE must also consider the loss of soluble neutron-absorbing isotopes through pin holes and cracks in the SNF cladding and its effect on steady-state criticality consequence.

3. The DOE must also include other types of steady-state criticality consequences, especially with respect to internal criticality, in its consequence analysis approach.

4. The DOE must develop and present a request for approval of a methodology for transient criticality.

5. The DOE needs to develop and present, for NRC acceptance, the modeling approach for transient criticality consequence.

6. The DOE needs to develop a validation approach for the power model for steady-state criticality consequence.

7. The DOE is required to develop a validation approach for a transient criticality consequence model.

In the October 23–24, 2000, Technical Exchange , the DOE indicated the previous Open Items have been addressed in the Topical Report, Rev. 01, which will be issued in January 2001. The staff will review and assess the Topical Report, Rev. 01, and provide the results of the assessment in the next revision of the IRSR. Therefore, the closure of the criticality consequence methodology will be dependent on the review and acceptance of the Topical Report, Rev. 01.

Modeling Approach

With respect to evaluation of the DOE modeling approach, the staff cannot evaluate the accuracy and acceptability of the equations used and the associated approaches because of the unavailability of any validation results regarding the model.

The inherent assumption in the foregoing approach is that the given configuration has a negative reactivity feedback associated with the changes in the moderator temperature. This may be true for a significant number of WPs with degraded internal components and intact assemblies. However, there may be some configurations with large gaps between the intact assemblies, because of degradation of internal components, which may cause a positive reactivity feedback from the changes in the moderator temperature. Another type of configuration that may not be covered by the above approach is the presence of other moderators such as silica. DOE indicated that no configuration has been found thus far that would exhibit higher reactivity with moderators other than water.

Provided DOE continues to identify and examine all possible configurations, especially with respect to moderators other than water, the staff agrees that, for a steady-state criticality condition to be sustained, with water as the moderator with positive reactivity coefficient, the amount of incoming water must be equivalent to the quantity of water being removed from the WP. A decrease in the drip or evaporation rates could disrupt the sustained criticality conditions.

In its second part of the request, DOE proposes the "Use of the drip rate probability distribution as a function of time".... As indicated by the DOE, the drip rate comes primarily from the climate model and mountain-scale hydrology model.

Staff acceptance of the drip rate depends on the satisfactory resolution of climate change, hydrologic effects of climate change, present-day shallow infiltration, deep percolation, matrix diffusion, and the other related subissues in the pertinent IRSRs. Therefore, staff acceptance of the DOE proposed approach about using the drip rate probability distribution as a function of time is pending the complete and satisfactory resolution of the related subissues.

In its third request item, DOE requests the acceptance of the methodology for "Determination of radionuclide increment from depletion code (ORIGEN-S) as a function of power, integrated over the duration of criticality (Section 4.4.1.1 of the TR as augmented in the response to RAI)." The DOE states "... the power level used to determine the burnup/depletion will be based on a specified probability distribution, " instead of the averaging method indicated.

The staff considers the approach in determining power is not part of the request at this point. As indicated by the response to the RAI, the approach has changed since the submittal of the TR. The staff agrees that a depletion analysis using the power integrated during criticality should be performed to determine the incremental increase in radionuclide inventory. However, this agreement is contingent on the following conditions:

- An acceptable approach for including uncertainty of power,
- Demonstration of the appropriateness and validity of the depletion code, and
- Inclusion of the impact of heat from steady-state criticality on the corrosion rate.

Validation Approach

With respect to model validation, the staff believes that most of the computer models that have been developed are based on well-known physics formulae. It is the combination of these well-known formulae that is used to build a model and performs a validation to provide assurance that the combination of the formulae can predict the behavior of the system. Hand calculations are simply model verification rather than model validation. The staff realizes that a steady-state criticality within the YM environment for thousands of years is not something for which one can find benchmark experiments or construct scale-model experiments. The staff believes that natural analogs may be an approach that the DOE can use to validate the power model and the steady-state criticality consequence model as a whole. The natural analogs may be more appropriate for an integral type of validation of the steady-state external criticality consequence model.

With regard to the approach for the depletion model, the staff assumes the validation approach presented by the DOE for the isotopic section would also apply to the depletion part of the steady-state criticality consequence analysis. Therefore, the same conditions and open items identified earlier would apply to this section. With respect to postclosure, the isotopic models can be validated only for the decay constants. This validation may be performed by using the

chemical assays across a time range, and extrapolation can be made using the established trend.

Model Implementation, Data, and Analyses

The reports identified by the DOE in the October 23–24, 2000, Technical Exchange as examples of model implementation, data, and analysis with respect to the consequence component of the criticality subissue will be reviewed by the staff. In addition, the DOE agreed to provide information on how the increase in the radiation fields due to the criticality event affects the consequence evaluation because of increased radiolysis inside the WP and at the surfaces of nearby WPs. Therefore, the closure of the criticality analysis component with respect to model implementation, data, and analysis will be dependent on the staff review and acceptance of the reports that the DOE identified in the Technical Exchange.

5.5.7 Criticality Risk

5.5.7.1 U.S. Department of Energy Approach

The total risk associated with internal criticality is the combination of probability and consequences for all the possible scenarios and configurations of incremental dose to the member of the critical group at 20 km from the proposed YM site.

DOE proposed "to conduct detailed TSPA calculations using the incremented radionuclide inventory" if the initial PA evaluation indicates significant impact on the repository performance. DOE is planning to simulate the consequence of criticality by adding the incremented radionuclide inventory to the source term and performing TSPA analysis.

The DOE preliminary analysis for a single PWR WP becoming critical at a steady-state condition for 10,000 years indicates that the increase in the inventory of the 36 TSPA isotopes is 24 percent. The increase in the isotopes that are important to the repository performance, I-129, Tc-99, Np-237, and U-234, are between 4 and 11 percent. Tc-99 provides the highest and earliest incremental dose, which is around 0.07 mrem/year. This dose appears to be unrealistically high to result from only a 4-percent increase in the inventory of Tc-99 in a single WP.

5.5.7.2 NRC Staff Evaluation

The staff evaluation of the DOE approach and positions has been conducted based on the following AC .

- DOE includes degradation of in-package criticality control system as FEP in the TSPA. DOE uses sound technical bases for selecting the design criteria that mitigate degradation of criticality control system or any potential impact of the in-package on repository performance; identifies all FEP that may increase the reactivity of the system inside the WP; identifies all the configuration classes and configurations that have

potential for nuclear criticality; and includes changes in radionuclide inventory and thermal conditions in their abstraction of EB degradation.

The staff believes the approach shown in Figure 1-1 of the RAI responses needs to be followed. The approach in Figure 1-1 of the RAI responses indicates that a probability and consequence analyses will be performed for any critical configurations regardless of their probability. The staff believes other consequences such as additional heat buildup and mechanical disruption from transient criticality need to be included in the criticality consequences and in the criticality risk.

Secondly, DOE indicated in technical exchanges that it is planning to give all the consequence/probability results to DOE/TSPA people for inclusion or exclusion in the TSPA. The DOE/TSPA need to identify how the criticality FEP included in its database correspond to the configuration classes identified by the DOE in the TR, and what the basis is for the statement "criticality during the first 10,000 years is screened out on the basis of low probability" (Swift, 2000). DOE proposed only an approach in calculating the probability for critical configurations. It is not clear how the DOE/TSPA has concluded more than 30 critical configuration classes can be screened out based on probability.

In order to close this component of Subissue 5

1. The DOE must include other consequences, such as heat buildup and further degradation of the WP and WFs in its risk analyses.

2. The DOE must demonstrate a consistency between the TR criticality FEP and the FEP in the TSPA FEP database.

3. The DOE must provide the basis for claims that all criticality scenarios and configurations to be screened out based on probability.

In the October 23–24, 2000, Technical Exchange, the DOE alluded to the above items. With respect to including all consequences of criticality in addition to the radionuclide buildup in the risk analysis, the DOE stated that "any significant mechanical effects of the criticality will be evaluated by modifying the degradation characteristics of the affected barriers, and any affected model parameters will be modified." The DOE indicated that Topical Report, Rev. 01, addresses this requested information. Closure of this item is pending the staff review and acceptance of the Topical Report, Rev. 01.

With regard to consistency between the TR criticality FEP and the FEP database, the DOE provided the staff with FEP mapping tables at the October 23–24, 2000, Technical Exchange. The closure of this item is pending the staff review of the mapping tables and the DOE responding to issues raised by the review.

With respect to providing a basis for screening criticality, the DOE stated, in the Technical Exchange, that "in-package criticality has been excluded from the TSPA on the basis of low

probability for the regulatory period." The DOE cited two reports as the documentation for low probability:

- Probability of Criticality Before 10,000 Years, CAL-EBS-NU-000014 (draft in progress)
- Analyses to Support Screening of System-Level Features, Events, and Processes for the Yucca Mountain Total System Performance Assessment-Site Recommendation, ANL–WIS–MD–00019 (draft in progress)

However, the DOE has proposed to perform a "what-if" analysis that would evaluate the impact of a single WP early (pre-10,000-year) criticality event. Beyond the 10,000-year regulatory period, the DOE stated that "all probability/consequence pairs will be evaluated for inclusion in at least one TSPA sensitivity analysis." The DOE has decided to treat criticality in a sensitivity analysis instead of including in the TSPA basecase. The staff closure of this item is pending the DOE providing and NRC reviewing and accepting the CAL–EBS–NU–000014 calculations, ANL–WIS–MD–00019 report, the "what-if" analysis, the sensitivity analyses for most significant probability/consequence criticality scenarios, and addressing the issues associated with the criticality FEP in the FEP database prior to LA.

5.5.8 Status and Path to Resolution

The resolution of the in-package criticality subissue is proceeding through the use of TR, SER, and this IRSR. The criticality TR is the document in which the DOE is presenting the details of the methodology and modeling approach for postclosure disposal criticality. The criticality SER is the document in which the staff presents its assessment of the criticality TR. The IRSR is the document in which the staff provides the status of its technical interaction with the DOE, through the TR/SER, and other issues that may not have been covered in the TR/SER.

The previous sections provided the status of the NRC and the DOE staff interactions on the seven components of the criticality subissue; summarized the results of the criticality SER on the TR, Rev. 0; and identified information needed with respect to modeling implementation, data, and analyses. Therefore, the criticality subissue is closed, pending the DOE providing, and NRC reviewing and accepting, prior to LA, the following reports, analyses, calculations, and information, as listed in the transcripts of the NRC/DOE Technical Exchange.[23]

- Disposal Criticality Analysis Methodology Topical Report, Rev. 01, addressing all 28 Open Items in the SER (expected January 2001)
- Modified Disruptive Events FEP AMR, revised FEP database, and the Analyses to Support Screening of System-Level Features, Events, and Processes for the Yucca

[23]Schlueter, J., Letter (October 27) to S. Brocoum, U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting Related to Criticality (ML003763270). Washington, DC: U.S. Nuclear Regulatory Commission. 2000.

Mountain Total System Performance Assessment-Site Recommendation (expected January 2001)

- Probability of Criticality Before 10,000 Years calculation (received November 2000)
- Updated Calculation of Probability of Criticality for EDA II Waste Package Design, CAL–UDC–MD–0000001, Revision 00 (CRWMS M&O, 1999c)
- Probability of Criticality for MOX SNF, CAL–EBS–NU–000007, Revision 00 (CRWMS M&O, 1999d)
- Waste Package Related Impacts of Plutonium Disposition Waste Forms in a Geologic Repository, TDR–EBS–MD–000003, Revision 01 (CRWMS M&O, 2000bb), for application to the Pu-ceramic-containing WP
- EQ6 Calculation for Chemical Degradation of Shippingport LWBR (Th/U oxide) Spent Nuclear Fuel Waste Packages, CAL–EDC–MD000008, Revision 00 (not received)
- EQ6 Calculation for Chemical Degradation of Pu-Ceramic Waste Packages: Effects of Updated Materials Composition and Rates, CAL–EDC–MD–000003, Revision 00 (CRWMS M&O, 2000cc)
- Probability of a PWR Uncanistered Fuel Waste Package Postclosure Criticality (CRWMS M&O, 1998e)
- Results from NNWSI Series 3 Spent Fuel Dissolution Tests (Wilson, 1990a)
- The list of validation reports and their schedules. The geochemical model validation reports for Geochemistry Model Validation Report: Degradation and Release and Geochemistry Model Validation Report: Material Accumulation are expected to be available during 2001. The other reports are expected to be available during FY2002, subject to the results of detailed planning and scheduling.
- Provide information on how the increase in the radiation fields from the criticality event affects the consequence evaluation, because of increased radiolysis inside the WP and at the surfaces of nearby WPs or demonstrate how the current corrosion and dissolution models encompass the range of chemical conditions and corrosion potentials that would result from this increase in radiolysis. DOE has stated that the preliminary assessment (calculation) of radiolysis effects from a criticality event will be available to NRC during February 2001. The final assessment of these conditions will be available to NRC prior to LA.
- The "what-if" analysis to evaluate the impact of an early criticality, assuming a WP failure. DOE has stated that it would provide the requested analyses prior to LA. Actual schedule to be provided pending DOE planning process.

- Sensitivity analyses that will include the most significant probability/consequence criticality scenarios. DOE has stated that it would provide the requested analyses prior to LA. Actual schedule to be provided pending DOE planning process.

Any NRC concern not specifically covered in this section is dealt with a risk-informed approach (i.e., the concern may not be important in PA).

5.6 SUBISSUE 6: THE EFFECTS OF ALTERNATE ENGINEERED BARRIER SUBSYSTEM DESIGN FEATURES ON CONTAINER LIFETIME AND RADIONUCLIDE RELEASE FROM THE ENGINEERED BARRIER SUBSYSTEM

This subissue is concerned with the effects of alternate design features (e.g., DS, ceramic coatings, and backfill) that may be used in the proposed repository. Based on the current design for the SR, only the DS is now included among the alternate features. The DOE is considering the incorporation of a Ti-alloy DS to divert groundwater that may enter the drift away from the WPs, thereby extending the lifetimes of the WPs and delaying radionuclide release (CRWMS M&O, 2000d). The main components important to this subissue in examining the DS are thermal embrittlement and EAC of Ti-Pd alloys and uniform and localized corrosion of Ti-Pd alloys.

Model abstractions that apply to this subissue are

- ENG1 Degradation of Engineered Barriers
- ENG2 Mechanical Disruption of Engineered Barriers
- ENG3 Quantity and Chemistry of Water Contacting the WPs and WFs
- ENG4 Radionuclide Release Rates and Solubility Limits

5.6.1 Description of the U.S. Department of Energy Approach

The description of the DOE approach in the following sections is based on the WP Degradation PMR and supporting AMRs. In the NRC/DOE Technical Exchange and Management Meeting on CLST,[24] DOE agreed to provide additional information through revised AMRs or other documents prior to or at the time of the LA, as described in detail in Section 5.1.3.

5.6.1.1 Thermal Embrittlement and Environmentally Assisted Cracking of Ti Drip Shield

The DOE approach consists of examining the possible environments to which the DS may be exposed (e.g., temperature, and chemistry of incoming water) and evaluating the effects of these conditions on the possible failure modes and rates for Pd-bearing Ti alloys (in particular Ti grades 7 and 16). Failure modes considered include thermal embrittlement, EAC, [consisting of

[24]NRC/DOE Technical Exchange and Management Meeting on the Key Technical Issue: Container Life and Source Term, Las Vegas, NV, September 12–13, 2000.

SCC and HE or hydride-induced cracking (HIC)], uniform corrosion, and localized corrosion (pitting and crevice).

The possibility for thermal embrittlement of Ti used in DS construction was excluded for further analysis because it was considered to have a low probability of occurrence in the FEP analysis (CRWMS M&O, 2000b).

EAC was examined in two main parts: SCC and HIC. Analyses of these failure modes was based on the assumption that backfill will be present in the repository and, thus, precludes the possibility of increased stresses associated with rockfall. Since the issuance of the PMR on WP degradation Revision 00 (CRWMS M&O, 2000b) and also noted in the introduction of the PMR, the backfill option is no longer being considered. Because no new information on the effects of its removal is currently available from the DOE, this discussion only considers the situation in which backfill is still included. The PMR (CRWMS M&O, 2000b) and corresponding AMR (CRWMS M&O, 2000s) made a clear distinction between SCC and HIC. Within this framework, SCC was precluded as a likely failure mode because the stress levels would be insufficient for SCC to occur due to the presence of backfill. Furthermore, if SCC did occur, it was claimed that any cracks that developed would be plugged by corrosion products and, therefore, would not be available for the transport of water and subsequent dripping onto the WP. The approach taken by DOE to evaluate HIC is based on the assumption that the dominant cathodic reaction occurring on the metal surface during passive (uniform) dissolution is hydrogen evolution, and it is assigned a reaction rate equal to the passive dissolution rate observed from coupon testing. Of the hydrogen gas produced from this cathodic reaction, a fraction (between 0.02 to 0.10) will enter into the metal as hydrogen atoms, which may then lead to a loss in ductility (i.e., embrittlement). HIC is said to be possible once a critical hydrogen concentration has been exceeded. Based on the uniform corrosion rates observed from coupon testing and the assumptions involved with the fraction of hydrogen eventually adsorbed into the metal lattice, HIC was concluded not to have a significant effect on DS life expectancy during the 10,000-year performance period.

5.6.1.2 Uniform and Localized Corrosion of Ti Drip Shield

According to the WP Degradation PMR (CRWMS M&O, 2000b) and the general corrosion and localized corrosion of the DS AMR (CRWMS M&O, 2000r), Ti grade 16 coupons were exposed for a period of 1 year to a variety of environmental conditions. The tests showed there was little influence of temperature from 60 to 90 °C nor was there a significant influence of testing environment; all tests were conducted in variants of J-13 well water. A wide variation in the measured weight loss (resulting in corrosion rates of ~ -1,700 to 150 nm/yr) was reported. This variability was explained as resulting from differences in the postexposure cleaning procedures used to remove corrosion product buildup. Similar tests were conducted using creviced specimens with no significant attack observed under the crevice former. It was noted that the corrosion rates were similar for the uniform corrosion coupons and the crevice corrosion coupons, and it was assumed then that the main operational corrosion mode for the creviced specimens was also uniform passive corrosion of the exposed surfaces. Based on the

maximum corrosion rates observed (350 nm/yr for creviced specimens), it was concluded that failure of Ti alloy DS would be unlikely within the 10,000-year performance period.

A limited set of CPP experiments was also performed to examine localized corrosion susceptibility. Based on experiments which were conducted in SSW at 120 °C and in SCW at 90 °C (the nominal compositions for these solutions are shown in Table 2), no localized corrosion was noted even when polarization was conducted to 2.5 $V_{Ag/AgCl}$. A critical threshold potential was noted in the polarization scans near 1 $V_{Ag/AgCl}$, and was believed to be associated with oxygen evolution (CRWMS M&O, 2000r).

5.6.2 Staff Evaluation of the U.S. Department of Energy Approach

5.6.2.1 Thermal Embrittlement and Environmentally Assisted Cracking of Ti Drip Shield

Acceptance Criteria

The AC applicable to this subissue are based on the degradation of EB and include

- The description of engineered barriers, design features, degradation processes, physical phenomena, and couplings that may affect the degradation of the engineered barriers is adequate. For example, it includes materials and methods used to construct the engineered barriers and considers degradation processes such as uniform corrosion, pitting corrosion, crevice corrosion, stress corrosion cracking, intergranular corrosion, microbially influenced corrosion, dry-air oxidation, hydrogen embrittlement, as well as the effects of wet and dry cycles, material aging and phase stability, welding, and initial defects on the degradation modes for the engineered barriers.

- Sufficient technical bases for the inclusion of FEP related to degradation of engineered barriers in the Total System Performance Assessment abstractions are provided.

- Parameters used to evaluate the degradation of engineered barriers in the safety case are adequately justified (e.g., laboratory corrosion tests, site-specific data such as data from drift scale tests, in-service experience in pertinent industrial applications, and test results not specifically performed for the Yucca Mountain site, etc.). DOE describes how the data were used, interpreted, and appropriately synthesized into the parameters.

- Sufficient data have been collected on the characteristics of the engineered components, design features, and the natural system to establish initial and boundary conditions for the Total System Performance Assessment abstraction of degradation of engineered barriers.

- Data on the degradation of the engineered barriers, (e.g., general and localized corrosion, microbial influenced corrosion, galvanic interactions, hydrogen embrittlement, and phase stability) used in the Total System Performance Assessment abstraction are

based on laboratory measurements, site specific field measurements, industrial analog and/or natural analog research, and tests designed to replicate the range of conditions that may occur at the Yucca Mountain site. As appropriate, sensitivity or uncertainty analyses used to support the DOE Total System Performance Assessment abstraction are adequate to determine the possible need for additional data.

- Degradation models for the processes that may be significant to the performance of the engineered barriers are adequate. For example, DOE models consider the possible degradation of the engineered barriers as a result of uniform and localized corrosion processes, stress corrosion cracking, microbial influenced corrosion, hydrogen embrittlement, and incorporate the effects of fabrication processes, thermal aging, and phase stability.

- For those degradation processes that the Total System Performance Assessment abstraction indicates are significant to the performance of the engineered barriers, DOE provides appropriate parameters based on techniques that may include laboratory experiments, field measurements, industrial analogs, and process-level modeling studies conducted under conditions relevant to the range of environmental conditions within the WP emplacement drifts. DOE also demonstrates the capability to predict the degradation of the engineered barriers in laboratory and field tests.

- For the selection of parameters used in conceptual and process-level models of engineered barrier degradation that can be expected under repository conditions, assumed range of values and probability distributions are not likely to underestimate the actual degradation and failure of engineered barriers as a result of corrosion.

- Alternative modeling approaches of FEP are consistent with available data and current scientific understanding and consider the results and limitations appropriately in the abstraction.

- Numerical corrosion models used to calculate the lifetimes of the engineered barriers are adequate representations, considering the associated uncertainties in the expected long-term behaviors, the range of conditions (including residual stresses) and the variability in engineered barrier fabrication processes (including welding).

- Evidence is sufficient to show that models used to evaluate performance are not likely to underestimate the actual degradation and failure of engineered barriers as a result of corrosion or other degradation processes.

- DOE uses alternative modeling approaches consistent with available data and current scientific understanding, and evaluates their model results and limitations using tests and analyses that are sensitive to the processes modeled. For example, for processes such as uniform corrosion, localized corrosion, and stress corrosion cracking of the engineered barriers, DOE considers alternative modeling approaches to develop its

understanding of environmental conditions and material factors are significant to these degradation processes.

- The description of geological and engineering aspects of design features, physical phenomena, and couplings that may affect mechanical disruption of engineered barriers is adequate. For example, the description may include materials used in the construction of engineered barrier components, environmental effects (e.g., temperature, water chemistry, humidity, radiation, etc.) on these materials, and mechanical failure processes and concomitant failure criteria used to assess the performance capabilities of these materials. Conditions and assumptions in the Total System Performance Assessment abstraction of mechanical disruption of engineered barriers are readily identified and consistent with the body of data presented in the description.

- The Total System Performance Assessment abstraction of mechanical disruption of engineered barriers uses assumptions, technical bases, data, and models that are appropriate and consistent with other related DOE abstractions. For example, assumptions used for mechanical disruption of engineered barriers are consistent with the Total System Performance Assessment abstraction of degradation of engineered barriers. The descriptions and technical bases provide transparent and traceable support for the abstraction of mechanical disruption of engineered barriers.

- Sufficient data have been collected on the geology of the natural system, engineering materials, and initial manufacturing defects to establish initial and boundary conditions for the Total System Performance Assessment abstraction of mechanical disruption of engineered barriers.

- Data on geology of the natural system, engineering materials, and initial manufacturing defects used in the Total System Performance Assessment abstraction are based on appropriate techniques. These techniques may include laboratory experiments, site-specific field measurements, natural analog research, and process-level modeling studies. As appropriate, sensitivity or uncertainty analyses used to support the DOE Total System Performance Assessment abstraction are adequate to determine the possible need for additional data.

- Engineered barrier mechanical failure models for disruption events are adequate. For example, these models may consider effects of prolonged exposure to the expected emplacement drift environment, material test results not specifically designed or performed for the Yucca Mountain site, and engineered barrier component fabrication flaws.

- Process-level models used to represent mechanically disruptive events within the emplacement drifts at the proposed Yucca Mountain repository are adequate. Parameter values are adequately constrained by Yucca Mountain site data such that the effects of mechanically disruptive events on engineered barrier integrity are not underestimated.

Parameters within conceptual models for mechanically disruptive events are consistent with the range of characteristics observed at Yucca Mountain.

- Uncertainty is adequately represented in parameter development for conceptual models, process-level models, and alternative conceptual models considered in developing the Total System Performance Assessment abstraction of mechanical disruption of engineered barriers. This may be done either through sensitivity analyses or use of conservative limits.

- DOE uses appropriate methods for nondestructive examination of fabricated engineered barriers, the type, size, and location of fabrication defects that may lead to premature failure as a result of rapidly initiated engineered barrier degradation. DOE specifies and justifies the allowable distribution of fabrication defects in the engineered barriers and assesses the effects of defects that cannot be detected on the performance of the engineered barriers.

NRC Staff Evaluation

Though not considered important by the DOE, thermal embrittlement of Ti alloys has been reported based on thermally driven redistribution of nearly insoluble impurities from grain interiors to grain boundaries (Nesterova, et al., 1980). This redistribution results in embrittlement of the material with negligible change in strength (though wide variations in ductility are observed) and increased intergranular fracture. As discussed in Section 4.6.2, such segregation tends to result in precipitation of finely dispersed particles at the grain boundaries. For CP Ti and α-Ti alloys that contain Ni and Fe as impurities, these precipitates have been identified as $Ti_2(Fe,Ni)$. Embrittlement has been noted at temperatures as low as 350 °C after 500 hours. However, the possibility of embrittlement at lower temperatures when exposed for longer periods has not been examined. DOE abstraction analyses of HE of Ti alloys could be used to capture any possible effects of thermal embrittlement on predicted drip shield life expectancy. In addition, the yield strength and the ultimate tensile strength of Ti grade 7 decrease significantly with temperatures reaching at approximately 250 °C values close to half of those at room temperature. As a consequence, the effect of temperature on the mechanical integrity of the DS should be examined.

EAC of Ti-Pd alloys has not been extensively examined. It is generally accepted that EAC of Ti alloys occurs through an HE-type mechanism probably related with hydride precipitation and cracking. Use by DOE of the minimum hydrogen concentration necessary for HE based on CP Ti is conservative. The technical basis for the fraction of hydrogen absorbed, especially considering the well-known catalytic properties of Pd for hydrogen generation, however, needs to be strengthened. In addition, reliance on the passive corrosion rates measured from weight loss coupons may lead to a nonconservative estimate of the quantity of hydrogen absorbed. The corrosion rates measured (approximately 10 to a few hundreds of nanometers per year) using weight loss methods, especially given the uncertainties concerning cleaning procedures, may be unreliable and nonconservative. Furthermore, in the AMR dealing with general and localized corrosion of the DS (CRWMS M&O, 2000r) it is concluded that the majority of the weight loss

measurements during coupon exposure tests was at or below the level of detection. Based on the electrochemical corrosion tests, much higher passive dissolution rates were observed (at least a factor of 30 larger and, in some cases, more than 400 times larger), which could lead to a more conservative estimate of the hydrogen concentration in the alloy after 10,000 years. This estimate suggests that HE of Ti may occur under anticipated repository conditions. It is suggested that DOE examine the possibility of enhanced hydrogen uptake and absorption in the Pd-bearing Ti alloys, especially grade 7 rather than grade 16 because the differences in Pd content of these materials could make a difference in the measured hydrogen uptake rates. It is also recommended that DOE confirm the low corrosion rates measured from weight loss experiments and from polarization data with long-term electrochemical tests designed to sensitively measure the passive/corrosion rate.

The technical concerns raised in this section are planned to be addressed by the DOE in future versions of the WP Degradation PMR and related AMRs as indicated in Section 5.6.3. on Status and Path to Resolution.

5.6.2.2 Uniform and Localized Corrosion of Ti Drip Shield

Acceptance Criteria

- The description of engineered barriers, design features, degradation processes, physical phenomena, and couplings that may affect the degradation of the engineered barriers is adequate. For example, it includes materials and methods used to construct the engineered barriers and considers degradation processes such as uniform corrosion, pitting corrosion, crevice corrosion, stress corrosion cracking, intergranular corrosion, microbially influenced corrosion, dry-air oxidation, hydrogen embrittlement, as well as the effects of wet and dry cycles, material aging and phase stability, welding, and initial defects on the degradation modes for the engineered barriers.

- Sufficient technical bases for the inclusion of FEP related to degradation of engineered barriers in the Total System Performance Assessment abstractions are provided.

- Parameters used to evaluate the degradation of engineered barriers in the safety case are adequately justified (e.g., laboratory corrosion tests, site-specific data such as data from drift scale tests, in-service experience in pertinent industrial applications, and test results not specifically performed for the Yucca Mountain site, etc.). DOE describes how the data were used, interpreted, and appropriately synthesized into the parameters.

- Data on the degradation of the engineered barriers, (e.g., general and localized corrosion, microbial influenced corrosion, galvanic interactions, hydrogen embrittlement, and phase stability) used in the Total System Performance Assessment abstraction are based on laboratory measurements, site specific field measurements, industrial analog and/or natural analog research, and tests designed to replicate the range of conditions that may occur at the Yucca Mountain site. As appropriate, sensitivity or uncertainty

analyses used to support the DOE Total System Performance Assessment abstraction are adequate to determine the possible need for additional data.

- For those degradation processes that the Total System Performance Assessment abstraction indicates are significant to the performance of the engineered barriers, DOE provides appropriate parameters based on techniques that may include laboratory experiments, field measurements, industrial analogs, and process-level modeling studies conducted under conditions relevant to the range of environmental conditions within the WP emplacement drifts. DOE also demonstrates the capability to predict the degradation of the engineered barriers in laboratory and field tests.

- For the selection of parameters used in conceptual and process-level models of engineered barrier degradation that can be expected under repository conditions, assumed range of values and probability distributions are not likely to underestimate the actual degradation and failure of engineered barriers as a result of corrosion.

- DOE uses alternative modeling approaches consistent with available data and current scientific understanding, and evaluates their model results and limitations using tests and analyses that are sensitive to the processes modeled. For example, for processes such as uniform corrosion, localized corrosion, and stress corrosion cracking of the engineered barriers, DOE considers alternative modeling approaches to develop its understanding of environmental conditions and material factors are significant to these degradation processes.

- Numerical corrosion models used to calculate the lifetimes of the engineered barriers are adequate representations, considering the associated uncertainties in the expected long-term behaviors, the range of conditions (including residual stresses) and the variability in engineered barrier fabrication processes (including welding).

- Evidence is sufficient to show that models used to evaluate performance are not likely to underestimate the actual degradation and failure of engineered barriers as a result of corrosion or other degradation processes.

NRC Staff Evaluation

Though considerable data have been obtained examining the possibility and rates associated with uniform and localized corrosion, several areas of clarification are suggested. As mentioned previously, DOE needs to confirm the low corrosion rates measured from weight loss experiments with other tests designed to sensitively measure the passive-corrosion rate. This confirmation is particularly important because it appears there is an inconsistency between the AMR on general and localized corrosion (CRWMS M&O, 2000r) and the PMR (CRWMS M&O, 2000b). The AMR claims that the weight loss measurements are at or below the reliable detection limit, yet these values are used for life prediction purposes in the PMR. Of possibly greater importance is the lack of experimental work examining the possible detrimental effects of fluoride on the corrosion behavior of Ti. Though present in some test environments at low

levels, the presence of other species, such as Ca and Si, limit the concentration of free fluoride available for complexation with Ti (Schutz and Grauman, 1985).

From the perspective of localized corrosion, though little or no localized corrosion has been observed thus far, the localized corrosion behavior of Ti-Pd alloys has not been extensively studied. It has been observed that, under relatively aggressive conditions, these materials still exhibit high crevice corrosion resistance (Brossia and Cragnolino, 2000a). In the presence of fluoride, however, significant attack has been reported, and, in fact, some crevice corrosion in chloride-fluoride environments has been observed (Brossia and Cragnolino, 2000b). In addition, the possible detrimental effects of fabrication methods, such as weldments, have not been evaluated and further evaluation should be provided once the design has been finalized.

The technical concerns raised in this section are planned to be addressed by the DOE in future versions of the WP Degradation PMR and related AMRs as indicated in Section 5.6.3. on Status and Path to Resolution.

5.6.3 Status and Path to Resolution

This subissue is considered closed, pending additional information, as discussed in the previous two subsections. The path to resolution is based on DOE's presentation and the agreements reached in the NRC/DOE Technical Exchange and Management Meeting on CLST regarding this subissue. Any NRC concern not specifically covered in this section is dealt with a risk-informed approach (i.e., the concern may not be important in PA). The agreements summarized below are abstracted from the transcripts of the meeting.[25]

DOE agreed to provide documentation on several components of this subissue that are similar to those for the containers as discussed in Section 5.1.3. These components are the chemical composition and the physical characteristics of the environment in contact with the WP and the drip shield, alternative methods to measure corrosion rates or justification of the current approach, and corrosion rate data from the LTCTF. In addition, DOE will provide documentation on what it assumes are the nondeleterious effects of the fluoride anion and trace heavy metal cations on corrosion modes and rates. An approach similar to that proposed for Alloy 22 will be used. The documentation will be available in the revised AMR titled General Corrosion and Localized Corrosion of the Drip Shield (ANL-EBS-MD-000004) to be completed by LA.

SCC testing of Ti will be conducted using an approach similar to that adopted for Alloy 22. The data will be documented in the revised AMR titled Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier and the Stainless Structural Material (ANL-EBS-MD-000005), to be completed by LA. Regarding hydride embrittlement, DOE will provide additional justification for the use of a value of 400-ppm hydrogen as a threshold criterion for the occurrence of embrittlement or perform a sensitivity analysis using a lower value. DOE will

[25]Schlueter, J., Letter (October 4) to S. Brocoum, U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Key Technical Issue: Container Life and Source Term (ML003760868). Washington, DC: U.S. Nuclear Regulatory Commission. 2000.

conduct tests comparing various Ti alloys, such as Ti grade 2 (commercial purity Ti), with grades 7 and 16 (Ti-Pd alloys) and grades 5 and 24 (Ti-6Al-4V alloy, without and with Pd as alloying element) to determine the hydrogen threshold in hydrogen-charged notched tensile specimens and to evaluate the hydrogen pickup of galvanically coupled specimens in the LTCTF. Additional justification will be presented in the report Review of Expected Behavior of Alpha Titanium Alloys under Yucca Mountain Condition (TDR-EBS-MD-000015), which will be available in January 2001. In the same report, the technical basis for the assumed fraction of hydrogen absorbed into Ti as a result of corrosion reactions will be provided.

An important factor in the consideration of mechanical failure of the drip shield as a result of rockfall is the decrease in tensile mechanical properties of Ti alloys with increasing temperature above 200 °C. DOE will provide temperature distribution (CCDF) of the drip shield as a function of time under the current EBS design in the next revision of the AMR on Multiscale Thermohydrological Model (ANL–EBS–MD–000049), which will be available in January 2001.

DOE agreed to provide the justification for not including the rockfall effect and deadload from drift collapse on the consideration of SCC for drip shield. The documentation for the rockfall and dead-weight effects will be presented in the next revision of the SCC AMR (ANL-EBS-MD-000005) prior to LA. DOE agreed to provide documentation justifying that shell elements include normal and transverse stresses in the calculations, and more accurate results for thin elements using far fewer elements. This justification will be documented in the next revision of AMR titled Design Analysis for the Ex Container Components (ANL-XCS-ME-000001). DOE stated that it will demonstrate how the Tresca failure criterion bounds a fracture mechanics approach to calculating the mechanical failure of the drip shield. DOE stated that they believe the current approach of using American Society of Mechanical Engineers (ASME) Code is appropriate for this application. Additional justification for this conclusion will be included in the next revision of AMR titled Design Analysis for the Ex-Container Components (ANL-XCS-ME-000001) to be completed prior to LA. Rockfall calculations taking into consideration drip shield wall thinning due to corrosion, hydride embrittlement of titanium, and rockfalls of multiple rock blocks will also be included in this AMR. Seismic calculations addressing the load of fallen rock on the drip shield will be included in the next revision of this AMR. DOE stated that it will demonstrate that the drip shield mechanical analysis addressing seismic excitation is consistent with the design basis earthquake covered in the SDS KTI. DOE stated that the same seismic evaluations of drip shield (revision of AMRs ANL-UDC-MD-000001 and ANL-XCS-ME-000001) will support both the SDS KTI and the CLST KTI, therefore consistency is ensured.

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APPENDIX A

Table A-1. Status of U.S. Nuclear Regulatory Commission site characterization analysis open items on waste package and release from engineered barrier system

Item ID	Source	Title	Status	KTI
Comment 5	SCA	Interpretation of substantially complete containment	Closed	CLST
Comment 6	SCA	Performance assessment: hypothesis testing table and alternative conceptual models		All
Comment 25	SCA	Rationale on additional testing on waste and interactions between and among radionuclides on sorption	Closed	CLST ENFE RT
Comment 28	SCA	Sorption on particulates and colloids	Closed, pending	RT ENFE CLST
Comment 30	SCA	Solubility modeling	Closed, pending	ENFE RT CLST
Comment 44	SCA	Overall goal is not consistent with substantially complete containment	Closed	CLST
Comment 47	SCA	Relationship of postclosure tectonics to the waste package and the engineering barrier system requirement	Closed, pending	SDS CLST
Comment 79	SCA	Adequacy of waste package corrosion tests for the repository		ENFE CLST
Comment 80	SCA	Performance goals consistent with interpretation and intent of substantially complete containment	Closed	CLST

APPENDIX A

Table A-1. Status of U.S. Nuclear Regulatory Commission site characterization analysis open items on waste package degradation and radionuclide release from engineered barrier subsystem (cont'd)

Item ID	Source	Title	Status	KTI
Comment 81	SCA	Adequacy of program in stress corrosion cracking behavior of waste packages	Closed	CLST ENFE
Comment 82	SCA	There is an inadequate discussion on how the waste package performance may be verified at the time of license application		CLST
Comment 83	SCA	The term "uniform corrosion" is misleading	Closed	CLST
Comment 84	SCA	Issue resolution strategy and testing package for the waste package and engineering barrier system do not take into account the full range of likely natural conditions that might affect performance of the barrier		CLST SDS ENFE
Comment 85	SCA	Performance Assessment: Temporal changes in the state of stress due to corrosion of the container is not accounted for	Closed	CLST
Comment 86	SCA	Degradation modes of copper-based alloys do not appear to agree with scientific literature	Closed	CLST
Comment 87	SCA	Adequacy of effects of dissimilar metal contacts causing corrosion	Closed, pending	CLST
Comment 88	SCA	Assumption of reduced uncertainties on stress corrosion cracking because of the unsaturated zone	Closed, pending	CLST

APPENDIX A

Table A-1. Status of U.S. Nuclear Regulatory Commission site characterization analysis open items on waste package degradation and radionuclide release from engineered barrier subsystem (cont'd)

Item ID	Source	Title	Status	KTI
Comment 89	SCA	Construction materials may change the local pH and affect the corrosion of the metal containers and the leach rates of radionuclides from the glass		ENFE CLST
Comment 90	SCA	Consideration of varying oxygen concentrations on the corrosion of metal containers	Closed	CLST ENFE
Comment 91	SCA	Waste Package/Performance Assessment: Consideration of alternative canisters for carbon-14 releases	Closed	CLST
Comment 97	SCA	Adequacy of evidence to eliminate iodine as an important radionuclide	Closed, pending	RT CLST
Comment 118	SCA	The monitoring and testing activities should include long-term in situ and long-term waste package activities		CLST TSPAI
Question 30	SCA	Water quality as related to waste package design		ENFE CLST
Question 31	SCA	Integrity of spent fuel cladding	Closed, pending	CLST
Question 32	SCA	Container "similarity" for borosilicate glass waste vs. spent fuel	Closed	CLST
Question 34	SCA	Meaning of "undetected defective closures" in waste package fabrication and handling design goals	Closed, pending	CLST

APPENDIX A

Table A-1. Status of U.S. Nuclear Regulatory Commission site characterization analysis open items on waste package degradation and radionuclide release from engineered barrier subsystem (cont'd)

Item ID	Source	Title	Status	KTI
Question 35	SCA	Acceptance criteria for helium leak results	Closed	CLST
Question 36	SCA	Explanation and justification for use of corrosive surface finishing chemicals on waste package prior to emplacement	Closed, pending	CLST
Question 37	SCA	Basis for 10 cm or more of free fall for canister and contents	Closed	CLST
Question 38	SCA	Basis for mm scratch criterion to avoid emplacement of damaged canisters	Closed, pending	CLST
Question 39	SCA	Meaning of "unusual process history" as a criterion to avoid emplacement of damaged canisters	Closed, pending	CLST
Question 40	SCA	Basis for using a factor of 2 for corrosion for rate for borehole liner in comparison to container material	Closed	CLST
Question 43	SCA	Anticipated operational occurrences considered part of normal conditions on the preclosure design and analysis	Closed	SDS CLST
Question 44	SCA	Basis for assumed numbers of breached assemblies or canisters	Closed, pending	RDTME CLST
Question 45	SCA	Waste package: investigation of particulate source terms, retention factors, and plate-out of waste package during accident conditions	Closed, pending	CLST

APPENDIX A

Table A-1. Status of U.S. Nuclear Regulatory Commission site characterization analysis open items on waste package degradation and radionuclide release from engineered barrier subsystem (cont'd)

Item ID	Source	Title	Status	KTI
Question 46	SCA	Basis for stricter containment of long half-life isotopes	Closed	CLST
Question 47	SCA	What is the origin of the stated definition of a container failure	Closed	CLST
Question 48	SCA	Selection of peer review panel on waste package	Closed	CLST TSPAI
Question 49	SCA	Effects of low temperature oxidation on containers	Closed	CLST
Question 50	SCA	Assumption that stress propagation results in corrosion	Closed	CLST
Question 51	SCA	Impacts of INEL and Hanford high-level wastes on the YM Program	Closed	CLST
Question 52	SCA	Leaching properties specification will require the producer to control leaching characteristics of the glass waste	Closed	CLST
Question 53	SCA	Specification of cooling rate of the glass waste	Closed	CLST
Question 54	SCA	Release rates of radionuclides from spent fuels in J-13 water	Closed	CLST
Question 58	SCA	Flexibility of the Exploratory Shaft Facility design to accommodate *in situ* testing of the waste package, if required	Closed	RDTME CLST

APPENDIX B

Table B-1. Relationships between integrated subissues and key technical issues (U.S. Nuclear Regulatory Commission, 2000a)

KTI Subissue*	Integrated Subissues													
	ENG 1	ENG 2	ENG 3	ENG 4	UZ 1	UZ 2	UZ 3	SZ 1	SZ 2	Direct 1	Direct 2	Dose 1	Dose 2	Dose 3
USFIC1					■									■
USFIC2					■			■						■
USFIC3					■									■
USFIC4			■			■	■							
USFIC5								■	■			■		■
USFIC6							■		■					
TEF1	■		■			■								
TEF2	■		■			■								
TEF3														
ENFE1			■			■								
ENFE2	■		■											
ENFE3			■	■										
ENFE4				■			■							
ENFE5				■										
CLST1	■	■	■							■				
CLST2	■	■								■				
CLST3			■	■										
CLST4			■	■										
CLST5	■	■	■	■										
CLST6	■	■	■	■										
RT1							■		■					
RT2									■					
RT3							■		■					■
RT4							■		■					
TSPAI1 †														
TSPAI2 †														
TSPAI3	■	■	■	■	■	■	■	■	■	■	■	■	■	■
TSPAI4 †														
IA1 †														
IA2		■								■	■		■	■
SDS1 ‡		■						■						
SDS2		■												
SDS3		■	■		■	■	■	■	■					
SDS4 ‡		■												
RDTME1 †														

APPENDIX B

Table B-1. Relationships between integrated subissues and key technical issues (U.S. Nuclear Regulatory Commission, 2000a) (cont'd)

KTI Subissue*	Integrated Subissues													
	ENG 1	ENG 2	ENG 3	ENG 4	UZ 1	UZ 2	UZ 3	SZ 1	SZ 2	Direct 1	Direct 2	Dose 1	Dose 2	Dose 3
RDTME2														
RDTME3														
RDTME4 †														

ENG1 ENG–Degradation of Engineered Barriers
ENG2 ENG–Mechanical Disruption of Engineered Barriers
ENG3 ENG–Quantity and Chemistry of Water Contacting Waste Packages and Waste Forms
ENG4 ENG–Radionuclide Release Rates and Solubility Limits
UZ1 GEO–Climate and Infiltration
UZ2 GEO–Flow Paths in the Unsaturated Zone
UZ3 GEO–Radionuclide Transport in the Unsaturated Zone
SZ1 GEO–Flow Paths in the Saturated Zone
SZ2 GEO–Radionuclide Transport in the Saturated Zone
Direct1 GEO–Volcanic Disruption of Waste Packages
Direct2 GEO–Airborne Transport of Radionuclides
Dose1 BIO–Dilution of Radionuclides in Groundwater due to Well Pumping
Dose2 BIO–Redistribution of Radionuclides in Soil
Dose3 BIO–Lifestyle of the Critical Group

*A description of the KTI subissues is provided in Appendix B of TSPAI IRSR (U.S. Nuclear Regulatory Commission, 2000a).
†These subissues are addressed in areas other than model abstraction.
‡The influence of SDS4 (Tectonic model) and SDS1 (Faulting) on Direct1 (Volcanic Disruption of Waste Packages) will be discussed in scenario analysis in future revisions of this report. This is a result of SDS1 and SDS4 potentially affecting the probability of igneous activity.

U.S. Nuclear Regulatory Commission, *Issue Resolution Status Report, Key Technical Issue, Total System Performance Assessment and Integration*, Revision 3, Washington, DC, U.S. Nuclear Regulatory Commission, 2000a.

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
EBS (Backfill and drip shield)			
1.1.03.01.00	Error in waste or backfill emplacement	Excluded: Repository will be closed according to regulatory requirements, and deviations from design will be detected and corrected.	Accept: Backfill will be excluded from design based on thermal limitations
1.2.02.03.00	Fault movement shears waste container	Excluded: Low probability	Addressed in Structural Deformation and Seismicity (SDS) IRSR
1.2.03.02.00	Seismic vibrations cause waste container and drip shield failure	Excluded: Based on analysis that suggests that WP rock interactions will not lead to mechanical disruption	Addressed in SDS IRSR
2.1.03.04.00	Hydride cracking of waste containers and drip shields	Excluded: Preliminary calculations show time taken to attain critical hydrogen concentration in Ti drip shield may be longer than time for failure by general corrosion.	Accept: However, drip shield material may also include higher strength Ti-4Al-4V alloy, which may be more prone to hydrogen embrittlement
2.1.03.05.00	Microbially mediated corrosion of WP and drip shield	Partly excluded: Ti alloys are not susceptible to MIC	Accept

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.03.07.00	Mechanical impact of waste container	Excluded: Calculations indicate rockfall will not damage WP. Seismic vibrations are argued to not affect WP pending additional analyses. Internal pressurization due to gas generation is calculated to be too low. The swelling of corrosion products is also calculated not to exert stress on Alloy 22 WP	Reject: Effect of rockfall on WP and drip shield integrity needs to be further evaluated. Accept: Gas pressurization and corrosion product swelling are likely to exert low stresses on WP in the current design
2.1.03.09.00	Copper corrosion	Excluded: Not considered for current design	Accept
2.1.03.10.00	Container healing	Excluded: Plugging of pits and holes in container can retard radionuclide release. Analysis can be complex; ignoring this effect is conservative	Accept
2.1.03.11.00	Container form	Excluded: Container form is standardized through design and included in the TSPA	Accept
2.1.07.01.00	Rockfall (large block)	Excluded: Based on low consequence	This issue needs to be resolved through activities in the RDTME KTI
2.1.07.05.00	Creeping of metallic materials in the EBS	Excluded: Creep data on similar alloys, (e.g., Alloy 625), indicate negligible creep even at 650 °C	Accept

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.09.03.00	Volume increase of corrosion products	Excluded: Low consequence due to swelling of corrosion products	Accept: EDA II design removed carbon steel as an outer or inner overpack. Although other alloys do not generate voluminous corrosion products, the effect should be evaluated if local penetration of outer overpack can occur.
2.1.09.09.00	Electrochemical effects in WP and EBS	Excluded: The basis for exclusion seems to involve arguments related to the generation of electric fields in the drift due to the presence of various metallic materials	Reject: The argument about electric fields from metallic materials is a misunderstanding of the role of electrochemical processes on corrosion. Because the corrosion of metallic materials is an electrochemical process, this cannot be excluded. The galvanic effects between Ti and Alloy 22 may be small because of passive behavior of these alloys.

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.11.05.00	Differing thermal expansion of repository components	Excluded: Based on thermal stress magnitude being small compared to effects of rockfall and liner failure	Reject: Because rockfall was excluded in another FEP, rejection of thermal stresses on the basis of significant rockfall effect seems to be inconsistent. Additionally, differential thermal stresses due to closure welding can generate significant circumferential stresses (up to yield point) of WP materials. DOE needs to perform more detailed analysis before excluding this FEP.
2.1.11.06.00	Thermal sensitization of containers increasing fragility	Excluded: Based on drip shield	Accept: Ti alloys may undergo thermal induced embrittlement only at high temperatures. Intermediate temperatures (~200 °C) can reduce significantly the ultimate tensile strength of some Ti alloys.
In-Package Chemistry			
2.1.12.07.00	Radioactive gases in waste and EBS	Excluded: Low consequence. Inhalation dose low relative to other doses, except for C-14. Also, gases would readily dissipate from repository.	Accept

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.01.04.00	Spatial heterogeneity of emplaced waste	Excluded: Time scale of diffusion in aqueous phase is rapid compared to degradation rate of WP components. Excluded: Spatial heterogeneity of waste forms (WFs) throughout the repository, including individual WP temperatures	Reject: DOE not shown adequate technical basis for assuming that diffusion rates are much faster than reaction rates, especially in metallic components. Spatial heterogeneity may influence in-package chemistry locally within WP and lead to higher dissolution rates and solubility than predicted assuming homogeneity of waste. In the NRC/DOE Technical Exchange, DOE agreed to provide additional justification in a revised AMR, sensitivity studies and, if needed, plans for testing.
2.1.02.10.00	Cellulosic degradation	Excluded: Low probability of presence due to waste acceptance criteria	Accept: Need to verify this as part of quality control and performance confirmation programs

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.03.06.00	Internal corrosion of waste container	Partly excluded: Corrosion of inner overpack and internal components of WP are included after breach, but excluded prior to breach. Rationale cited: Control of water allowed in WP and filling it with inert gas prior to WP closure. N-reactor fuel may consume any excess water due to corrosion.	Accept: Need to verify this as part of quality control and performance confirmation programs
2.1.08.07.00	Pathways for unsaturated flow and transport in the waste and EBS	Partly excluded: Inclusion of transport pathways inside the WP would delay release of radionuclides and, therefore, excluding them is conservative	Accept: However, neglecting transport pathways inside the container need not be equivalent to spatial homogeneity of waste (see FEP 2.1.01.04.00)
2.1.08.08.00	Induced hydrological changes in waste and EBS	Partly excluded: Changes in hydrological properties of WF are excluded because uncertainties are small in relation to overall uncertainties of in-package chemistry	Accept
2.1.09.01.00	Properties of the potential carrier plume in the waste and EBS	Partly excluded: Changes in the chemistry of incoming water are slight compared to the more dramatic changes predicted in the in-package chemistry	Reject: It is not clear if DOE considered the carrier plume exiting the WP, which will be profoundly influenced by in-package outer chemistry

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.09.02.00	Interaction with corrosion products	Partly excluded: Potential beneficial effects from corrosion products in decreasing advective and diffusive transport of radionuclides and sorptive effects are excluded leading to conservatism	Reject: Corrosion products from the degradation of WP internal components (e.g., baskets) may cause local mechanical stresses and rupture due to volume expansion. Also, some corrosion products such as β-FeOOH can occlude chloride. Others such as magnetite can raise the redox potential. DOE should provide rationale on how these effects are considered in other ways to compensate neglecting this FEP.

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.09.07.00	Reaction kinetics in waste and EBS	Partly excluded: DOE assumed equilibrium with corrosion products between reaction time steps in the EQ3/6 calculations based on the assertion that the reaction transients between time steps are of low consequence.	Reject: This assumption may be in contradiction with an earlier FEP (2.1.01.04.00), which suggested that the transport rates are much faster than reaction rates. Many electrochemical processes governing WP internal components are far from equilibrium. Secondly, the kinetics of some redox reactions such as ferric/ferrous species on conductive surfaces are often much faster than kinetics of oxygen reduction. Information may lead to erroneous assumptions such as all reactions are governed by one common redox equilibrium dictated by oxygen reduction reaction. Further analysis needs to be performed to justify whether lack of consideration of reaction kinetics can lead to a bounding evaluation of in-package chemistry.

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "Included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.09.09.00	Electrochemical effects (electrophoresis, galvanic coupling in waste and EBS)	Excluded: Based on low consequence. The influence of fluid flow through a failed container on the in-package chemistry is much greater than any effect on the degradation of the SNF or HLW matrix that can be created by electrophoresis or electro-osmosis.	Partly reject: While it is accepted that electrophoresis or electro-osmosis are unlikely to cause degradation of in-package components, electrochemical effects encompass more phenomena than these two cited by DOE. Most in-package components, with the exception of HLW glass, can sustain electrochemical reactions. The galvanic interaction between SNF and cladding has been inadequately examined and potentially may be important. Further analysis needs to be performed to justify whether lack of consideration of reaction kinetics can lead to a bounding evaluation of in-package chemistry.

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.09.11.00	Waste-rock contact	Partly excluded: Drip shield and container, rock is not expected to come in direct contact with WF in the first 10,000years. Also, direct chemical interaction between rock and WF is unlikely. The rockfall effect on cladding was excluded in another FEP.	Accept (see rockfall effects on cladding FEP)
2.1.11.08.00	Thermal effects: chemical and microbiological changes in the waste and EBS	Partly excluded: for many radionuclides, temperature- specific solubility unavailable. Microbiological FEP excluded. Temperature effects for some species (e.g., U) included.	Reject: Some radionuclides may have retrograde solubility that may raise criticality potential. DOE needs to offer greater technical basis for excluding temperature effects on solubility of specific species. Microbial effects FEP is addressed elsewhere.
2.1.11.04.00	Temperature effects/ coupled processes in waste and EBS	Partly excluded: Temperature effects on in-package chemistry are not included due to lack of thermodynamic data, but are considered in various degradation models related to SNF, cladding, etc.	Accept: Temperature effects are considered in EQ3/6 calculations
2.1.11.09.00	Thermal effects on liquid or two-phase flow in waste and EBS	Partly excluded: Thermal effects on flow inside the WP are excluded, but outside the WP are included	Accept: Because temperatures are anticipated to be low after breach, thermal effects on flow may not be significant inside the WP

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.11.10.00	Thermal effects on diffusion (Soret effect) in waste and EBS	Excluded: Bounding analysis indicate that diffusion due to temperature gradients within the WF is insignificant	Accept
2.1.12.01.00	Gas generation	Excluded: Gas expected to escape the repository through fractures. Gas generation within WP expected to be low.	Accept
2.1.12.02.00	Gas generation (He) from fuel decay	Excluded: Low consequence due to small increase in internal pressure.	Accept
2.1.12.06.00	Gas transport in waste and EBS	Excluded: Low dose due to escaping CO_2 gas. C-14 assumed to be in aqueous environment.	Accept
2.1.09.08.00	Chemical gradients/ enhanced diffusion in waste and EBS	Excluded: DOE assumes WP to be a mixing cell. Rate of in-flow slow enough to prevent long-term gradients. Also, diffusive release from within WF is subsumed by more conservative assumptions involving exposed internal surfaces, failed cladding, etc.	Reject: Chemical gradients within WP are likely due to tight crevices present and cause enhanced dissolution and solubility of some radionuclides. DOE needs to justify, through analysis or experiments, the exclusion of this FEP or perform sensitivity studies.
2.1.12.04.00	Gas generation (CO_2, CH_4, H_2S) from microbial degradation	Excluded: Biological activity inside WP will be excluded because organic matter will be excluded	Accept: Need to verify as part of quality control (QC) and performance confirmation programs.

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.12.03.00	Gas generation (H_2) from metal corrosion	Excluded: Otic environment and fracture pathways may minimize hydrogen gas outside the WP. Influence of steel corrosion on H_2 inside WP is negligible and may reduce acidification	Accept
Commercial Spent Nuclear Fuel Matrix Degradation			
2.1.13.01.00	Radiolysis	Partly excluded: Gamma radiolysis not likely at long times when water contacts waste. Alpha radiolysis included in the SNF tests	Reject: Alpha radiolysis effects on environments containing thin water film or humid environments or in crevices may be different from those effects in flow-through tests, which were used in abstraction. Also, alpha radiolysis effects on glass WFs in co-disposal packages may need consideration. DOE needs to justify through analysis or sensitivity studies the exclusion of this FEP.
2.1.13.02.00	Radiation damage in waste and EBS	Excluded: Experimental data show little influence of burnup on degradation rate	Accept

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.08.07.05	Waste-form and backfill consolidation	Excluded: Consolidation would decrease surface area and hence is nonconservative. Assumption of water filling all void volume is conservative and consolidation not necessary.	Accept
2.1.02.04.00	Alpha recoil enhances dissolution	Excluded: Even when assuming all alpha decay results in alpha-recoil, analysis shows no significant increases in degradation rate of WFs	Accept
Cladding Degradation			
2.1.02.11.00	Water logged rods	Excluded: Moisture content controlled by waste acceptance criteria. Corrosion of cladding not expected at moisture level resulting from standard drying process	Accept: Will depend on implementation of QC controls
2.1.02.13.00	General corrosion of cladding	Excluded: Generalized corrosion of Zircaloy is low	Accept
2.1.02.14.00	Microbial corrosion of cladding	Excluded: Microbial activity screened out. Also, no experimental evidence of microbial corrosion of zirconium	Accept

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.02.15.00	Acid corrosion of cladding from radiolysis	Excluded: Zirconium has high corrosion resistance in acids like nitric	Accept
2.1.02.16.00	Localized corrosion of cladding	Included	Only fluoride induced localized corrosion is included. This form of corrosion is really uniform corrosion that occurs in patches. Under oxidizing conditions, chlorides can induce localized corrosion and need to be considered. DOE agreed in the NRC/DOE Technical Exchange to expand the technical basis for its analysis.
2.1.02.16.00	Localized corrosion (crevice corrosion) of cladding	Excluded: Zirconium does not suffer crevice corrosion	Accept: NRC experiments also indicate a lack of crevice corrosion of Zircaloy. There is a need to develop a better understanding of localized corrosion before confirming this exclusion because the data is limited.
2.1.02.18.00	High dissolved silica content of waters enhances cladding corrosion	Excluded: Silica is not corrosive to zircaloy	Accept

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.02.22.00	Hydride embrittlement of cladding	Excluded: In-package environment and cladding stresses are not conducive to hydride cracking	Reject:. While hydride embrittlement is not a significant process, pre-existing hydride reorientation and embrittlement of cladding depend upon temperature. In the DOE/NRC Technical Exchange, DOE agreed to provide additional information on cladding temperatures and stresses.
2.1.07.01.00	Rockfall	Excluded: Cladding perforation from other modes occurs before cladding collapse. Also, robust WPs	Accept
2.1.02.26.00	$FeCl_2$ degradation of cladding	Excluded: Based on the conditions not existing inside WP	Reject: The FEP should refer to $FeCl_3$ and not $FeCl_2$ because the latter is not sufficiently oxidizing to cause pitting. DOE has not established sufficient technical basis in the form of relevant numerical simulation and experiments to rule out the formation of $FeCl_3$. DOE agreed in the NRC/DOE Technical Exchange to provide additional justification on the in-package water chemistry.

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.09.28.00	Diffusion controlled cavity growth (DCCG)	Excluded: This mechanism has not been demonstrated in zirconium experimentally	Accept
2.1.02.21.00	Stress corrosion cracking (SCC) of cladding	Included	Only the iodine-induced SCC is included. DOE should consider chloride-induced SCC for conditions that can also lead to localized corrosion. DOE agreed in the NRC/DOE Technical Exchange to expand the technical basis for its analysis of SCC.
U.S. Department of Energy Spent Nuclear Fuel			
2.1.02.08.00	Pyrophoricity	Excluded: Scoping analysis showed that heat produced by a pyrophoric event is not sufficient to impact performance of DSNF or other adjacent WP	Accept
2.1.02.08.04	Acetylene generation from DSNF	Excluded: Only Peach Bottom fuel has the potential to generate acetylene gas. The gas is expected to disperse through fractures before explosions can occur	Accept
2.1.02.25.00	DSNF cladding degradation	Excluded: More than 80 percent of DSNF is N-reactor fuel and in poor condition. No credit is taken for cladding	Accept

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.11.03.00	Exothermic reactions in waste and EBS	Excluded: Possible temperature rise from exothermic reaction is small relative to radioactive decay	Reject: DOE needs to perform some calculations to confirm this assertion because DSNF will be co-disposed with HLW glass does not generate significant radioactive decay heat
2.1.12.08.00	Gas explosions	Excluded: Lack of oxygen, low water, and inert gas will preclude explosion before container breach. After breach, gas will disperse into repository	Accept
HLW Glass Degradation			
2.1.02.03.00	Glass degradation, alteration, and dissolution	Partly excluded: Phase separation and selective leaching are excluded because upper bound rate used for matrix dissolution	Accept: However, secondary FEPS such as 2.1.02.03.03 "Congruent Dissolution (in waste form)" and 2.1.02.03.08 "iron corrosion products" were not screened.
2.1.02.06.00	Glass recrystallization	Excluded: Controls will ensure phase separation and recrystallization do not occur	Accept
Dissolved Radionuclide Concentration			
2.1.09.10.00	Secondary phase effects on dissolved radionuclide concentrations	Excluded: Leads to conservative prediction of dissolved radionuclides	Accept

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.09.12.00	Rind formation in waste, EBS, and adjacent rock	Partly excluded: Rind formation may reduce radionuclide release and, hence, exclusion leads to conservative prediction	Accept
2.1.09.13.00	Complexation by organics in waste and EBS	Excluded: Organic material will be minimized by waste acceptance criteria. Drift temperatures may drive any volatiles	Accept
Colloids			
2.1.09.15.00	Formation of true colloids in waste and EBS	Excluded: True colloids would be expected to dissolve when solution is diluted	Accept. Probably covered by irreversible experiments.
2.1.09.18.00	Microbial colloid formation in the waste and transport EBS	Excluded: Microbial activity is screened out. Microbial activity may increase colloid size leading to settling out	Accept
2.1.09.19.00	Colloid sorption and transport in waste and EBS	Partly excluded: Modeling component only acts as source term and does not evaluate transport inside WP	Reject: Rationale for exclusion is not clear
2.1.09.20.00	Colloid filtration in waste and EBS	Excluded: Assumption of not filtering the colloids is conservative	Accept

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.10.01.00	Biological activity in waste and EBS	Excluded: Unlikely that biological activity will be sufficient to affect colloid mobility or WP corrosion. Organic matter will be minimized based on waste acceptance criteria	Reject: Lack of experimental evidence of lack of microbial activity under thermal or wet/dry conditions, and adjacent to WFs
2.1.13.03.00	Mutation	Excluded: Based on general principles that mutation may be harmful to organism and in absence of strong natural selection, unlikely to produce any definite change in phenotypes of organisms	Accept: Based on lack of experimental evidence to contrary
2.1.09.05.00	In-package sorption	Partly excluded: Sorption on stationary material will be beneficial	Accept: However, spike release may be an issue
In-Package Criticality			
2.1.14.00.00	Nuclear criticality (in wastes and EBS)	Header, see subentries: This category contains FEPs related to nuclear criticality in the waste and engineered barrier system.	NA

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.14.02.00	Criticality in-situ, nominal configuration, top breach The waste package (WP) internal structures and the waste form remain intact (nominal configuration). There is a breach near the top of the WP, which allows water to collect in the WP. Criticality then occurs in-situ.	Excluded: Commercial spent nuclear-fuel waste containers, have neutron absorbers added as amendments, such as boron, to reduce the likelihood that a critical assembly can form if the container is accidentally filled with water. This FEP has no stated mechanism to remove or separate the neutron absorber. Therefore, this process seems unlikely. Processes described in FEPs ISC-1 through ISC-6 are considered more probable. Whether it is physically possible to actually fill the container before heating from fissions drives up the temperature is also an open question. (Criticality evaluation will probably show that intact basket and rods will not go critica—J. Wilson, INEEL).	Reject: Insufficient information for exclusion. The results of criticality evaluations should be included. This primary FEP is excluded but contains an "included" secondary FEP (2.1.14.02.02).

APPENDIX C

Table C-1. U.S. Nuclear Regulatory Commission evaluation of U.S. Department of Energy rationale for exclusion of features, events, and processes related to waste package performance. The "included" features, events, and processes are generally not evaluated (cont'd)

Features, Events, and Processes Number	Title	U.S. Department of Energy Rationale	U.S. Nuclear Regulatory Commission Evaluation
2.1.14.04.00	Criticality in-situ, WP internal structures degrade at same rate as waste form, top breach The waste package (WP) internal structures degrade at the same rate as the waste form. There is a breach near the top of the WP, which allows water to collect in the WP. Significant amounts of the neutron absorber are flushed out the top of the WP. A slurry with insufficient neutron absorbing material forms at the WP bottom and DSNF criticality occurs in-situ.	Excluded: A screening argument must be developed for each category of DSNF and the proposed waste package configuration in which it is to be contained. The use of a more insoluble neutron absorber can ensure that the criticality limit (CL) is not exceeded. (Until WP bottom is pierced, insoluble poison should mix with slurry).	Reject: The FEP should not be excluded until appropriate screening arguments are developed. This primary FEP is excluded but contains two "included" secondary FEPs (2.1.14.04.01 and 2.1.14.04.02).