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DOC.20031208.0004
DOC.20031208.0004

2. Type of Mathematical Model

☐ Process Model ☒ Abstraction Model ☐ System Model

Describe Intended Use of Model

The Integrated Waste Package Degradation (IWPD) Model documented within this technical product produces profiles for the initial failure and subsequent number of penetrations in the waste packages and drip shields as a function of time. The IWPD Model is used directly in total system performance assessment (TSPA) analysis. The outputs of the IWPD Model are used as input for waste form degradation analysis and radionuclide release analysis from failed waste packages.

3. Title

WAPDEG Analysis of Waste Package and Drip Shield Degradation

4. DI (Including Rev. No. and Change No., if applicable):

ANL-EBS-PA-000001 REV 01

5. Total Attachments	6. Attachment Numbers - No. of Pages in Each
2	I – 12, II - 5

	Printed Name	Signature	Date
7. Originator	Kevin G. Mon Bryan E. Bullard G. Alda Behie	SIGNATURE ON FILE SIGNATURE ON FILE SIGNATURE ON FILE	12/5/03 12/05/03 12/05/03
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13. Remarks

Kevin Mon is responsible for the entire document.
Joon Lee is responsible for the conservatism discussions in Sections 6.3.6.3 and 6.3.6.4.
Bryan Bullard and Alda Behie made significant contributions.
Assistance with DIRS was provided by Erin Nicholls-Heckler.

TER-02-0015 is addressed in this report.

Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

For TSPA-LA.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

MODEL REVISION RECORD

2. Model Title:

WAPDEG Analysis of Waste Package and Drip Shield Degradation

3. DI (including Rev. No. and Change No., if applicable):

ANL-EBS-PA-000001 REV 01

4. Revision/Change No.	5. Description of Revision/Change
00	Initial Issue
00 ICN 01	Interim Change to incorporate changes due to the removal of backfill and new/revised upstream inputs Names of Alloy 22 outer barrier lids changed to outer closure lid and middle closure lid. Discussion added for recommended versus used uncertainty models Section 6.3.
01	Revision to incorporate changes for TSPA-LA. Incorporate changes in upstream process models. Conform to AP-SIII.10Q. The entire model documentation was revised because the changes were too extensive to use Step 5.8d)1) of AP-SIII.10Q.

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ACRONYMS AND ABBREVIATIONS

AP	Absorber Plate
CDF	Cumulative Distribution Function
CDSP	Co-Disposal
CFR	Code of Federal Regulations
CPP	cyclic potentiodynamic polarization
CSNF	Commercial Spent Nuclear Fuel
DHLW	Defense High Level Waste
DIRS	Document Input Reference System
DLL	Dynamic Link Library
DOE	U.S. Department of Energy
DS	Drip Shield
DTN	Data Tracking Number
EBS	Engineered Barrier System
FEPs	Features Events and Processes
GLM	General Linear Model
HAZ	Heat-Affected Zone
HLW	High Level Waste
IWPD	Integrated Waste Package Degradation
KTI	Key Technical Issue
LA	License Application
LC	Localized Corrosion
LLNL	Lawrence Livermore National Laboratory
LTCTF	Long Term Corrosion Test Facility
NG	Nuclear Grade
NRC	Nuclear Regulatory Commission
PAP	Performance Assessment Project
pdf	probability density function
PGV	peak ground velocity
RH	Relative Humidity
SC	Safety Category
SCC	Stress Corrosion Cracking
sd	standard deviation
SMR	Software Management Report
SNF	Spent Nuclear Fuel
SR	Site Recommendation
SSC	Silver-Silver Chloride (Ag/AgCl)
TSPA	Total System Performance Assessment
TSPAI	Total System Performance Assessment Integration
TWP	Technical Work Plan
UT	Ultrasonic Testing
WP	Waste Package
WPD	Waste Package Department
WPOB	Waste Package Outer Barrier
YS	Yield Strength

1. PURPOSE

As directed by a Technical Work Plan (TWP) (BSC 2002 [DIRS 161132]), an abstraction model of the degradation of the drip shields and waste packages in the engineered barrier system (EBS) of the repository at Yucca Mountain is developed. This activity is conducted by the Performance Assessment Project's (PAP) Waste Package Department (WPD). The purpose of this activity is to provide the PAP with estimates of waste package and drip shield degradation as a function of exposure time under exposure conditions anticipated in the repository. This abstraction model provides information useful to satisfy requirements of the Yucca Mountain Review Plan (NRC 2003 [DIRS 163274]). Comments by the Waste Package Peer Review Panel (Beavers, et al. 2002 [DIRS 158781]) were also considered. Several Features, Events, and Processes (FEPs) are also discussed (see Section 6.2, Table 17).

Abstractions of process models for the waste packages and drip shield degradation processes considered in the repository are incorporated into the Integrated Waste Package Degradation (IWPD) Model documented in this report. The output from the IWPD Model is a set of profiles (time-histories) for the failure (i.e. initial breach) and subsequent number of penetration openings in the waste package and drip shield as a function of time. The IWPD Model is used directly in total system performance assessment (TSPA) analysis. The IWPD Model includes general corrosion and stress corrosion cracking models for the waste package outer barrier as input to TSPA. The localized corrosion model is not included in the IWPD Model as a direct feed to TSPA. The outputs of the IWPD Model are used as input for waste form degradation analysis and radionuclide release analysis from failed waste packages. The analyses presented in this report are for the current repository design (BSC 2003 [DIRS 164069]). In this design, a drip shield is placed over the waste packages and no backfill is used.

It should be noted that the results of the analyses documented in Section 6.6 are for illustrative purposes only. The drip shield and waste package degradation profiles presented in Section 6.6 result from the use of representative thermal hydrologic history files (Section 6.3.13) produced for the purpose of allowing the IWPD Model to be exercised in this report. The actual drip shield and waste package degradation profiles which will be used in the TSPA-LA Model will make use of the thermal hydrologic history files appropriate for the repository. Also the results of the localized corrosion (pitting and crevice corrosion) are not presented in this report because evaluation of this degradation mode would require (in addition to of the actual thermal hydrologic history files appropriate for the repository) in-drift geochemical inputs which will only be available to TSPA. Therefore, the localized corrosion model is implemented directly in TSPA. However, localized corrosion initiation and propagation models for the waste package outer barrier are discussed in Sections 4.1.4 and 6.3.6 and the rationale for exclusion of localized corrosion of the drip shield material is discussed in Section 6.3.5. Nonetheless the drip shield and waste package degradation profiles presented in Section 6.6 provide evidence that the IWPD Model implementation functions properly over a range of input parameter values.

The only limitations on the IWPD Model result from the abstracted models implemented within it. All models implemented within the IWPD Model were developed for the exposure conditions in the repository. Although the corrosion models in the *General Corrosion and Localized Corrosion of the Drip Shield* report were developed using information from a wide range of titanium alloys, the DS degradation models are primarily intended to apply to the corrosion of titanium-palladium alloys, in particular, to the Titanium Grade 7 alloy anticipated to be used for the drip shield (DS) plates (BSC 2003 [DIRS 161236], Section 1.2). The DS plates perform the water diversion function of the DS. One should note that the DS also has stiffeners and support beams composed of Titanium Grade 24. Degradation of Titanium Grade 24 is not modeled in this report. The discussion on SCC will be restricted to the waste package outer barrier (WPOB) and the DS plates, which are made of Alloy 22 and Titanium Grade 7, respectively. Degradation of the 316 stainless steel WP inner vessel is not modeled i.e. the IWPD Model does not take corrosion credit for the inner vessel of the WP. Several model limitations (too lengthy to be recounted here) associated with the localized corrosion implementation are discussed in Sections 4.1.4 and 6.3.6.

1.1 BARRIER CAPABILITIES

10 CFR 63 [DIRS 156605] defines a barrier as "any material, structure, or feature that, for a period to be determined by the Nuclear Regulatory Commission (NRC), prevents or substantially reduces the rate of movement of water or radionuclides from the Yucca Mountain repository to the accessible environment, or prevents the release or substantially reduces the release rate of radionuclides from the waste." 10 CFR 63.102(h) and 10 CFR 63.113(a) require that the repository system include multiple barriers, both natural and engineered. The capability of a barrier is defined by its ability to achieve one or more of the functions described above: i.e. the extent to which it can prevent or delay the movement of water or radionuclides, or prevent or reduce the release rate from the waste. In this document, two barriers are considered; the drip shield and the waste package. These barriers contribute to waste isolation by keeping water away from the waste forms while the barriers remain intact.

Drip shields will be installed over the waste packages prior to repository closure. The drip shield plates will be composed mainly of Titanium Grade 7. The drip shields divert any moisture that might seep from the drift walls, including condensed water vapor, around the waste packages to the drift floor for thousands of years. The drip shields will be made of Titanium Grade 7 with Titanium Grade 24 stiffeners and support beams, which provides corrosion resistance and structural strength. The drip shields limit any damage arising to waste packages in the event of expected rockfalls, as the emplacement drifts degrade over time. Because of the low corrosion rate of titanium, the initial breaches of the drip shields due to corrosion degradation processes will not occur until approximately 35,000 years (Section 6.3.3), and the median estimate of the mean time to initial breaching of drip shields is approximately 310,000 years (Section 6.6). Therefore, even in the event of a breach of a waste package before its corresponding drip shield, advective transport of radionuclides cannot occur until after approximately 35,000 years and is likely to be delayed even longer.

Waste packages prevent any contact between water and waste as long as they are intact, and limit water flow and potential radionuclide migration even after the waste packages are breached. The waste packages have a dual-metal design containing two concentric cylinders. The inner vessel cylinder is a 50 mm thick layer of 316 stainless steel. The outer barrier cylinder is a 20 mm or 25 mm thick layer of Alloy 22, a corrosion resistant nickel-based alloy. Alloy 22 protects the 316 stainless steel inner vessel from corrosion, while the 316 stainless steel inner vessel provides structural support for the thinner Alloy 22 outer cylinder. The general corrosion rates of Alloy

22 are so low that it is not expected that any waste packages would be breached by general corrosion or stress corrosion cracking during the first 10,000 years: models indicate that the time to initial breaching of the waste packages is on the order of one hundred thousand years (Section 6.6). Analyses of the potential for premature failures of waste packages by processes other than corrosion (e.g., improper heat treatment or damage by rockfall) indicate a very low probability that packages would be breached before 10,000 years. Even after that time, the slow failure rate of waste packages, and the low rate of water movement through them, would limit releases of radionuclides for many tens of thousands of years.

2. QUALITY ASSURANCE

The Quality Assurance (QA) program applies to the development of this technical product. The Technical Work Plan entitled *Waste Package Materials Data Analyses and Modeling* (BSC 2002 [DIRS 161132]) determined that this activity is subject to the *Quality Assurance Requirements and Description* (QARD) DOE/RW-0333P (DOE 2003 [DIRS 162903]) requirements. All waste package configurations have been determined to be important to waste isolation in accordance with AP-2.22Q and therefore are classified as Safety Category (SC) on the *Q-List* (BSC 2003 [DIRS 165179], Appendix A; BSC 2003 [DIRS 164554], Section 6.4.2). The drip shields have been determined to be important to waste isolation in accordance with AP-2.22Q and therefore are classified as Safety Category (SC) on the *Q-List* (BSC 2003 [DIRS 165179], Appendix A; BSC 2003 [DIRS 164554], Section 6.4.2).

The inputs to this report are documented according to the AP-3.15Q, *Managing Technical Product Inputs* procedure. The methods used to control the electronic management of data as required by AP-SV.1Q, *Control of the Electronic Management of Information*, were accomplished in accordance with the technical work plan. The process for control of the electronic management of information on evaluation of work activities/processes/process functions, outlined in Section 5.0 of AP-SV.1Q, is followed to ensure accuracy, completeness, and security of information and data used in preparation of this report. Examples of process controls mentioned in AP-SV.1Q are (a) access to the information contained on personal computer is password protected; (b) secured backup copies are appropriately labeled and stored before changes are made and kept until the changes are confirmed and correct; (c) physical electronic media (tape, diskette, CD-ROM, etc.) are appropriately labeled; and (d) for non-physical electronic media, transport mechanisms can be e-mail, TCP/IP, Netbios, etc. and methods of receipt verification may include visual inspection, transmission verification settings, check sums, application information integrity check, etc.

This document is prepared in accordance with AP-SIII.10Q, *Models,* and reviewed in accordance with AP-2.14Q, *Document Review*.

3. USE OF SOFTWARE

3.1 EXCEL 97 SR-2

Excel 97 SR-2 is a commercial off-the-shelf software program used in this report. The computations performed in this report using Excel use only standard functions and are documented in sufficient detail to allow an independent technical reviewer to reproduce or verify the results by visual inspection or hand calculation without recourse to the originator. The formulas or algorithms used and a listing of inputs to and outputs from the formulas or algorithms are sufficiently documented to allow results to be reproduced. Therefore this software is exempt from the AP-SI.1Q, *Software Management,* procedure. Excel 97 SR-2 is appropriate for its intended use because it offers the mathematical and graphical functionality necessary to perform and document the numerical manipulations used in this report. Excel 97 SR-2 was executed on a Optiplex GX260 Workstation (CRWMS M&O tag 152849, located in the Summerlin Offices, Las Vegas, Nevada) equipped with the Windows 2000 operating system.

3.2 SIGMAPLOT 8.0

SigmaPlot 8.0 is a commercial off-the-shelf software program used in this report. No computations are performed in this report using SigmaPlot 8.0. Therefore this software is exempt from the AP-SI.1Q, *Software Management,* procedure. SigmaPlot 8.0 is appropriate for its intended use because it offers the graphical functionality necessary to perform and document the plots used in this report. SigmaPlot 8.0 was executed on a Optiplex GX260 Workstation (CRWMS M&O tag 152849, located in the Summerlin Offices, Las Vegas, Nevada) equipped with the Windows 2000 operating system.

3.3 MATHCAD 2001I PROFESSIONAL

MathCad 2001i Professional is a commercial off-the-shelf software program used in this report. The computations performed in this report using MathCad 2001i Professional use only standard functions and are documented in sufficient detail to allow an independent technical reviewer to reproduce or verify the results by visual inspection or hand calculation without recourse to the originator. The formulas or algorithms used and a listing of inputs to and outputs from the formulas or algorithms are sufficiently documented to allow results to be reproduced. Therefore this software is exempt from the AP-SI.1Q, *Software Management,* procedure. MathCad 2001i Professional is appropriate for its intended use because it offers the mathematical and graphical functionality necessary to perform and document the numerical manipulations used in this report. MathCad 2001i Professional was executed on a Optiplex GX260 Workstation (CRWMS M&O tag 152849, located in the Summerlin Offices, Las Vegas, Nevada) equipped with the Windows 2000 operating system.

3.4 WAPDEG V. 4.07

The WAste Package DEGradation (WAPDEG) software (BSC 2002 [DIRS 161240]) was developed, in accordance with AP-SI.1Q, *Software Management*, to implement the models documented in this report. The WAPDEG software is qualified and is used in this report in accordance with AP-SI.1Q, *Software Management*. The following information is used to identify the WAPDEG software:

Software Title: WAPDEG

Software Tracking Number: 10000-4.07-00

Version Number: 4.07

This software was obtained from the Software Configuration Manager in accordance with appropriate procedures. The WAPDEG software was executed on a Optiplex GX260

Workstation (CRWMS M&O tag 152849, located in the Summerlin Offices, Las Vegas, Nevada) equipped with the Windows 2000 operating system. WAPDEG version 4.07 is an appropriate tool for this application, because it was specifically designed to calculate drip shield and waste package failure profiles. The software was used within its range of validation.

3.5 CWD V. 2.0

Software routine Closure Weld Defects (CWD) (BSC 2003 [DIRS 162809]) was developed, in accordance with AP-SI.1Q, *Software Management*, to implement the abstraction results of the probability of the occurrence and size of weld flaws in the closure-lid welds of the Alloy 22 waste package outer barrier. The CWD software routine is qualified and is used in this report in accordance with AP-SI.1Q, *Software Management*. The following information is used to identify the CWD software routine:

Software Title: CWD

Software Tracking Number: 10363-2.0-00

Version Number: 2.0

This software was obtained from the Software Configuration Manager in accordance with appropriate procedures. The CWD software routine was executed on a Optiplex GX260 Workstation (CRWMS M&O tag 152849, located in the Summerlin Offices, Las Vegas, Nevada) equipped with the Windows 2000 operating system. This software routine is appropriate for this application as it was developed to implement the results of the analyses. The CWD software routine was used within its range of validation.

3.6 SCCD V. 2.01

Software routine Stress Corrosion Cracking Dissolution (SCCD) (BSC 2000 [DIRS 161757]) was developed, in accordance with AP-SI.1Q, *Software Management*, to implement the abstraction results of the stress and stress intensity factor profiles in the closure-lid welds of the Alloy 22 waste package outer barrier. The SCCD software routine is qualified and is used in this technical product in accordance with AP-SI.1Q, *Software Management*. The following information is used to identify the SCCD software routine:

Software Title: SCCD

Software Tracking Number: 10343-2.01-00

Version Number: 2.01

This software was obtained from the Software Configuration Manager in accordance with appropriate procedures. The SCCD software routine was executed on a Optiplex GX260 Workstation (CRWMS M&O tag 152849, located in the Summerlin Offices, Las Vegas, Nevada) equipped with the Windows 2000 operating system. This software routine is appropriate for this application as it was developed to implement the results of the analyses. The SCCD software routine was used within its range of validation.

3.7 GOLDSIM V. 7.50.100

The GoldSim software (BSC 2003 [DIRS 161572]) is acquired software controlled in accordance with AP-SI.1Q, *Software Management*. The GoldSim software was used to pass input to the WAPDEG software and software routines listed in this Section. The GoldSim software is fully qualified and is used in this technical product in accordance with AP-SI.1Q, *Software Management*. The following information is used to identify the GoldSim software:

Software Title: GoldSim

Software Tracking Number: 10344-7.50.100-00

Version Number: 7.50.100

This software was obtained from the Software Configuration Manager in accordance appropriate procedures. The GoldSim software was executed on a Optiplex GX260 Workstation (CRWMS M&O tag 152849, located in the Summerlin Offices, Las Vegas, Nevada) equipped with the Windows 2000 operating system. GoldSim is an appropriate tool for this application, because it has the capabilities to interface with external software routines and was specifically configured to call the WAPDEG software and the software routines discussed in this Section. The GoldSim code was used within its range of validation.

4. INPUTS

This document may be affected by technical product input information that requires confirmation. Any changes to the document that may occur, as a result of completing the confirmation activities, will be reflected in subsequent revisions. The status of the input information quality may be confirmed by review of the Document Input Reference System (DIRS) database.

4.1 DIRECT INPUT

Treatment of uncertainties in inputs will also be discussed in Section 6.

Table 1. Summary of IWPD Model Inputs

Input Name	Input Source	DTN	Input Value
21 PWR Waste Package Configuration Dimensions	*Repository Design, Waste Package, Project 21-PWR Waste Package with Absorber Plates, Sheet 1 of 3, Sheet 2 of 3, and Sheet 3 of 3* (BSC 2001 [DIRS 157812])	N/A	See Section 4.1.1
5 HLW/1 DOE Short Waste Package Configuration Dimensions	*Repository Design, Waste Package Project 5 DHLW/DOE SNF - Short Waste Package, Sheet 1 of 3, Sheet 2 of 3, and Sheet 3 of 3* (BSC 2001 [DIRS 157817])	N/A	See Section 4.1.1

Input Name	Input Source	DTN	Input Value
5 HLW/1 DOE Long Waste Package Configuration Dimensions	*Repository Design, Waste Package Project 5 DHLW/DOE SNF - Long Waste Package, Sheet 1 of 3, Sheet 2 of 3, and Sheet 3 of 3* (BSC 2001 [DIRS 157818])	N/A	See Section 4.1.1
Drip Shield Configuration Dimensions	*Repository Design Project, Repository/PA IED Interlocking Drip Shield and Emplacement Pallet.* (BSC 2003 [DIRS 165304], Tables 1and 5)	N/A	See Section 4.1.1
Waste Package Inventory Information	*Repository Design Project, RDP/PA IED Typical Waste Package Components Assembly (2).* (BSC 2003 [DIRS 163855], Table 11)	N/A	See Section 4.1.1
Distance from Invert to WP Centerline	*Repository Design Project, Repository/PA IED Emplacement Drift Configuration 1 of 2* (BSC 2003 [DIRS 164069])	N/A	See Section 4.1.1
Weld Volumes	*Repository Design Project, RDP/PA IED Typical Waste Package Components Assembly (5).* (BSC 2003 [DIRS 164610], Table 18 and 19)	N/A	See Section 4.1.5
Drip shield general corrosion rate (Titanium Grade 7)	*General Corrosion and Localized Corrosion of the Drip Shield* (BSC 2003 [DIRS 161236], Section 6.3.5)	MO0306SPAGLCDS.001 [DIRS 163912]	See Section 4.1.2
Alloy 22 waste package outer barrier general corrosion inputs	*General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.3)	SN0308T0506303.004 [DIRS 164840]	See Section 4.1.3
Alloy 22 waste package outer barrier localized corrosion inputs	*General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.4)	SN0308T0506303.003 [DIRS 164839]	See Section 4.1.4
Weld flaw analysis inputs	*Analysis of Mechanisms for Early Waste Package/Drip Shield Failure* (BSC 2003 [DIRS 164475]) *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234]) BSC 2001 [DIRS 157812], BSC 2001 [DIRS 157817], and BSC 2001 [DIRS 157818]	LL030607012251.065 [DIRS 163968]	See Section 4.1.5

Input Name	Input Source	DTN	Input Value
Stress intensity factor (K_I) vs depth	*Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234])	LL030607012251.065 [DIRS 163968]	See Section 4.1.6
Stress coefficients for outer and middle closure lids	*Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234])	LL030607012251.065 [DIRS 163968]	See Section 4.1.6
Yield strength, YS (various temperatures)	N/A	MO0003RIB00071.000 [DIRS 148850]	See Section 4.1.6
Slip dissolution inputs	*Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234])	LL030607012251.065 [DIRS 163968]	See Section 4.1.7
Waste package outer barrier microbial induced corrosion inputs	*General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.5)	SN0308T0506303.004 [DIRS 164840]	See Section 4.1.8
Waste package early failure inputs	*Analysis of Mechanisms for Early Waste Package/Drip Shield Failure* (BSC 2003 [DIRS 164475])	N/A	See Section 4.1.9

4.1.1 Waste Package and Drip Shield Design Input

In this report, as in the TSPA-SR Model (CRWMS M&O 2000 [DIRS 153246], Table 4.1-1), two nominal waste package (WP) configurations are considered. The first waste package configuration is referred to as the Commercial Spent Nuclear Fuel (CSNF) WP configuration (CRWMS M&O 2000 [DIRS 153246], Table 4.1-1) for which the 21 PWR AP WP configuration parameters are used (BSC 2001 [DIRS 157812]). The second WP configuration is Co-Disposal (CDSP) waste package configuration (CRWMS M&O 2000 [DIRS 153246], Table 4.1-1) whose length is considered to be the average length of the 5 HLW/1 DOE SNF Long (BSC 2001 [DIRS 157818]) and Short (BSC 2001 [DIRS 157817]) WP configurations. The waste package inventory information for the repository is shown in Table 2. Note that commercial spent nuclear fuel containing WP configurations (e.g., 21 PWR AP) and naval fuel containing WP configurations (i.e. Naval Short and Long) are represented by the CSNF WP configuration and HLW containing WP configurations (e.g., 5 HLW Long Only) are represented by the CDSP WP configuration.

Table 2. Waste Package Inventory Information (BSC 2003 [DIRS 163855], Table 11).

Waste Package Configuration	Nominal Quantity for LA	Nominal WP Configuration
21 PWR AP	4299	CSNF
21 PWR CR	95	CSNF
12 PWR AP Long	163	CSNF
44 BWR AP	2831	CSNF
24 BWR AP	84	CSNF

Waste Package Configuration	Nominal Quantity for LA	Nominal WP Configuration
5 IPWF	0	N/A
5 HLW Short/1 DOE SNF Short	1147	CDSP
5 HLW Long/1 DOE SNF Long	1406	CDSP
2 MCO/2 HLW	149	CDSP
5 HLW Long/1 DOE SNF Short	31	CDSP
5 HLW Long Only	679	CDSP
Naval Short	144	CSNF
Naval Long	156	CSNF

Based on Table 2, the total number of WPs represented by the CSNF and CDSP WP configurations in the repository are 7772 and 3412, respectively.

The 21-PWR waste package configuration is an appropriate representation of the CSNF waste package configuration since the 21 PWR AP WP is the most common WP configuration in the repository (BSC 2003 [DIRS 163855], Table 11). The 5 HLW/1 DOE SNF (Co-Disposal) Long and Short waste package configurations are appropriate representations of the CDSP WP configuration since these are the most common High-Level Waste (HLW) waste package configurations in the repository (BSC 2003 [DIRS 163855], Table 11).

Relevant waste package and drip shield dimensions were obtained from Information Exchange Drawings (BSC 2003 [DIRS 165406]; BSC 2003 [DIRS 164069]) or design products listed on Information Exchange Drawings (BSC 2003 [DIRS 165406]) and are presented in Table 3.

Table 3. Waste Package and Drip Shield Dimensions.

Input Name	Input Source	Input Value
21-PWR Waste Package Outer Barrier (Shell) Outer Diameter (OD)	BSC 2001[DIRS 157812] Sheet 2 of 3	1564 mm
21-PWR Waste Package Inner Barrier Length	BSC 2001[DIRS 157812] Sheet 2 of 3	4775 mm
21 PWR AP Waste Package Outer Barrier Thickness	BSC 2001[DIRS 157812] Sheet 3 of 3	20 mm
5 HLW/1 DOE SNF Short Waste Package Outer Barrier (Shell) Outer Diameter (OD)	BSC 2001[DIRS 157817] Sheet 2 of 3	2030 mm
5 HLW/1 DOE SNF Short Waste Package Outer Barrier (Shell) Nominal Outer Diameter	BSC 2001[DIRS 157817] Sheet 1 of 3	2110 mm
5 HLW/1 DOE SNF Short Waste Package Inner Barrier Length	BSC 2001[DIRS 157817] Sheet 2 of 3	3200 mm
5 HLW/1 DOE SNF Short Waste Package Outer Barrier Thickness	BSC 2001[DIRS 157817] Sheet 3 of 3	25 mm
5 HLW/1 DOE SNF Long Waste Package Outer Barrier (Shell) Outer Diameter (OD)	BSC 2001[DIRS 157818] Sheet 2 of 3	2030 mm
5 HLW/1 DOE SNF Long Waste Package Inner Barrier Length	BSC 2001[DIRS 157818] Sheet 2 of 3	4827 mm
5 HLW/1 DOE SNF Long Waste Package Outer Barrier Thickness	BSC 2001[DIRS 157818] Sheet 3 of 3	25 mm
Drip Shield Plate Thickness	BSC 2003 [DIRS 165304], Table 5	15 mm
Interior Height of Drip Shield	BSC 2003 [DIRS 165304], Table 1	2715.62 mm
Distance from Invert to WP Centerline for 5 DHLW	BSC 2003 [DIRS 164069]	1282 mm

The Waste Package Outer Barrier (Shell) Outer Diameter and Waste Package Inner Barrier Length are used to calculate the waste package surface area for use in determining the fraction of area subject to stress corrosion cracking. The Waste Package Outer Barrier Thickness is used indirectly in the formulation of inputs to the model (see Section 6.3.2), while the Drip Shield Thickness is used directly in the WAPDEG_Inputs element of the IWPD Model (see Table I-1, Row 40). Since these are design-related parameters, there is no uncertainty treatment for these parameters.

The 5 HLW/1 DOE SNF Short Waste Package Outer Barrier (Shell) Nominal Outer Diameter, Interior Height of Drip Shield, and the Distance from Invert to WP Centerline for 5 DHLW are used in Section 6.3.8 in an analysis of the potential for rockfalls causing contact between the WP and DS.

The information listed in Table 3 are design-related parameters which were obtained from controlled and confirmed sources and thus do not require data tracking numbers.

4.1.2 Drip Shield General Corrosion Inputs

Details of the general corrosion rate distributions used for the under side and top side of the drip shield (DS) are developed in the report entitled *General Corrosion and Localized Corrosion of the Drip Shield* (BSC 2003 [DIRS 161236], Section 6.3.5) and are tracked with DTN: MO0306SPAGLCDS.001 [DIRS 163912]. These inputs are qualified. In the report entitled *General Corrosion and Localized Corrosion of the Drip Shield*, general corrosion rates of Titanium Grade 16 are taken to be representative of those for Titanium Grade 7 (BSC 2003 [DIRS 161236], Section 1.1). Also see Section 6.3.3 of this report for a discussion of the DS general corrosion conceptual model and Section 6.5.6 for discussion of implementation. The general corrosion rate cumulative distribution function applicable to the under side of the DS is shown in Table 4. The general corrosion rate cumulative distribution function applicable to the top side of the DS is shown in Table 5.

Table 4. CDF for General Corrosion Rates for Under Side of the Drip Shield (BSC 2003 [DIRS 161236], Section 6.3.5) (DTN: MO0306SPAGLCDS.001 [DIRS 163912]).

Sample	Rate (mm/yr)	CDF
1	0.00000000E+00	0.0000
2	7.90540100E-06	0.2500
3	7.90899600E-06	0.3125
4	7.91733600E-06	0.3750
5	7.99205500E-06	0.4375
6	1.59679640E-05	0.5000
7	1.60740360E-05	0.5625
8	2.35658240E-05	0.6250
9	2.37302160E-05	0.6875
10	2.40329080E-05	0.7500
11	3.99976910E-05	0.8125
12	7.14961090E-05	0.8750
13	7.91641200E-05	0.9375
14	1.12788228E-04	1.0000

Table 5. CDF for General Corrosion Rates for the Top Side of the Drip Shield (BSC 2003 [DIRS 161236], Section 6.3.5) (DTN: MO0306SPAGLCDS.001 [DIRS 163912]).

Sample	Rate (mm/yr)	CDF
1	0.00000000E+00	0.00000000E+00
2	4.18430800E-06	1.42857143E-01
3	7.90540100E-06	1.78571429E-01
4	7.90899600E-06	2.14285714E-01
5	7.91733600E-06	2.50000000E-01
6	7.99205500E-06	2.85714286E-01
7	1.59679640E-05	3.21428571E-01
8	1.60740360E-05	3.57142857E-01
9	1.65389750E-05	3.92857143E-01
10	2.10450870E-05	4.28571429E-01
11	2.35658240E-05	4.64285714E-01
12	2.37302160E-05	5.00000000E-01
13	2.40329080E-05	5.35714286E-01
14	2.52784890E-05	5.71428571E-01
15	3.99976910E-05	6.07142857E-01
16	4.26207080E-05	6.42857143E-01
17	4.28647310E-05	6.78571429E-01
18	5.15303020E-05	7.14285714E-01
19	6.33683700E-05	7.50000000E-01
20	6.49668830E-05	7.85714286E-01
21	7.14961090E-05	8.21428571E-01
22	7.91641200E-05	8.57142857E-01
23	8.22028960E-05	8.92857143E-01
24	1.11563286E-04	9.28571429E-01
25	1.12788228E-04	9.64285714E-01
26	3.19409704E-04	1.00000000E+00

These inputs are appropriate for their intended use because they provide a very reasonable estimate of the general corrosion behavior of Titanium Grade 7 subjected to the expected exposure conditions in the repository.

DTN: MO0306SPAGLCDS.001 [DIRS 163912] contains a file called ANL_EBS_MD_000004_REV_01.zip. Within this file is a file called 1_Year_CDFs.pdf. 1_Year_CDFs.pdf contains the general corrosion rates for the top and under sides of the DS used in this technical product.

The variation in these inputs are considered to be entirely due to uncertainty (BSC 2003 [DIRS 161236], Section 6.3.5). Therefore, a single general corrosion rate should be sampled from each distribution and applied to all DSs in the repository. The general corrosion rate sampled for the outside surface of the DS should be independent of the general corrosion rate sampled for the inner surface of the DS because the environments above and below the DS are not expected to be significantly correlated (BSC 2003 [DIRS 161236], Section 6.3.5).

4.1.3 Alloy 22 Waste Package Outer Barrier General Corrosion Inputs

4.1.3.1 Primary Alloy 22 General Corrosion Rate Distribution

In the report entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.3) (DTN: SN0308T0506303.004 [DIRS 164840]), general corrosion rates determined from 5-year weight loss samples with the crevice geometry were used to generate a cumulative distribution function for the general corrosion rate (R_o) used in the IWPD Model at an exposure temperature of 60°C (333.15 K). The *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* report (BSC 2003 [DIRS 161235], Section 6.4.3) states that R_o (in nm/yr) is given by a Weibull distribution (Evans, et al. 1993 [DIRS 112115], Chapter 41) with scale parameter, α, equal to 8.88 nm/yr, shape parameter, β, equal to 1.62, and location parameter, θ, equal to 0. This is a two-parameter Weibull distribution since the location parameter, θ, is zero. The parameters are summarized in Table 6.

Table 6. Primary General Corrosion Rate Distribution

Input Name	Input Source	Input Value	Units
Weibull Scale, α	BSC 2003 [DIRS 161235], Section 6.4.3 DTN: SN0308T0506303.004 [DIRS 164840]	8.88	nm/yr
Weibull Shape, β	BSC 2003 [DIRS 161235], Section 6.4.3 DTN: SN0308T0506303.004 [DIRS 164840]	1.62	N/A

The cumulative distribution function (CDF) for a two-parameter Weibull distribution is given by (Evans, et al. 1993 [DIRS 112115], Chapter 41)

$$CDF(x) = 1 - \exp\left(-\left(\frac{x}{\alpha} \right)^{\beta} \right) \quad \text{(Eq. 1)}$$

Also see Section 6.3.4 of this report for a discussion of the conceptual model and Section 6.5.7 for discussion of implementation.

These inputs are appropriate for their intended use because they provide a very reasonable estimate of the general corrosion behavior of Alloy 22 subjected to the expected exposure conditions in the repository.

DTN: SN0308T0506303.004 [DIRS 164840] contains a file called WPOBrev01GC_Model.zip. Within this file is a file called Base Case GC Rate CDF.xls. Base Case GC Rate CDF.xls contains a worksheet called Base Case GC Rate. Cell B1 of the Base Case GC Rate worksheet contains the Weibull scale (identified as s = 8.88) and Cell B2 contains the Weibull shape (identified as b = 1.62).

These general corrosion rates are applied to the Alloy 22 waste package outer barrier surfaces when the exposure temperature is 60°C (333.15 K). The variation in the primary general corrosion rate distribution used for the Alloy 22 waste package outer barrier is considered to be entirely due to variability on the surface of the waste packages (BSC 2003 [DIRS 161235, Section 6.4.3), i.e. the general corrosion rate distribution is passed to the WAPDEG software used in the IWPD Model. As discussed in the report entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.3), the uncertainty in the general corrosion rate is contained in its temperature dependent terms presented in the next section of this report.

4.1.3.2 Temperature Dependence of Alloy 22 General Corrosion

The Alloy 22 general corrosion rate is considered a function of exposure temperature. The temperature dependence follows an Arrhenius relationship, i.e.,

$$R = \exp\left[C_o - \frac{C_1}{T}\right] \quad \text{(Eq. 2)}$$

where

R = general-corrosion rate
T = temperature (Kelvin)
C_o = intercept term
C_1 = slope term (Kelvin)

The intercept term (C_o) is determined from the relationship between Equations 1 and 2 evaluated when the exposure temperature is 60°C (333.15 K). The variation in the general corrosion rate intercept term is considered to be entirely due to variability at the crevice patch size level. Also see Section 6.3.4 of this report for a discussion of the conceptual model for patch sizes and Section 6.5.7 for discussion of implementation.

The slope term (C_1) is sampled from a truncated (at ±3 standard deviations) normal distribution with a mean of 3116.47 and a standard deviation of 296.47 (BSC 2003 [DIRS 161235], Section 6.4.3) (DTN: SN0308T0506303.004 [DIRS 164840]). (Note that the sign of the slope term in this report is negative with respect to the slope term in the *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.3) to be consistent with the input requirements of the WAPDEG software).

Table 7. General Corrosion Slope Term (C_1) Distribution

Input Name	Input Source	Input Value	Units
Normal mean	BSC 2003 [DIRS 161235], Section 6.4.3 DTN: SN0308T0506303.004 [DIRS 164840]	3116.47	K
Normal standard deviation	BSC 2003 [DIRS 161235], Section 6.4.3 DTN: SN0308T0506303.004 [DIRS 164840]	296.47	K
Truncation	BSC 2003 [DIRS 161235], Section 6.4.3	±3 standard deviations	N/A

These inputs are appropriate for its intended use because it provides a very reasonable estimate of the temperature variation in the general corrosion behavior of Alloy 22 subjected to the expected exposure conditions in the repository.

DTN: SN0308T0506303.004 [DIRS 164840] contains a file called WPOBrev01GC_Model.zip. Within this file is a subdirectory called GC Base Case Model. The GC Base Case Model subdirectory contains a file called GC_TempDep_Reg.xls. GC_TempDep_Reg.xls contains a worksheet called TDep_RegOut1. Cell H6 of the TDep_RegOut1 worksheet contains the normal mean and Cell J6 contains the normal standard deviation for the general corrosion temperature dependence slope term, C_1.

The variation in the general corrosion rate slope term is considered to be entirely due to uncertainty (BSC 2003 [DIRS 161235], Section 6.4.3). For each realization of the Integrated Waste Package Degradation Model, a single general corrosion rate slope term is sampled and applied to the Alloy 22 waste package outer barrier surfaces to model variation in the Alloy 22 general corrosion rate with exposure temperature. Spatial and temporal variability of the exposure temperature in the repository lead to spatial and temporal variability in the general corrosion rates used to model general corrosion of Alloy 22.

4.1.4 Waste Package Outer Barrier Localized Corrosion Inputs

The localized corrosion (LC) model used in this report is documented in the report entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.4) (DTN: SN0308T0506303.003 [DIRS 164839]). The LC model for the waste package outer barrier (WPOB) consists of a LC initiation model and a LC propagation rate model. LC initiates when the open circuit potential, or corrosion potential (E_{corr}) is equal to or greater than a critical threshold potential (E_{rcrev}, the crevice repassivation potential), that is, ΔE ($= E_{rcrev} - E_{corr}) \leq 0$.

The following limitations are identified for the application of the localized corrosion model for Alloy 22 (BSC 2003 [DIRS 161235], Section 1.2):

- Temperature from 20°C up to boiling temperature of $CaCl_2$-containing brines.
- Solution pH from 2 to 12.
- Chloride concentration from a very low non-zero value to 25 molal (*m*, moles/kg water). A value of 0.001 *m* is recommended for the chloride concentration for solutions with no chloride.
- Nitrate concentration from a very low non-zero value to 6 molal (*m*, moles/kg water). A value of 0.001 *m* is recommended for the nitrate concentration for solutions with no nitrate.
- The nitrate to chloride concentration ratio from zero to 1.0 for the crevice repassivation potential model. For solutions with the ratio greater than 1.0, the ratio is limited to 1.0. This ratio range is not applied to the corrosion potential model.

Note that no localized corrosion of the WPOB is expected for any water chemistries with the nitrate concentration greater than the upper bound (6 *m*). Because only nitrate ions are accounted for in the localized corrosion model for the inhibitive effect, the model results for solutions with significant amounts of other potentially inhibitive ions such as carbonate and sulfate (in addition to nitrate ions) are highly conservative. The model results for the beneficial effects of the inhibitive ions combined with the alkaline pH conditions of the typical carbonate waters in the repository are consistent with the experimental observations on the immunity of Alloy 22 to localized corrosion in those waters (BSC 2003 [DIRS 161235], Section 1.2).

Further discussion of conceptual model for Alloy 22 localized corrosion is presented in Section 6.3.6.

4.1.4.1 Waste Package Outer Barrier Crevice Repassivation Potential Inputs

The crevice repassivation potential (E_{rcrev}) is expressed as follows.

$$E_{rcrev} = E^{o}_{rcrev} + \Delta E^{NO_3^-}_{rcrev} \qquad \text{(Eq. 3)}$$

where E^{o}_{rcrev} is the crevice repassivation potential in the absence of nitrate ions (which tend to inhibit LC initiation), and $\Delta E^{NO_3^-}_{rcrev}$ is the crevice repassivation potential changes resulted from the inhibiting effect of nitrate ion in solution (BSC 2003 [DIRS 161235], Section 6.4.4).

The crevice repassivation potential of the mill-annealed and as-welded Alloy 22 in the absence of inhibitive nitrate ion is expressed as follows (BSC 2003 [DIRS 161235], Section 6.4.4).

$$E^{o}_{rcrev} = a_o + a_1 T + a_2 pH + a_3 \log([Cl^-]) + a_4 T \times \log([Cl^-]) \qquad \text{(Eq. 4)}$$

where E^{o}_{rcrev} is in mV vs. the Silver-Silver Chloride (SSC) reference electrode, a_o, a_1, a_2, a_3, and a_4 are constants, T is the temperature (°C), and $[Cl^-]$ is the chloride ion concentration. The median estimated regression coefficients are: a_o = 214.089, a_1 = -3.696, a_2 = 25.284, a_3 = -252.181, and a_4 = 1.414. The covariance matrix resulting from the least squares fitting was determined to be (BSC 2003 [DIRS 161235], Section 6.4.4) (DTN: SN0308T0506303.003 [DIRS 164839]):

$$CV = \begin{bmatrix} 2197.7 & -15.159 & -83.254 & -1805.2 & 15.897 \\ -15.159 & 0.22667 & -1.2402 & 18.767 & -0.19963 \\ -83.254 & -1.2402 & 31.826 & -32.372 & 0.74246 \\ -1805.2 & 18.767 & -32.372 & 2906.5 & -28.677 \\ 15.897 & -0.19963 & 0.74246 & -28.677 & 0.29946 \end{bmatrix} \qquad \text{(Eq. 5)}$$

The entire variance of the model is due to uncertainty. It is recommended that the uncertainty of the parameter coefficients of the above model be limited to ±2 sd (BSC 2003 [DIRS 161235], Section 6.4.4).

The effect of nitrate ions on the crevice repassivation potential is represented as follows.

$$\Delta E^{NO_3^-}_{rcrev} = b_o + b_1 [NO_3^-] + b_2 \frac{[NO_3^-]}{[Cl^-]} \qquad \text{(Eq. 6)}$$

where $\Delta E^{NO_3^-}_{rcrev}$ is in mV vs. SSC, b_o, b_1 and b_2 are constants and other parameters are defined as before. The parameter coefficients resulting from the fitting procedure were determined to be: $b_0 = $-50.959, $b_1 = 115.867$, and $b_2 = 1045$. The effect of the interaction of the competing aggressive ions (e.g., chloride ions) and inhibitive nitrate ions on the crevice repassivation potential is represented with the ratio of the concentrations of the two competing ions and the concentration of nitrate ion. The linear relationship between $\Delta E^{NO_3^-}_{rcrev}$ and the concentration ratio is applicable for concentration ratios between 0.1 and 1.0 (BSC 2003 [DIRS 161235], Section 6.4.4). Because the effect of the measurement uncertainty has already been captured in the crevice repassivation potential model with no nitrate ion present, only the mean value of the $\Delta E_{rcrev}^{NO_3^-}$ is used to determine the crevice repassivation potential (E_{rcrev}) (BSC 2003 [DIRS 161235], Section 6.4.4).

Variability in the crevice repassivation potential among waste packages is included through the temporally and spatially varying waste package temperature and chemistry exposure conditions.

4.1.4.2 Waste Package Outer Barrier Long-Term Corrosion Potential Inputs

The long-term corrosion potential model (E_{corr}) for the WPOB is expressed as follows (BSC 2003 [DIRS 161235], Section 6.4.4):

$$E_{corr} = c_o + c_1 T + c_2 pH + c_3 [Cl^-] + c_4 \log\left(\frac{[NO_3^-]}{[Cl^-]}\right) \quad \text{(Eq. 7)}$$

where E_{corr} is the long-term corrosion potential in mV vs. SSC, c_o, c_1, c_2, c_3, and c_4 are coefficients of the model parameters, and other parameters are defined as before. The median estimated regression coefficients are: $c_0 =$ 365.511, $c_1 =$ 1.853, $c_2 =$-48.091, $c_3 =$-29.641, and $c_4 =$ -4.263. The covariance matrix resulting from the least squares fitting was determined to be (BSC 2003 [DIRS 161235], Section 6.4.4) (DTN: SN0308T0506303.003 [DIRS 164839]):

$$CV = \begin{bmatrix} 1082.5 & -10.818 & -31.492 & 0.77527 & -37.167 \\ -10.818 & 0.13976 & -0.029431 & -0.1269 & 0.37478 \\ -31.492 & -0.029431 & 6.3919 & 0.42229 & 0.59728 \\ 0.77527 & -0.1269 & 0.42229 & 3.7299 & 6.1905 \\ -37.167 & 0.37478 & 0.59728 & 6.1905 & 18.711 \end{bmatrix} \quad \text{(Eq. 8)}$$

The purpose of this corrosion potential model is *to estimate the long-term steady-state open-circuit corrosion potential of Alloy 22* for a range of exposure conditions related to the repository. The model *should not be used for short-term transient conditions* (BSC 2003 [DIRS 161235], Section 6.4.4). The entire variance of the model is due to uncertainty. As with the crevice repassivation potential model, it is recommended that the uncertainty of the parameter coefficients of the corrosion potential model be limited to ±2 sd. Note that the above corrosion potential model, in conjunction with the crevice repassivation potential model, is to be used to evaluate *the long-term localized corrosion susceptibility of the WPOB* and is not intended for modeling of short-term transient behavior (BSC 2003 [DIRS 161235], Section 6.4.4).

Variability in the corrosion potential among waste packages is included through the temporally and spatially varying waste package temperature and chemistry exposure conditions.

4.1.4.3 Waste Package Outer Barrier Localized Corrosion Penetration Rate Inputs

In the localized corrosion penetration rate model, localized corrosion propagates at a (time-independent) constant rate (BSC 2003 [DIRS 161235], Section 6.4.4). The localized corrosion penetration rates for the WPOB range from 12.7 to 1270 μm/yr with the median value of 127 μm/yr, as shown in Table 8 (converted to mm/yr). The LC penetration rate follows a log-uniform distribution between the bounds (BSC 2003 [DIRS 161235], Section 6.4.4). The entire variance in the penetration rate is due to uncertainty.

Table 8. Distribution of Localized Corrosion Rates for Alloy 22 (DTN: SN0308T0506303.003 [DIRS 164839]).

Input Name	Input Source	Input Value	Units
LogUniform lower bound	BSC 2003 [DIRS 161235], Section 6.4.4 DTN: SN0308T0506303.003 [DIRS 164839]	1.27E-2	mm/yr
LogUniform upper bound	BSC 2003 [DIRS 161235], Section 6.4.4 DTN: SN0308T0506303.003 [DIRS 164839]	1.270	mm/yr

4.1.5 Weld Flaw Inputs

This section lists the design information inputs to the Integrated Waste Package Degradation (IWPD) Model weld flaw analysis for the Alloy 22 waste package outer barrier (or outer shell) closure-lid welds. Most of these inputs can be found in the *Analysis of Mechanisms for Early Waste Package/Drip Shield Failure* (BSC 2003 [DIRS 164475]).

Table 9. Manufacturing Defect Analysis Inputs and Their Sources

	Input Source	Input Value	Units
Fraction of embedded weld flaws to propagate (Depth of plate to be included for embedded flaws)	BSC 2003 [DIRS 161234], Table 8-1 DTN: LL030607012251.065 [DIRS 163968]	0.25	N/A
Fraction of weld flaws capable of propagation based on orientation	BSC 2003 [DIRS 164475], Table 12	0.008	N/A
Characteristic weld flaw size for PND (location parameter)	BSC 2003 [DIRS 164475], Table 11	2.5	mm
Shape factor for PND	BSC 2003 [DIRS 164475], Table 11	3	N/A
Lower limit for PND (detection threshold)	BSC 2003 [DIRS 164475], Table 11	0.005	N/A
Sample weld diameter, D	BSC 2003 [DIRS 164475], Table 6 and Section 6.2.1.1.2	60.765	in
Weld cross section dimensions	BSC 2003 [DIRS 164475], Figure 1 and Table 6	See Figure 1 and Table 10	N/A
Number of sample welds	BSC 2003 [DIRS 164475], Section 6.2.1.1.2	16	N/A
Number of sample flaws, n_f	BSC 2003 [DIRS 164475], Table 11	7	N/A
Cumulative size of sample flaws S_f	BSC 2003 [DIRS 164475], Attachment I, p. I-3	31.75	mm
Flaw size parameter	BSC 2003 [DIRS 164475], Equation 2	Gamma distribution with a mean of n_f / S_f and a standard deviation of $\mathrm{sqrt}(n_f)/S_f$ [(a)]	mm^{-1}
Flaw density parameter	BSC 2003 [DIRS 164475], Equation 12	Gamma distribution with a mean of $(n_f + ½)/ V_f$ and a standard deviation of $\mathrm{sqrt}(n_f + ½)/ V_f$ [(a)]	mm^{-3}
CSNF WP outer closure lid weld volume	BSC 2003 [DIRS 164610], Table 19	1350189	mm^3

	Input Source	Input Value	Units
CSNF WP middle closure lid weld volume	BSC 2003 [DIRS 164610], Table 18	490478	mm^3
CDSP WP outer closure lid weld volume	BSC 2003 [DIRS 164610], Table 19	1753091	mm^3
CDSP WP middle closure lid weld volume	BSC 2003 [DIRS 164610], Table 18	639901	mm^3
Weld Thickness (*th*)	BSC 2001 [DIRS 157812], BSC 2001 [DIRS 157817], and BSC 2001 [DIRS 157818], Sheet 3 of 3	25 for outer closure lid 10 for middle closure lid (same for CSNF and CDSP WPs)	mm

(a) Equations 2 and 12 in BSC 2003 [DIRS 164475] are pdfs of gamma distributions (Evans, et al. [DIRS 112115], Section 18). V_f is the cumulative volume of sample welds analyzed (see Section 6.3.8.2).

Figure 1 shows a schematic of the weld samples which were analyzed to determine the distributions used in the analysis of weld flaws (BSC 2003 [DIRS 164475], Figure 1 and Table 6).

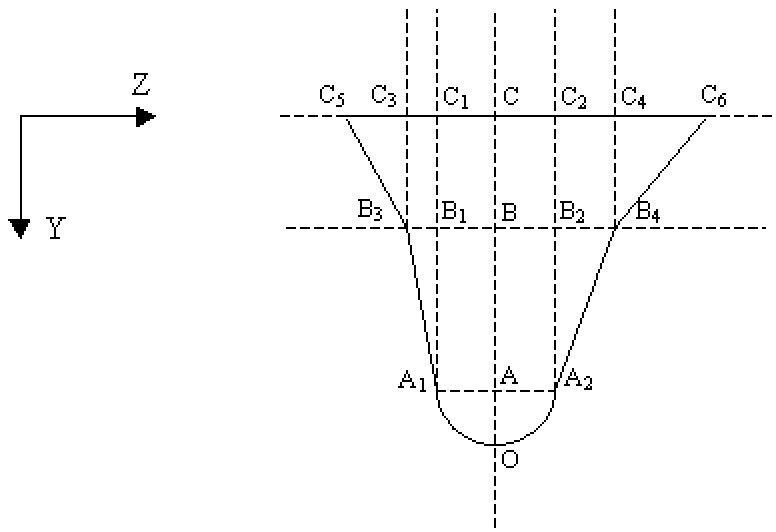


Figure 1. Schematic Representation of The Cross Section of the Alloy 22 Weld Analyzed (BSC 2003 [DIRS 164475], Figure 1).

Table 10. Weld Dimensions

Input Description	Input Source	Input Value	Units
Radius of the half-circle A_1OA_2, d_{AO}	BSC 2003 [DIRS 164475], Table 6	0.125	in
Distance OC, d_{OC}	BSC 2003 [DIRS 164475], Table 6	0.97	in
Distance BC, d_{BC}	BSC 2003 [DIRS 164475], Table 6	0.43	in
Angle $B_3A_1B_1$, θ_2	BSC 2003 [DIRS 164475], Table 6	3	degrees
Angle $C_5B_3C_3$, θ_1	BSC 2003 [DIRS 164475], Table 6	25	degrees
Angle $B_2A_2B_4$, θ_3	BSC 2003 [DIRS 164475], Table 6	6	degrees
Angle $C_4B_4C_6$, θ_4	BSC 2003 [DIRS 164475], Table 6	29	degrees

This design information was obtained from controlled sources.

4.1.6 Stress and Stress Intensity Factor Profile Inputs

Inputs to this analysis include stress and stress intensity factor profiles (stress or stress intensity factor versus depth) and slip dissolution model parameters appropriate for both the outer closure and middle closure lids of the waste package outer barrier. Table 11 summarizes these inputs, their sources, data tracking numbers (DTNs), and table numbers. All slip dissolution model parameters can be found in the report entitled *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234]).

Table 11. Stress and Stress Intensity Factor Profile Inputs and Their Sources

Input Name	Input Source	Input Value
Stress Profile Equation	BSC 2003 [DIRS 161234], Table 8-1 DTN: LL030607012251.065 [DIRS 163968]	Equation 9
Stress Profile Coefficients	BSC 2003 [DIRS 161234], Table 8-1 DTN: LL030607012251.065 [DIRS 163968]	See Table 12
Stress Intensity Factor Profiles	BSC 2003 [DIRS 161234], Table 8-2 and Table 8-3 DTN: LL030607012251.065 [DIRS 163968]	See Table 13
Yield strength, YS (various temperatures)	DTN: MO0003RIB00071.000 [DIRS 148850]	338 MPa at 366 K 283 MPa at 477 K
Stress variation with angle	BSC 2003 [DIRS 161234], Table 8-1 DTN: LL030607012251.065 [DIRS 163968]	Equation 10
Stress intensity factor variation with angle	BSC 2003 [DIRS 161234], Table 8-1 DTN: LL030607012251.065 [DIRS 163968]	Equation 11
Uncertain scaling factor for stress and stress intensity factor profiles, *z*	BSC 2003 [DIRS 161234], Section 6.4.5 DTN: LL030607012251.065 [DIRS 163968]	Truncated normal (at ±3 sd) with a mean of 0 and a standard deviation (sd) of 5% of YS

These inputs are qualified.

The hoop stress (σ in MPa) as a function of depth (x in mm) in the closure weld regions of the Alloy 22 waste package outer barrier is given by a third order polynomial equation of the form (BSC 2003 [DIRS 161234], Equation 23; DTN: LL030607012251.065 [DIRS 163968]):

$$\sigma(x,0) = A_0 + A_1 \cdot x + A_2 \cdot x^2 + A_3 \cdot x^3 \qquad \text{(Eq. 9)}$$

where the values of the coefficients (A_i's) are given in Table 12. The variation in the stress profile with depth is variability. The second argument in the stress function is used to represent angular variation as discussed later in this section.

Table 12. Stress Coefficients Used in the IWPD Model for the Outer and Middle Closure Lids of Waste Package Outer Barrier in Metric Units (i.e. Stress in MPa). The Stress Coefficients are Found in (BSC 2003 [DIRS 161234], Table 8-1, DTN: LL030607012251.065 [DIRS 163968]).

Coefficient	Outer Closure Lid Laser Peened	Middle Closure Lid As-Welded	Units
A_0	-292.607	219.908	MPa
A_1	178.277	56.494	MPa/mm
A_2	-14.135	-20.848	MPa/mm^2
A_3	0.320	1.083	MPa/mm^3

Table 13 lists the stress intensity factor versus depth profiles for the outer and middle closure lids of the Alloy 22 waste package outer barrier. The stress intensity factor is a scale factor defining the magnitude of the crack tip stress field. The variation in the stress intensity factor profile with depth is variability. As these are the results of intermediate calculations, as many digits are possible are retained to avoid round-off errors.

Table 13. Stress Intensity Factor (K_I) Vs. Depth Tables (due to Sz Hoop Stress) for the Outer and Middle Closure-Lids of Waste Package Outer Barrier. The K_I Profile for the Laser-Peened Waste Package Outer Barrier Outer Lid (Outer Closure Lid) is Found in (BSC 2003 [DIRS 161234], Table 8-3, DTN: LL030607012251.065 [DIRS 163968]). The Profile for the As-Welded Waste Package Outer Barrier Middle Lid is found in (BSC 2003 [DIRS 161234], Table 8-2, DTN: LL030607012251.065 [DIRS 163968]).

Outer Closure Lid		Middle Closure Lid	
K_I (MPa•m$^{1/2}$)	Depth (mm)	K_I (MPa•m$^{1/2}$)	Depth (mm)
-5.6943	0.3988	7.5754	0.1593
-6.4965	0.8001	10.9665	0.3203
-6.1528	1.1989	13.7144	0.4797
-5.1372	1.6002	16.1330	0.6407
-3.6697	1.9990	18.3358	0.8000
-1.8824	2.4003	20.3775	0.9593
0.1212	2.7991	22.3816	1.1203
2.2821	3.2004	24.3197	1.2797
4.5533	3.5992	26.1726	1.4407
6.8939	3.9980	27.9459	1.6000
9.2702	4.3993	29.6433	1.7593
11.6543	4.7981	31.2668	1.9203
14.0165	5.1994	32.8922	2.0797
16.3364	5.5982	34.5292	2.2407
18.6024	5.9995	36.1060	2.4000
20.8003	6.3983	37.6220	2.5593
22.9177	6.7970	39.0762	2.7203
24.9441	7.1984	40.4676	2.8797
26.9023	7.5971	41.8264	3.0407
28.8612	7.9985	43.2168	3.2000
30.7287	8.3972	44.5479	3.3593
32.5008	8.7986	45.8181	3.5203
34.1745	9.1973	47.0265	3.6797
35.7479	9.5987	48.1718	3.8407
37.2200	9.9974	49.2531	4.0000
38.4530	10.3962	50.3451	4.1593
39.5674	10.7975	51.3729	4.3203
40.5636	11.1963	52.3351	4.4797
41.4432	11.5976	53.2313	4.6407

Outer Closure Lid		Middle Closure Lid	
K_I (MPa•m^{½})	Depth (mm)	K_I (MPa•m^{½})	Depth (mm)
42.2086	11.9964	54.0602	4.8000
42.8627	12.3977	54.8214	4.9593
43.4439	12.7965	55.4811	5.1203
43.9342	13.1978	56.0586	5.2797
44.3269	13.5966	56.5637	5.4407
44.6272	13.9954	56.9965	5.6000
44.8409	14.3967	57.3567	5.7593
44.9743	14.7955	57.6444	5.9203
45.0329	15.1968	57.7587	6.0797
45.0208	15.5956	57.6946	6.2407
44.9464	15.9969	57.5522	6.4000
44.8182	16.3957	57.3322	6.5593
44.6449	16.7945	57.0353	6.7203
44.4361	17.1958	56.6626	6.8797
44.2112	17.5946	56.1419	7.0407
43.9968	17.9959	55.3276	7.2000
43.7750	18.3947	54.4422	7.3593
43.5578	18.7960	53.4878	7.5203
43.3569	19.1948	54.6294	7.6797
43.1853	19.5961	56.2191	7.8407
43.0560	19.9949	57.7865	8.0000

The variation in the stress profile with depth is due to variability. The provided hoop stress state was determined to vary with angle (θ) around the circumference of the Alloy 22 waste package outer and middle closure-lid welds ($\theta = 0$ point arbitrarily chosen) according to the following functional form (BSC 2003 [DIRS 161234], Section 6.4.5) (DTN: LL030607012251.065 [DIRS 163968]):

$$\sigma(x,\theta) = \sigma(x,0) - (17.236893)\cdot(1-\cos(\theta)) \qquad \text{(Eq. 10)}$$

Note that $\sigma(x, 0)$ (defined in Equation 9) uses the stress coefficients (A_i) defined in Table 12 with x in units of mm. Based on the angular stress variation in Equation 10, the stress intensity factor variation with angle is given by (BSC 2003 [DIRS 161234], Section 6.4.5) (DTN: LL030607012251.065 [DIRS 163968]):

$$K_I(x,\theta) = K_I(x)\cdot\left(\frac{\sigma(Thck,\theta)}{\sigma(Thck,0)}\right) \qquad \text{(Eq. 11)}$$

where $Thck$ is the lid thickness and $K_I(x)$ is given by the values in Table 13. The variation of the stress and stress intensity factor profiles with angle is due to variability (BSC 2003 [DIRS 161234], Section 6.4.5).

The uncertainty in the stress and stress intensity factor profiles is introduced through a scaling factor, z. The scaling factor, z, which is sampled from a normal distribution with a mean of zero and a standard deviation of 5 percent of the yield strength, YS, with an upper bound of 15 percent of the YS and a lower bound of –15 percent of the YS (BSC 2003 [DIRS 161234], Section 6.4.5).

The stress relation, accounting for uncertainty, is given by

$$\sigma_u(x,\theta,z) = \sigma(x,\theta)\cdot\left(\frac{\sigma(Thck,\theta)+z}{\sigma(Thck,\theta)}\right) \quad \text{(Eq. 12)}$$

and the stress intensity factor relation is given by

$$K_{Iu}(x,\theta,z) = K_I(x,\theta)\cdot\left(\frac{\sigma(Thck,\theta)+z}{\sigma(Thck,\theta)}\right) = K_I(x,0)\cdot\left(\frac{\sigma(Thck,\theta)+z}{\sigma(Thck,0)}\right) \quad \text{(Eq. 13)}$$

The inputs discussed in this section is appropriate for its intended use because it provides a very reasonable estimate of the stress and stress intensity factor profiles for the outer and middle closure lids of waste package outer barrier.

The uncertainty treatment of these inputs is encompassed in the parameter *z* which is sampled once per realization of the Integrated Waste Package Degradation Model for each closure lid (i.e. a different value of *z* may be sampled for each lid in a given realization).

The stress and stress intensity factor profiles for the waste package outer barrier closure lids are technical product output information obtained from controlled and confirmed sources.

4.1.7 Slip Dissolution Inputs

The Slip Dissolution Model for stress corrosion cracking requires a threshold stress, a stress intensity factor threshold, an incipient crack size, and crack growth rate parameters (which are functions of *n*, the repassivation slope). These inputs and their sources are listed in Table 14.

Table 14. Slip Dissolution Inputs Used in the IWPD Model and Their Sources

Input Name	Input Source	Input Value	Units
Threshold stress	BSC 2003 [DIRS 161234], Table 8-1 DTN: LL030607012251.065 [DIRS 163968]	0.9*YS at 473 K	MPa
Incipient crack size	BSC 2003 [DIRS 161234], Table 8-1 DTN: LL030607012251.065 [DIRS 163968]	0.05	mm
Fraction of embedded weld flaws to propagate	BSC 2003 [DIRS 161234], Table 8-1 DTN: LL030607012251.065 [DIRS 163968]	0.25	N/A
Threshold stress intensity factor, K_{ISCC}	BSC 2003 [DIRS 161234], Section 6.3.5 DTN: LL030607012251.065 [DIRS 163968]	Equation 14	MPa $m^{1/2}$
Repassivation slope, *n*	BSC 2003 [DIRS 161234], Table 8-1 DTN: LL030607012251.065 [DIRS 163968]	Truncated normal (at ±2 sd) with a mean of 1.304 and sd of 0.16.	N/A

The threshold stress is defined as the minimum stress at which cracks initiate on a "smooth" surface. These cracks are referred to in this report as incipient cracks (to distinguish them from weld flaws) and typically form at local surface defects such as grain boundary junctions and surface roughness. Incipient cracks are 0.05 mm in length (BSC 2003 [DIRS 161234], Table 8-1).

Weld flaws are already nucleated and thus do not require a stress threshold to nucleate. However, most weld flaws are embedded within the material and therefore not exposed to the environment. As general corrosion proceeds, some initially embedded weld flaws may be exposed to the environment (BSC 2003 [DIRS 161234], Section 6.2.2) while others are "corroded away." This evolution of the number of defects is not considered in detail. It has been recommended that a conservative approach would be to consider the fraction of weld flaws embedded within the outer ¼ of the weld thickness (BSC 2003 [DIRS 161234], Section 6.2.2) to be capable of propagation by the slip-dissolution model.

If the stress intensity factor at the crack tip is below the threshold stress intensity factor, no crack growth will occur. The threshold stress intensity factor, K_{ISCC}, is given as a function of the repassivation slope, n and V_{gc} (which equals 7.23 nm/yr and is expressed in units of mm/s for use in Equation 14) (BSC 2003 [DIRS 161234], Section 6.3.5):

$$K_{ISCC} = \left(\frac{V_{gc}}{\overline{A}} \right)^{1/\overline{n}} \qquad \text{(Eq. 14)}$$

$\overline{A}$ and $\overline{n}$ are functions of n, as discussed below. The threshold stress intensity factor is applied to both incipient cracks and weld flaws. The variations in the threshold stress and stress intensity factor distributions are entirely due to uncertainty. The thresholds are sampled once per realization of the IWPD Model (i.e. the same value of these thresholds is used for each lid in a given realization).

Once crack growth initiates the crack(s) grow at a velocity given by (BSC 2003 [DIRS 161234], Table 8-1) (DTN: LL030607012251.065 [DIRS 163968]):

$$V_t = \overline{A}\left(K_I\right)^{\overline{n}} \qquad \text{(Eq. 15)}$$

where V_t is the crack growth rate in mm/s, and K_I is the stress intensity factor in $MPa(m)^{1/2}$. Parameters, $\overline{A}$ and $\overline{n}$, in the above equation are expressed in terms of the repassivation slope, n, as follows.

$$\overline{A} = 7.8x10^{-2} n^{3.6} \left(4.1x10^{-14}\right)^{n} \qquad \text{(Eq. 16)}$$

$$\overline{n} = 4n \qquad \text{(Eq. 17)}$$

In the IWPD Model, the parameter n is represented by a truncated normal distribution (at ±2 sd) with a mean of 1.304, a sd of 0.16. The variation in the repassivation slope, n, is entirely due to uncertainty. The repassivation slope is sampled once per realization of the IWPD Model (i.e. the same value of n is used for each lid in a given realization).

The inputs discussed in this section are appropriate for their intended use because they provide very reasonable estimates of the stress corrosion crack growth characteristics for the outer and middle closure lids of the Alloy 22 waste package outer barrier. The slip dissolution parameters for the waste package outer barrier closure lids are technical product output information obtained from controlled and confirmed sources.

4.1.8 Waste Package Outer Barrier Microbially Influenced Corrosion Inputs

The treatment of microbially influenced corrosion (MIC) of the Alloy 22 waste package outer barrier requires a threshold relative humidity for microbial activity and a general corrosion rate multiplier to model the affect of microbial activity. These inputs and their sources are listed in Table 15.

Table 15. Waste Package Outer Barrier Microbially Influenced Corrosion Inputs and Their Sources

Input Name	Input Source	Input Value	Units
MIC Threshold RH	BSC 2003 [DIRS 161235], Section 6.4.5 DTN: SN0308T0506303.004 [DIRS 164840]	0.9	fraction
General Corrosion Rate MIC enhancement factor	BSC 2003 [DIRS 161235], Section 6.4.5 DTN: SN0308T0506303.004 [DIRS 164840]	Uniform over the range (1, 2)	N/A

According to the upstream report entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.5) (DTN: SN0308T0506303.004 [DIRS 164840]), general corrosion rates should be enhanced to model the effect of MIC above 90% relative humidity. The parameter value for the threshold RH above which MIC takes place is fixed (i.e. no uncertainty or variability).

The upstream report recommends the general corrosion rate of the waste package outer barrier be enhanced due to MIC by a factor between 1 and 2 (i.e. no enhancement up to the general corrosion rate being doubled) (BSC 2003 [DIRS 161235], Section 6.4.5) (DTN: SN0308T0506303.004 [DIRS 164840]). Thus, the general corrosion rate enhancement factor will be sampled from a uniform distribution with an upper bound of 2 and a lower bound of 1. The same upstream report recommends that, while bacteria preferentially colonize weldments, heat affected zones, and charged regions, the general corrosion rate enhancement factor is to be applied to the entire waste package surface (BSC 2003 [DIRS 161235], Section 6.4.5) (DTN: SN0308T0506303.004 [DIRS 164840]). The variation in the general corrosion rate MIC enhancement factor is entirely due to uncertainty (BSC 2003 [DIRS 161235], Section 6.4.5).

The parameters discussed in this section are appropriate for their intended use because they provide a very reasonable estimate of the affects of microbial action on the waste package outer barrier. The parameters are technical product output information obtained from controlled and confirmed sources.

4.1.9 Waste Package Early Failure Inputs

Several mechanisms which could result in early failure of the WP were considered in the *Analysis of Mechanisms for Early Waste Package/Drip Shield Failure* (BSC 2003 [DIRS 164475]). It was determined that improper heat treatment, improper stress mitigation, and mishandling of the WP could have adverse consequences on WP performance (BSC 2003 [DIRS 164475], Section 6.4.8). The probabilities of occurrence for these three mechanisms were combined to yield an overall probability of WP early failure. The number of WPs affected per realization is given by a Poisson distribution with an uncertain intensity. These values and their sources are summarized in Table 16.

Table 16. Waste Package Early Failure Inputs and Their Sources

Input Name	Input Source	Input Value	Units
Evaluation probability per WP (Uncertain Poisson intensity)	BSC 2003 [DIRS 164475], Section 7, Table 20	Log normal distribution with a median of 7.2×10^{-6} and an error factor of 15 truncated at 7.44213E-3	per WP
Number of Early Failed WP per realization	BSC 2003 [DIRS 164475], Section 7, Table 20	Poisson distribution with intensity given above.	# WP/realization

The "Evaluation probability per WP" distribution is sampled once per realization (i.e. it is an uncertainty distribution). The sampled value is then multiplied by the number of WPs per realization to give the Poisson intensity for the distribution for the number of early failed WPs per realization. The Poisson distribution is sampled once per realization to give the number of affected WPs in the realization. In this representation, variation in the number of early failed WPs is expressed as variability deriving from a discrete Poisson distribution with an uncertain intensity parameter. The uncertain intensity parameter is the product of the uncertain rate of WP failures (log normally distributed) and the number of WPs in a realization. Also see Section 6.3.12 of this report for a discussion of the conceptual model and Section 6.5.12 for discussion of implementation (including a discussion of a marginal distribution that incorporates uncertainty).

The following recommendations are made in the *Analysis of Mechanisms for Early Waste Package/Drip Shield Failure* (BSC 2003 [DIRS 164475], Section 6.4.8) for evaluating the consequences of WP early failure of the Alloy 22 WPOB:

- A failure of the WP outer barrier shell and outer and middle closure lids should be assumed as well as the failure of the stainless steel structural inner vessel and closure lid.
- The affected WPs should be assumed to fail immediately upon initiation of degradation processes.
- The entire WP surface area should be considered affected by WP early failure.
- The materials of the entire affected area should be assumed lost upon failure of the WPs because the affected area will be subjected to stress corrosion cracking and highly enhanced localized and general corrosion.

The inputs are technical product output information obtained from controlled and confirmed sources.

4.2 CRITERIA

The Waste Package Technical Work Plan (TWP) (BSC 2002 [DIRS 161132], Attachment C, Table C5) has identified the following acceptance criteria (AC) based on the requirements mentioned in the *Project Requirements Document* (PRD) (Canori and Leitner 2003 [DIRS 161770]) and the *Yucca Mountain Review Plan* (NRC 2003 [DIRS 163274]):

1. System Description and Demonstration of Multiple Barriers (NRC 2003 [DIRS 163274], Section 2.2.1.1.3; Canori and Leitner 2003 [DIRS 161770], PRD-002/T-014, PRD-002/T-016)

Specific requirements involve identification of multiple barriers (natural and engineered), describing the capabilities of these barriers to isolate waste, and providing technical bases for capabilities descriptions consistent with the postclosure performance objectives. To comply with these requirements, the following acceptance criteria are identified in the Waste Package TWP (BSC 2002 [DIRS 161132], Attachment C, Table C5):

- AC1: Identification of Barriers is Adequate
- AC2: Description of Barrier Capability to Isolate Waste is Acceptable.
- AC3: Technical Basis for Barrier Capability is Adequately Presented

2. Degradation of Engineered Barriers (NRC 2003 [DIRS 163274], Section 2.2.1.3.1.3; Canori and Leitner 2003 [DIRS 161770], PRD-002/T-015)

Specific requirements include describing deterioration or degradation of engineered barriers and modeling degradation processes using data for performance assessment, including total system performance assessment (TSPA). Consideration of uncertainties and variabilities in model parameters and alternative conceptual models are also required. To fulfill these requirements, the following acceptance criteria are identified in the Waste Package TWP (BSC 2002 [DIRS 161132], Attachment C, Table C5):

- AC1: System Description and Model Integration are Adequate
- AC2: Data are Sufficient for Model Justification
- AC3: Data Uncertainty is Characterized and Propagated Through the Model Abstraction
- AC4: Model Uncertainty is Characterized and Propagated Through the Model Abstraction
- AC5: Model Abstraction Output is Supported by Objective Comparisons

3. Quantity and Chemistry of Water Contacting Waste Packages and Waste Forms (NRC 2003 [DIRS 163274], Section 2.2.1.3.3.3; Canori and Leitner 2003 [DIRS 161770], PRD-002/T-015)

Specific requirements include describing deterioration or degradation of engineered barriers and modeling degradation processes using data for performance assessment, including total system performance assessment (TSPA). Consideration of uncertainties and variabilities in model parameters and alternative conceptual models are also required. To fulfill these requirements, the following acceptance criteria are identified in the Waste Package TWP (BSC 2002 [DIRS 161132], Attachment C, Table C5):

- AC1: System Description and Model Integration are Adequate
- AC2: Data are Sufficient for Model Justification
- AC3: Data Uncertainty is Characterized and Propagated Through the Model Abstraction

- AC4: Model Uncertainty is Characterized and Propagated Through the Model Abstraction
- AC5: Model Abstraction Output is Supported by Objective Comparisons

4.3 CODES AND STANDARDS

The process of implementing these models is consistent with the methodology described in the ASTM Standard Practice C-1174 for prediction of the long-term behavior of EBS components in a geologic repository (ASTM C 1174-97 1998 [DIRS 105725]).

5. ASSUMPTIONS

No assumptions were made in the development of this report.

6. MODEL DISCUSSION

This section provides modeling objectives and the conceptual model for the waste package and drip shield degradation used in the Integrated Waste Package Degradation (IWPD) Model. The implementation of the abstraction models of the process-level models for the degradation processes considered are described. The IWPD Model results are discussed in terms of a set of profiles for waste package and drip shield failure and average number of penetrations as a function of time. The results of all analyses documented in this report are tracked by DTN: MO0310MWDWAPAN.002 [DIRS 165800]. A complete list of corroborating/supporting data and information used in model development can be found in the corresponding DIRS. The data and information is identified as being used in Section 6 and carries a status of Reference Only.

6.1 MODELING OBJECTIVES

The U.S. Department of Energy is currently evaluating the long-term (>10,000 years) performance of the repository for the disposal of spent nuclear fuel (SNF) and high-level nuclear waste (HLW) at Yucca Mountain, Nevada. The Yucca Mountain site is located approximately 100 miles Northwest of Las Vegas, Nevada. The radioactive waste will be placed inside the waste package, part of the Engineered Barrier System (EBS), and placed approximately 300 m below ground. The release of radionuclides from the EBS into the geosphere will depend on a robust drip shield and waste package design, among other EBS components.

The License Application (LA) waste package design consists of two layers: an Alloy 22 outer barrier and a 316 stainless steel inner vessel (BSC 2003 [DIRS 165406]). A drip shield with Titanium Grade 7 water diversion plates will be placed over the waste package (BSC 2003 [DIRS 164069]). The space between the drip shield and the emplacement drift is open for air circulation and there is no backfill material used. Although the stainless steel inner vessel provides structural stability to the Alloy 22 outer barrier, no other performance credit is taken for the WP inner vessel. The WP outer barrier has two Alloy 22 closure lids (referred to as the WP outer barrier outer and middle closure lids). The 316 stainless steel WP inner vessel has one 316 stainless steel closure lid (referred to as the WP inner vessel closure lid). The WP outer barrier closure lids are welded to the WP outer barrier and the WP inner vessel closure lid is welded to the WP inner vessel after the waste form (spent nuclear fuel and/or glassified high-level nuclear waste) is loaded.

Over the emplacement period, the drip shield and waste package are potentially subject to various degradation processes including general corrosion, localized corrosion, and stress corrosion cracking. Generally, the effects of other processes important to degradation of the drip shields and waste packages (e.g., MIC, aging and phase instability, radiolysis, weld flaws, mechanisms of early failure, etc.) are considered in terms of their effect on these three processes. The Integrated Waste Package Degradation (IWPD) Model developed in this technical product is used directly in total system performance assessment (TSPA) analysis to evaluate degradation of the drip shields and waste packages with time. In addition to the DS and WP design inputs discussed above, the primary inputs to the IWPD Model are documented in the reports summarized below:

- *General Corrosion and Localized Corrosion of the Drip Shield* (BSC 2003 [DIRS 161236])
  - General corrosion inputs for the Titanium Grade 7 DS (Section 4.1.2). The general corrosion treatment for the Titanium Grade 7 DS includes an uncertain distribution of general corrosion rates.
  - Localized corrosion initiation criteria.

- *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235])
  - General corrosion inputs for the Alloy 22 WPOB (Section 4.1.3). The general corrosion treatment for the Alloy 22 WPOB includes a variability distribution of general corrosion rates applicable at 60°C and an uncertain distribution for an Arrhenius-type temperature-dependence.
  - An uncertain distribution for a general corrosion rate multiplier to represent the effect of MIC on general corrosion (Section 4.1.8).
  - Localized corrosion initiation inputs (Section 4.1.4).
  - Localized corrosion growth rate inputs (Section 4.1.4).

- *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234])
  - Stress and stress intensity factor profiles for the closure weld regions of the Alloy 22 WPOB (Section 4.1.6). These inputs include an angular variability treatment and an uncertainty treatment.
  - Slip Dissolution Model inputs such as stress and stress intensity factor thresholds for the closure weld regions of the Alloy 22 WPOB and SCC crack growth velocity inputs (Section 4.1.7). These inputs are 100% uncertain.
  - An assessment of the area of the Alloy 22 WPOB subject to SCC. This input is neither uncertain nor variable.

- *Analysis of Mechanisms for Early Waste Package/Drip Shield Failure* (BSC 2003 [DIRS 164475])
  - Inputs for the number and size of weld flaws (Section 4.1.5).
  - Inputs for the mechanisms of early failure and their consequences (Section 4.1.9).

The IWPD Model uses a stochastic simulation approach and provides a description of the variation of waste package and drip shield degradation as a function of time for specific design and thermohydrologic exposure conditions. The objectives of the IWPD Model are:

- To provide a representation of waste package degradation processes in the repository;
- To capture the effects of uncertainty and variability both in exposure conditions and degradation processes over a geologic time scale

The TSPA-LA waste package degradation analysis simulates the behavior of a few hundred waste packages (see Section 6.5). Effects of spatial and temporal variations in the exposure conditions over the repository are modeled by explicitly incorporating relevant exposure condition histories into the analysis. The exposure condition parameters that were considered to vary over the repository are relative humidity and temperature at the waste package surface. In addition, potentially variable corrosion processes within a single waste package are represented by dividing the waste package surface into subareas called "patches" and stochastically sampling the degradation model parameter values for each patch. The use of patches explicitly represents the variability in degradation processes within a single waste package at a given time.

In the TSPA-LA analysis, uncertainty in waste package degradation is analyzed with multiple realizations of the IWPD Model. For each realization, values are sampled for the uncertain degradation parameters and passed to the IWPD Model. Each realization is a complete IWPD Model simulation, of a given number of waste packages, explicitly considering variability in the degradation processes. Accordingly, each of the IWPD Model outputs (i.e. the fraction of the total number of waste packages and drip shields failed versus time and of the average number of patch and crack penetrations per failed waste package (or drip shield)) are reported as a group of "degradation profile curves" (resulting from the multiple realizations) which represent the potential range of the output parameters. For example, the waste-package failure time profiles are reported with a group of curves representing the cumulative probability of waste package failures as a function of time. The outputs of the IWPD Model are used as input for waste form degradation analysis and radionuclide release analysis from failed waste packages conducted within the Total System Performance Assessment Model.

6.2 FEATURES, EVENTS, AND PROCESSES INCLUDED IN MODEL

The development of a comprehensive list of features, events, and processes (FEPs) potentially relevant to post-closure performance of the potential Yucca Mountain repository is an ongoing, iterative process based on site-specific information, design, and regulations. The approach for developing an initial list of FEPs, in support of TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), was documented in Freeze et al. (2001 [DIRS 154365]). The initial FEP list contained 328 FEPs, of which 176 were included in TSPA-SR models (CRWMS M&O 2000 [DIRS 153246], Tables B-9 through B-17). To support TSPA-LA, the FEP list was re-evaluated in accordance with the *Enhanced FEP Plan* (BSC 2002 [DIRS 158966], Section 3.2). As documented in the Technical Work Plan for this technical product (BSC 2002 [DIRS 161132], Attachment C, Table C3), the Features, Events, and Processes listed in Table 17 are included in the TSPA-LA and are addressed in this report. Note that the TSPA-SR FEPs were renumbered for TSPA-LA. The first column in Table 17 lists the TSPA-LA FEP numbers.

Table 17. Table of Included FEPs

FEP No.	FEP Name	Section Where Disposition is Described	Summary of Disposition in TSPA-LA
2.1.03.01.0A	General corrosion of waste packages	Section 6.3.4	Included in Integrated Waste Package Degradation (IWPD) Model as a mechanism for creating patch openings in waste packages. Because general corrosion is likely to be operative for the most of the repository operation period, it is one of the key corrosion processes that could lead to degradation and failure of waste packages in the repository. General corrosion due to dry-air oxidation, aqueous corrosion of the waste package outer barrier, microbially influenced corrosion and aging and phase instability are discussed in the *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235]) model report. It was concluded in the *General Corrosion and Localized Corrosion of the Waste Package Outer Barrier* model report (BSC 2003 [DIRS 161235], Section 8.1) that although dry air oxidation occurs, it results in a negligible amount of barrier thinning over repository time scales (only ~93 µm even if the waste package outer barrier (WPOB) were exposed for 10,000 years at 350°C). Therefore, dry oxidation does not need to be considered in TSPA analyses. Penetration rates for aqueous general corrosion are provided in Section 6.4.3 of the *General Corrosion and Localized Corrosion of the Waste Package Outer Barrier* model report (BSC 2003 [DIRS 161235]). General corrosion rates of the WPOB were estimated using weight-loss data of Alloy 22 samples after 5-year exposure in the Long-Term Corrosion Testing Facility (BSC 2003 [DIRS 161235], Section 6.4.3). Based on these test results, the general corrosion rate of 7.32 nm/yr is used as the base case general corrosion rate of the WPOB. For TSPA, the general corrosion progresses uniformly over a large surface at a time independent constant rate and the depth of penetration or thinning of the WPOB by general corrosion is equal to the general corrosion rate multiplied by the time the waste package is exposed to an environment under which general corrosion occurs. Details of the general corrosion rate distributions used for the Alloy 22 Waste Package Outer Barrier (WPOB) are given in *General Corrosion and Localized Corrosion of the Waste Package Outer Barrier* model report (BSC 2003 [DIRS 161235]). The Alloy 22 general corrosion rate is considered to be a function of exposure temperature. The temperature dependence follows an Arrhenius relationship, i.e., $R = \exp\left[C_o - \frac{C_1}{T}\right]$

FEP No.	FEP Name	Section Where Disposition is Described	Summary of Disposition in TSPA-LA
			where R = general-corrosion rate T = temperature (Kelvin) C_o = intercept term C_1 = slope term as discussed in the report entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.3). The slope term is determined from short-term polarization resistance data for Alloy 22 specimens tested for a range of sample configurations, metallurgical conditions, and exposure conditions (BSC 2003 [DIRS 161235], Section 6.4.3). The intercept term, C_o, is determined from the general corrosion rate distribution derived from the weight loss of the 5-year crevice geometry samples exposed in the LTCTF (BSC 2003 [DIRS 161235], Section 6.4.3) and the value of the slope term, C_1. The general corrosion rate distribution derived from the weight loss of the 5-year crevice geometry samples exposed in the LTCTF are considered to represent the distribution of long-term general corrosion rates of the WPOB at 60°C (333.15 K). Therefore, $$\ln(R_o) = C_o - \frac{C_1}{333.15}$$ or $$C_o = \ln(R_o) + \frac{C_1}{333.15}$$ where R_o is the general corrosion rate distribution from the 5-year crevice geometry samples. Substituting for C_o, $$R = \exp\left[\ln(R_o) + C_1\left(\frac{1}{333.15} - \frac{1}{T}\right)\right]$$ The *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* report (BSC 2003 [DIRS 161235], Section 6.4.3) states that R_o is given by a Weibull distribution. The patch size used to model the WPs is four times the area of the crevice geometry sample size. Conceptually, the method employed corresponds to using the highest of four sampled corrosion rates (from the two-parameter Weibull distribution) to model general corrosion of the WP patch. This approach is conservative and appropriate for this application. The approach is conservative because it is probable that not all four samples from the Weibull distribution will have the highest rate, therefore, a more realistic representation of the overall general corrosion rate would be the average of the four sampled

FEP No.	FEP Name	Section Where Disposition is Described	Summary of Disposition in TSPA-LA
			corrosion rates. However, this approach would not account for the fact that one fourth of the patch has the maximum of the four sampled corrosion rates. On this basis the proposed approach is conservative and appropriate for this application. The effect of this method is to shift the median corrosion rate to higher values and to decrease the probability of sampling lower corrosion rates. The effect of microbial activity on the general corrosion process of the WPOB is represented in TSPA analyses with a rate enhancement factor (BSC 2003 [DIRS 161235], Table 6-1). Comparative analysis of the corrosion rates from the polarization resistance technique showed insignificant effects of welds and thermal aging of the WPOB on the general corrosion rates (BSC 2003 [DIRS 161235], Table 6-1). It was also concluded that the aging of both the base metal and welds of the WPOB under the thermal conditions expected in the repository is not significant for the regulatory time period (BSC 2003 [DIRS 161235], Table 6-1) and is of negligible consequence to radiological exposures to the RMEI and radionuclide releases to the accessible environment. Aging and phase instability and their effects on general corrosion are also discussed in FEP 2.1.11.06.0B, Thermal sensitization of drip shields. Section 6.3.4 of the *WAPDEG Analysis of Waste Package and Drip Shield Degradation* report (ANL-EBS-PA-000001), discusses how general corrosion of the Alloy 22 waste package outer barrier is temperature dependent and discusses details of the drip shield general corrosion conceptual model and its incorporation into the IWPD Model. The IWPD Model produces waste package degradation profiles consisting of the fraction of waste packages failed versus time and the average (per failed waste package) number of patch openings versus time. The degradation profiles are used as input into the TSPA model.
2.1.03.01.0B	General corrosion of drip shields	Section 6.3.3	Included in Integrated Waste Package Degradation (IWPD) Model as a mechanism for creating patch openings in drip shields. General corrosion due to dry-air oxidation, humid-air and aqueous general corrosion, microbially influenced corrosion and aging and phase instability of the Titanium Grade 7 drip shield are discussed in the *General Corrosion and Localized Corrosion of the Drip Shield* (BSC 2003 [DIRS 161236]) model report. It was concluded in the *General Corrosion and Localized Corrosion of the Drip Shield* report (BSC 2003 [DIRS 161236], Section 6.2) that although dry air oxidation occurs, it results in a negligible amount of barrier thinning over repository time scales (only ~2,129 nm even if the DS were exposed for 10,000 years at 200°C). Therefore, dry oxidation does not need to be considered in the TSPA analyses.

FEP No.	FEP Name	Section Where Disposition is Described	Summary of Disposition in TSPA-LA
			Penetration rates for general corrosion are provided in the *General Corrosion and Localized Corrosion of the Drip Shield* report (BSC 2003 [DIRS 161236]) and are used in TSPA analyses. Both humid-air and aqueous corrosion processes are considered part of general corrosion (BSC 2003 [DIRS 161236], Section 6.3). General corrosion rates of the DS were estimated with weight-loss data of Titanium Grade 16 samples after 1 to 5-year exposure in the Long-Term Corrosion Testing Facility (BSC 2003 [DIRS 161236], Section 6.3). Based on these test results, the penetration (or oxidation) rates range from 10 to 100 nm/yr (BSC 2003 [DIRS 161236], Section 6.3). The DS corrosion rates range from 0 to 320 nm/yr (BSC 2003 [DIRS 161236], Section 6.3). The DS outer surface may be exposed to a more complicated chemistry and geometry than the DS inner surface since dust and/or mineral films (from evaporation of dripping water) may form crevices on the DS outer surfaces. In contrast, the inner surfaces of the DS will not be exposed to dripping water nor significant dust film formation (BSC 2003 [DIRS 161236], Section 6.3). Therefore, the general corrosion of the inner surface and the outer surface of the drip shield are modeled by using different sets of corrosion data (BSC 2003 [DIRS 161236], Section 6.3). The variation in these inputs are considered to be entirely due to uncertainty (BSC 2003 [DIRS 161236], Section 6.3.4). For each realization of the Integrated Waste Package Degradation Model, a single general corrosion rate is sampled from each general corrosion rate distribution and applied to all DSs. Using this conceptual model for DS general corrosion, all DSs in the repository fail by general corrosion at the same time. The maximum general corrosion rate for the CDF applied to the under side of the DS is approximately 1.13E-04 mm/yr and the maximum general corrosion rate for the CDF applied to the top side of the DS is approximately 3.20E-04 mm/yr (BSC 2003 [DIRS 161236], Section 6.3.4); therefore, the earliest possible DS failure by general corrosion is about 35,000 years. Section 6.3.3 of the *WAPDEG Analysis of Waste Package and Drip Shield Degradation* report (ANL-EBS-PA-000001) report discusses details of the drip shield general corrosion conceptual model and its incorporation into the IWPD Model. The IWPD Model produces drip shield degradation profiles consisting of the fraction of drip shields failed versus time and the average (per failed drip shield) number of patch openings versus time. The degradation profiles are used as input into the TSPA model.
2.1.03.02.0A	Stress corrosion cracking (SCC) of waste packages	Section 6.3.8	Included in Integrated Waste Package Degradation (IWPD) Model as a mechanism for creating crack openings in waste packages. SCC of the waste package barrier is included in TSPA as part of waste

FEP No.	FEP Name	Section Where Disposition is Described	Summary of Disposition in TSPA-LA
			package degradation analyses. The *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* model report (BSC 2003 [DIRS 161234], Section 6) provides input to the IWPD Model for waste package degradation. As discussed in the *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* report (BSC 2003 [DIRS 161234], Section 6), the slip dissolution/film rupture model was used to assess the failure (or lack of it) of the WP due to the SCC crack propagation for given manufacturing cracks and/or cracks initiated by the combined effects of stress and environment. The threshold stress intensity factor is based on the theory that there exists a threshold value for the stress intensity factor such that there is no growth of a pre-existing crack or flaw having a stress intensity factor less than the threshold value. The stress intensity factor provides a criterion for determining if an SCC crack will reach an arrest state or enter propagation phase. The application of the SCC models to the WP also requires input of weld residual stress profiles and stress intensity factor profiles along with uncertainty and variability (BSC 2003 [DIRS 161234]). These input data were developed for the 25-mm outer lid (subjected to laser peening) and the as-welded 10-mm middle lid. The *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* report (BSC 2003 [DIRS 161234]) also provides other needed input for a complete TSPA for the degradation of the waste package due to SCC effects in the following areas: threshold stress for crack initiation, size, density and orientation distributions for manufacturing flaws or defects, and an estimate of crack opening size. Because, among other exposure condition parameters, tensile stress is required to initiate SCC and the waste package closure welds are the only places with such tensile stresses, only the waste package closure welds are considered subject to SCC (BSC 2003 [DIRS 161234]). The outer fabrication welds of the waste container will be fully annealed before waste is loaded into the waste containers (Plinski 2001 [DIRS 156800], Section 8.1.7) and are not subject to SCC. The presence of stable "liquid" water is required to initiate corrosion processes (including SCC) that are supported by electrochemical corrosion reactions. SCC due to thermal stresses will not occur. Thermal expansion/stress of in-drift EBS components is not a credible source of stress in the repository.

FEP No.	FEP Name	Section Where Disposition is Described	Summary of Disposition in TSPA-LA
			See Section 6.3.8 of the *WAPDEG Analysis of Waste Package and Drip Shield Degradation* report (ANL-EBS-PA-000001). The IWPD Model produces waste package degradation profiles consisting of the fraction of waste packages failed versus time and the average (per failed waste package) number of crack openings versus time. The degradation profiles are used as input into the TSPA model.
2.1.03.03.0A	Localized corrosion of waste packages	Section 6.3.6	Included in Integrated Waste Package Degradation Model. See Section 6.3.7 of the *WAPDEG Analysis of Waste Package and Drip Shield Degradation* report (ANL-EBS-PA-000001). Localized corrosion (pitting and crevice corrosion) is a type of corrosion in which the attack progresses at discrete sites or in a non-uniform manner. The rate of localized corrosion is generally much higher than the rate of general corrosion, and, if occurs, it could lead to a rapid failure of the waste packages. While the drip shield performs its design function and prevents seepage water from directly contacting the underlying waste package, solutions that form on the waste package surface from evaporative concentration of the leachate from the dust have neutral to alkaline pH and contain significant concentrations of inhibitive ions such as nitrate. Localized corrosion of the WPOB in such environments is not expected to occur (although the possibility exists for localized corrosion to occur under these conditions) (BSC [161235], Section 6.2). A possible scenario for the WPOB to be potentially subjected to localized corrosion in the repository is drip shield failure coupled with direct contact of seepage water on the waste package surface during the first few hundred years of active thermal perturbation after repository closure. A seepage water with a characteristic chemistry could evolve to highly concentrated chloride-containing brines by evaporative concentration. After the active thermal perturbation period, the waste package temperature slowly decreases with time. Once it cools to the temperature that is lower than the minimum temperature for localized corrosion initiation in highly concentrated chloride-containing brines, the waste packages are completely immune to localized corrosion (BSC 2003 [161235], Section 6.2). The localized corrosion model consists of two components: initiation and propagation. Localized corrosion of the WPOB occurs when the open circuit corrosion potential (E_{corr}) is equal to or greater than a certain critical potential ($E_{critical}$). Once initiated, localized corrosion of the WPOB propagates at a (time-independent) constant rate. This is highly conservative because it is known that the localized corrosion rate generally decreases with time.
2.1.03.05.0A	Microbially influenced	Section 6.3.9	Included in Integrated Waste Package Degradation Model as a multiplier on the general corrosion rate for

FEP No.	FEP Name	Section Where Disposition is Described	Summary of Disposition in TSPA-LA
	corrosion (MIC) of waste packages		waste packages. See Section 6.3.9 of the *WAPDEG Analysis of Waste Package and Drip Shield Degradation* report (ANL-EBS-PA-000001). The waste package is subject to MIC when the relative humidity at the waste package surface is above 90% (BSC 2003 [DIRS 161235], Section 6.4.5). Effect of MIC on general corrosion of the WPOB is represented by a general corrosion enhancement factor. The enhancement factor was determined from the comparative analysis of the corrosion rates from the short-term polarization resistance test of samples in abiotic and biotic conditions. The enhancement factor has a uniform distribution between 1 and 2. In the MIC model, the abiotic general corrosion rate is multiplied by the enhancement factor when the exposure conditions on the waste package surface warrant MIC of the WPOB. The IWPD Model produces waste package degradation profiles consisting of the fraction of waste packages failed versus time and the average (per failed waste package) number of patch openings versus time. The degradation profiles are used as input into the TSPA model.
2.1.03.08.0A	Early failure of waste packages	Section 6.3.12.2	Included in Integrated Waste Package Degradation Model as a mechanism for waste package failure. See Section 6.3.12.2 of the *WAPDEG Analysis of Waste Package and Drip Shield Degradation* report (ANL-EBS-PA-000001). Several types of manufacturing defects which could potentially lead to early WP failure were considered. Of these only improper heat treatment and handling damage (including improper laser peening) were determined to be necessary for inclusion in TSPA models. The probabilities of occurrence of these manufacturing defects were added together, because they share the same consequence of increasing the susceptibility of the WP to stress corrosion cracking (BSC 2003 [DIRS 164475], Section 7). Among these defects, improper heat treatment is, by far, the dominant process in terms of probability (BSC 2003 [DIRS 164475], Section 7). The IWPD Model produces waste package degradation profiles consisting of the fraction of waste packages failed. The degradation profiles are used as input into the TSPA model.
2.1.03.10.0B	Healing of drip shields	Section 6.3.7	Plugging (or healing) of cracks, holes or pits in drip shields by corrosion products and mineral precipitates could occur in the repository. As discussed in Section 6.3.5 of the *WAPDEG Analysis of Waste Package and Drip Shield Degradation* report (ANL-EBS-PA-000001), localized corrosion of the DS will not occur under exposure conditions in the repository. Therefore, pits (assumed to be equivalent to holes) will not form on the DS material. As discussed in FEP 2.1.03.02.0A, Stress Corrosion Cracking (SCC) of Drip Shields, plugging of any cracks developed by SCC processes is expected. Drip shields are subject to SCC under the action of seismic-induced loading and rockfalls.

FEP No.	FEP Name	Section Where Disposition is Described	Summary of Disposition in TSPA-LA
			In the nominal case (in the absence of seismic-induced loading and rockfalls) even if SCC of the drip shield were to occur, cracks in passive alloys, such as Titanium Grade 7, tend to be tight (i.e. small crack opening displacement) (BSC 2003 [DIRS 161234], Section 6.3.7). As the crack grows through-wall, the tensile stresses normal to the crack walls are relieved, and the resulting crack faces continue to corrode at very low passive corrosion rates until the gap region of the tight crack opening is "plugged" by corrosion products and precipitates such as carbonate minerals. As discussed in *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* report (BSC 2003 [DIRS 161234], Section 6.3.7), SCC cracks are sealed in a few hundred years at most when water is allowed to flow through the cracks at the expected low flow rate. When the cracks are bridged by water, the sealing process may take thousands of years, but no flow occurs since the water is held by capillary forces. Following plugging of the crack, any solution flow through the crack would be dominated by an efficiency factor determined by the ratio of solution run-off on the drip shield surface compared to through crack flow which in turn is determined by scale porosity/permeability. Because of the expected high density of the calcite deposits and lack of pressure gradient to drive water through the crack, the probability of solution flow through the crack would approach zero (BSC 2003 [DIRS 161234], Section 6.3.7). Thus, the effective water flow rate through cracks in the drip shield will be extremely low and will not contribute significantly to the overall radionuclide release rate from the repository. The development of pits or holes from localized corrosion is not expected. Since the formation of corrosion products and precipitates precludes water flow through the drip shield, performance credit is taken for the ability of the DS to prevent water flow and protect the WP. Healing of drip shields is included in TSPA as part of waste package degradation analyses in that stress corrosion crack openings are not considered to compromise the water diversion design function of the drip shield.
2.1.03.11.0A	Physical form of waste package and drip shield	Section 6	The waste package, drip shield, and repository design are standardized for the YMP (BSC 2003 [DIRS 164069]). While there is more than one waste package configuration expected to be used in the repository, they are all similar in their general design, fabrication methodology, and dimensions (Plinski 2001 [DIRS 156800], Section 1). Therefore, there will be little variation in strength, dimensions, and shape of the waste packages used in the repository. Effects of different waste forms (CSNF, DSNF, and DHLW) on heat dissipation and physical and chemical conditions in the vicinity of the waste packages are indirectly included in the TSPA analysis through different thermal-

FEP No.	FEP Name	Section Where Disposition is Described	Summary of Disposition in TSPA-LA
			hydrologic-geochemical responses and their impacts on corrosion processes. Waste package and drip shield degradation modes are modeled in the *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235]) and the *General Corrosion and Localized Corrosion of the Drip Shield* (BSC 2003 [DIRS 161236]) model reports.

6.3 BASE-CASE CONCEPTUAL MODEL FOR INTEGRATED WASTE PACKAGE DEGRADATION MODEL

The License Application (LA) waste package (WP) design consists of two layers: an Alloy 22 waste package outer barrier (WPOB) and a 316 stainless steel WP inner vessel (BSC 2003 [DIRS 165406]). The highly corrosion resistant Alloy 22 WPOB is responsible for the long waste package lifetime. In this report, the only performance credit taken for the 316 stainless-steel inner vessel is for the structural support it provides to the WPOB before WP breach. Although the WP inner vessel would also provide some performance for waste containment and potentially act as a barrier to radionuclide transport after WPOB breach, the potential performance of this barrier is far less than that of the more corrosion resistant Alloy 22 WPOB. For this reason, the corrosion performance of the WP inner vessel is conservatively ignored in this report. The WPOB has two Alloy 22 closure lids. The WP closure lids are welded to the WPOB after the waste form (spent nuclear fuel and/or glassified high-level nuclear waste) is loaded. A drip shield (DS) with Titanium Grade 7 water diversion plates will be placed over the waste package (BSC 2003 [DIRS 164069]). The space between the DS and the emplacement drift is open for air circulation and there is no backfill material used.

Over the emplacement period, the DS and WP are potentially subject to various degradation processes including general corrosion, localized corrosion, and stress corrosion cracking. Generally, the effects of other processes important to degradation of the DSs and WPs (e.g., MIC, aging and phase instability, radiolysis, weld flaws, mechanisms of early failure, etc.) are considered in terms of their effect on these three processes. The Integrated Waste Package Degradation (IWPD) Model developed in this technical product is used directly in total system performance assessment (TSPA) analysis to evaluate degradation of the DSs and WPs with time.

The IWPD Model makes use of the WAPDEG software (BSC 2002 [DIRS 161240]). In the WAPDEG software corrosion models and events are specified to apply to specific "water conditions" (BSC 2002 [DIRS 162606], Section 3.2.3). For example, in the WAPDEG software, a general or localized corrosion model is specified to apply to a specific barrier and water condition. Events, such as stress corrosion cracking or microbially influenced corrosion, apply to a specific barrier, however, they may apply to multiple water conditions. Using this design, the effects of an Event can be identical under different water conditions, however, the effects of a Model (such as the general corrosion rate) cannot be correlated (beyond specifying identical inputs). For example, the general corrosion rate can be sampled from the same distribution under different water conditions, however the sampled values cannot be correlated. In the implementation discussed in this report, the water condition on the outside of the DS differs from that on the underside of the DS and the WP surface before DS failure. Upon DS failure, the WP is exposed to the water condition previously on the outside surface of the DS and the WP general corrosion model appropriate for the new water condition is applied.

6.3.1 Drip Shield Design Conceptual Model

The only drip shield (DS) degradation process modeled in the Integrated Waste Package Degradation (IWPD) Model implemented within the WAPDEG software is general corrosion (Section 6.3.3). General corrosion is modeled separately for the DS outer and inner surfaces. The DS outer surface uses a different general corrosion rate (Section 6.3.3) than the DS inner surface. As will be discussed in Section 6.3.3, the variation in the general corrosion rate of the DS is considered to be only due to uncertainty (i.e. there is no variability in the general corrosion rate on the inner and outer surfaces of the DS). For these reasons, unlike the waste packages, each DS is modeled as a single entity. The waste package (WP) surface is modeled as being composed of several subareas referred to as patches (see the following Section) in order to represent spatial variation in degradation processes on the WP surfaces.

The Drip Shield Plate Thickness (Table 3) is used directly in the input to the WAPDEG software (Section 6.5.6). The WAPDEG software does not require the DS surface area; it is only necessary that the number of DS patches (i.e. one) be specified.

6.3.2 Waste Package Design Conceptual Model

In the Integrated Waste Package Degradation (IWPD) Model, the Waste Package (WP) surface is divided into subareas referred to as patches (Figure 2) which are used to simulate variability across the barrier surfaces. It is at the patch-level that the degradation models are applied (e.g., each patch might have a different general corrosion rate, crack growth threshold, etc.). The IWPD Model outputs consist of the fraction of DS and WP failures versus time and the average (per failed DS or WP) number of pit, crack, and patch penetrations or each barrier versus time.

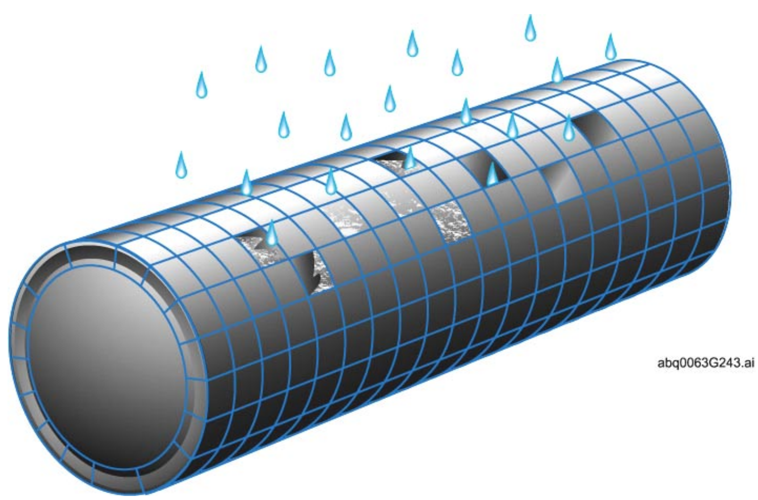


Figure 2. Schematic Representation of Waste Package Patches

As briefly discussed in Section 4.1.1, in this report two nominal waste package configurations are considered. This treatment is consistent with the approach used in the TSPA-SR Model

(CRWMS M&O 2000 [DIRS 153246], Table 4.1-1). The first waste package configuration is referred to as Commercial Spent Nuclear Fuel (CSNF) WP configuration (CRWMS M&O 2000 [DIRS 153246], Table 4.1-1) for which the 21-PWR waste package configuration parameters are used (BSC 2001 [DIRS 157812]). The 21-PWR waste package configuration is an appropriate representation of the CSNF waste package configuration since the 21-PWR WP is the most common WP configuration in the repository (BSC 2003 [DIRS 163855], Table 11). Using the WP configuration parameters listed in Table 3, the CSNF WP surface area is

$$\text{CSNF WP Surface Area} = \pi \cdot (1564\,\text{mm}) \cdot (4775\,\text{mm}) = 2.346 \cdot 10^7\ \text{mm}^2 \qquad \text{(Eq. 18)}$$

Note that the surface area of the closure lids was not considered. Because the CSNF WP surface area is primarily used to determine the fraction of WP surface area subjected to SCC (later in this section), it is conservative and appropriate to ignore the closure lid surface area in determining the total surface area.

The second waste package configuration is the Co-Disposal (CDSP) WP configuration (CRWMS M&O 2000 [DIRS 153246], Table 4.1-1) whose length is considered to be the average length of the 5 HLW/1 DOE SNF Long (BSC 2001 [DIRS 157818]) and Short (BSC 2001 [DIRS 157817]) WP configurations. The 5 HLW/1 DOE SNF (Co-Disposal) Long and Short waste package configurations are appropriate representations of the CDSP WP configuration since these are the most common High-Level Waste (HLW) waste package configurations in the repository (BSC 2003 [DIRS 163855], Table 11). Again using the WP configuration parameters listed in Table 3, the CDSP WP surface area is

$$\text{CDSP WP Surface Area} = \pi \cdot (2030\,\text{mm}) \cdot \left(\frac{(3200 + 4827)}{2} \text{mm} \right) = 2.560 \cdot 10^7\ \text{mm}^2 \qquad \text{(Eq. 19)}$$

The 5 HLW/1 DOE SNF Long (BSC 2001 [DIRS 157818]) and Short (BSC 2001 [DIRS 157817]) WP configurations both have the same WPOB outer diameter (2030 mm) as shown in Table 3.

The general corrosion model used for the WP is based on weight-loss measurements for samples exposed in the LTCTF (BSC 2003 [DIRS 161235], Section 6.4.3). For the WP outer barrier, samples with the crevice geometry were used to generate the general corrosion rate distribution (applied at 60°C). The crevice geometry samples have nominal dimensions of 2 inch x 2 inch x 1/8 inch and a 0.312 inch diameter hole in the center for sample mounting (BSC 2003 [DIRS 161235], Section 6.4.3). Therefore the exposed surface area, *A*, for a crevice geometry sample is calculated as follows

$$A = 2ab + 2bc + 2ac - \left(\frac{\pi d^2}{2} \right) + \pi dc \qquad \text{(Eq. 20)}$$

where *a* is the length of the specimen in mm, *b* is the width of the specimen in mm, *c* is the thickness of the specimen in mm, and *d* is diameter of hole in mm. Using the above mentioned dimensions (converted to mm), the exposed surface area for a crevice sample is found to be 5,787 mm^2. That part of the IWPD Model implemented within the WAPDEG software will use a patch size of about four (4) times this area (23,150 mm^2). This means that the CSNF WPs will be modeled with 1014 patches and the CDSP WPs will be modeled using 1106 patches. In

Section 6.3.4, the general corrosion rate distribution applied to the WPOB is modified to reflect this change in scale between the smaller crevice geometry sample size and the patch size.

Effectively, the WPOB is composed of two different regions; the closure lid region and the shell region. The WPOB shell region thickness, 20 mm for the CSNF WP configuration and 25 mm for the CDSP WP configuration (Table 3), is used indirectly in the formulation of inputs to the WAPDEG software. Both the CSNF and CDSP WP configurations have a similar closure lid configurations. The WPOB outer closure lid thickness (and weld thickness) is 25 mm for both the CSNF and CDSP WP configurations (Table 9). The WPOB middle closure lid thickness (and weld thickness) is 10 mm (Table 9). It is these thicknesses that are used as direct inputs to the WAPDEG software. The WAPDEG software is not capable of modeling the WPOB closure lid region and the shell region entirely independently. Therefore, both WPOB regions are modeled as being composed of two layers (Figure 3); the outer modeled layer is 25 mm thick and the inner modeled layer is 10 mm thick. Use of two layers is straightforward for the closure lid region of the WPOB. For the WPOB shell region, the general corrosion rate used for the modeled outer layer is very large (~10^{10} mm/yr) leading to instantaneous penetration. Effectively, the WPOB shell region of the modeled outer layer does not contribute to WP performance. The general corrosion rate used for the WPOB shell region of the modeled inner layer of the CSNF WP configuration is decreased by a factor of 20 mm / 10 mm = 2 (i.e. multiplied by a factor of 0.5). In this way, the modeled 10 mm inner layer "behaves" (in the model) like a 20 mm layer. Similarly, the general corrosion rate used for the WPOB shell region of the modeled inner layer of the CDSP WP configuration is decreased by a factor of 25 mm / 10 mm = 2.5 (i.e. multiplied by a factor of 0.4). In this way, the modeled 10 mm inner layer behaves (in the model) like a 25 mm layer.

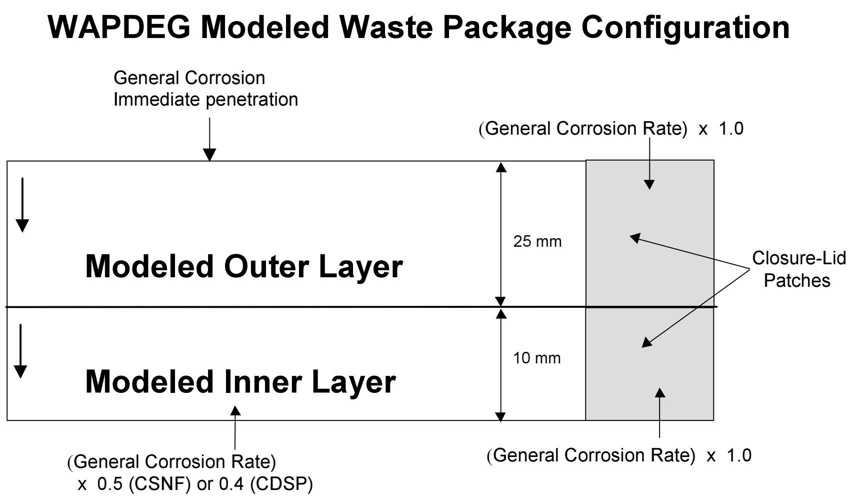


Figure 3. Schematic of Waste Package Configuration in IWPD Model Analysis to Implement SCC of Dual Closure-Lids of Waste Package Outer Barrier

6.3.2.1 Stress Corrosion Cracking Patches

That part of the IWPD Model which uses the WAPDEG software also requires a fraction of WP surface area subject to stress corrosion cracking (SCC). This area is the same as the fraction of the total surface area represented by the closure-lid patches identified in Figure 3 (the bulk of the closure lid is not modeled, only the closure lid weld region). As mentioned above, the area of a WP patch is 23,150 mm^2. Making the reasonable modeling assumption that the patches are square, the length of one side of a patch is about 152 mm. The closure-lid weld region can reasonably be represented as a cylinder one patch side wide and with the same radius as the waste package. This results in the fraction of area represented by the closure weld region for CSNF WPs being

$$\frac{\text{Closure–Lid Weld Region Area}}{\text{WP Surface Area}} = \frac{\pi(1564\,\text{mm})(152\,\text{mm})}{2.346x10^{7}\,\text{mm}^{2}} \approx 0.032 \qquad \text{(Eq. 21)}$$

or about 32 patches. For CDSP WPs the fraction of area represented by the closure weld region is

$$\frac{\text{Closure–Lid Weld Region Area}}{\text{WP Surface Area}} = \frac{\pi(2030\,\text{mm})(152\,\text{mm})}{2.560x10^{7}\,\text{mm}^{2}} \approx 0.038 \qquad \text{(Eq. 22)}$$

or about 42 patches.

Analyses presented in report entitled *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234], Section 6.5.1), indicate that the distance between two neighboring cracks would need to be greater than the plate thickness for the stress (and stress intensity factor) profile to be of sufficient magnitude to propagate a crack through-wall. Therefore, for the WPOB outer closure-lid (25 mm thick (Table 9)), and again making the modeling assumption that the patches are square (side length about 150 mm), one would expect about 6 cracks per patch to be able to propagate through-wall. For the WPOB middle closure-lid (10 mm thick (see Table 9)), one would expect about 15 cracks per patch to be able to propagate through-wall. The WAPDEG software (BSC 2003 [DIRS 161240]) models crack growth on a patch until the first crack penetrates, then ceases to model crack growth for any remaining cracks. That is, if, for example, 32 patches are subject to crack growth and all fail by cracking, only 32 crack penetrations (the first crack to penetrate on each patch) will be reported, regardless of how many cracks per patch were considered. Therefore, it is appropriate (and conservative) to multiply the number of crack penetrations reported by the WAPDEG software by the number of cracks per patch to get a measure of the total number of cracks (see Section 6.5.10).

6.3.3 Drip Shield General Corrosion Conceptual Model

Details of the general corrosion rate distributions used for the drip shield (DS) are given in the report entitled *General Corrosion and Localized Corrosion of the Drip Shield* (BSC 2003 [DIRS 161236], Section 6.3.5) and are tracked with DTN: MO0306SPAGLCDS.001 [DIRS 163912]. In that report, general corrosion rates of Titanium Grade 16 are taken to be representative of those for Titanium Grade 7 (BSC 2003 [DIRS 161236], Section 1.1). Also see Section 4.1.2 of this report for a discussion of the DS general corrosion inputs and Section 6.5.6 for discussion of implementation.

The DS outer surface may be exposed to a more complicated chemistry and geometry than the DS inner surface since dust and/or mineral films (from evaporation of dripping water) may form crevices on the DS outer surfaces. In contrast, the inner surfaces of the DS will not be exposed to dripping water nor significant dust film formation (BSC 2003 [DIRS 161236], Section 6.3.5). Therefore, the general corrosion of the inner surface and the outer surface of the drip shield are modeled by using different sets of corrosion data (BSC 2003 [DIRS 161236], Section 6.3.5). The general corrosion rate cumulative distribution function applicable to the under side of the DS is shown in Table 4. The general corrosion rate cumulative distribution function applicable to the top side of the DS is shown in Table 5.

The variation in these inputs are considered to be entirely due to uncertainty (BSC 2003 [DIRS 161236], Section 6.3.5). For each realization of the Integrated Waste Package Degradation Model, a single general corrosion rate is sampled from each general corrosion rate distribution and applied to all DSs. Using this conceptual model for DS general corrosion, all DSs in the repository fail by general corrosion at the same time.

One should note that the maximum general corrosion rate for the CDF applied to the under side of the DS (Table 4) is approximately 1.13E-04 mm/yr and the maximum general corrosion rate for the CDF applied to the top side of the DS (Table 5) is approximately 3.20E-04 mm/yr, therefore the earliest possible DS failure by general corrosion is about 35,000 years.

6.3.3.1 Influence of Fluoride on Corrosion of Titanium

Review of the titanium corrosion literature indicates that the presence of dissolved fluoride in a range of brine solutions can, under certain conditions, significantly increase the general corrosion rate of titanium alloys including Titanium Grade 7. Titanium alloys show enhanced susceptibility to general corrosion in environments containing fluoride, in particular, in acidic fluoride containing solutions corrosion is generally attributed to the formation of complexes such as TiF_6^{2-} and TiF_6^{3-}, which are soluble in electrolyte solutions. Analyses documented in the *General Corrosion and Localized Corrosion of the Drip Shield* report (BSC 2003 [DIRS 161236], Section 6.3.7) indicate that the direct incorporation of fluoride ions into the passive film leading to enhanced dissolution only occurred under acidic conditions. It was concluded that the formation of HF at low pH was the key step causing film dissolution and the establishment of active dissolution conditions (BSC 2003 [DIRS 161236], Section 6.3.7).

The importance of the condition of the passive film in resisting corrosion in neutral fluoride-containing solutions was also discussed (BSC 2003 [DIRS 161236], Section 6.3.7). If the fluoride ion was added to test solutions shortly after electrode immersion while the oxide film is growing, and hence defective, enhanced corrosion is observed. However, if the titanium oxide is allowed to grow for a sufficient period for the formation of a coherent oxide with a low defect concentration (~ 4 days), then the subsequent addition of fluoride ions has no observable effect. Clearly, the susceptibility of titanium to enhanced corrosion in fluoride-containing environments is associated with defects and flaws in the oxide (BSC 2003 [DIRS 161236], Section 6.3.7).

In the case of the DS application in the repository, there is an early period of dry air exposure. During this time, the drip shield would be subjected to a long period of thermal oxidation prior to aqueous exposure. Thermal treatments not only thicken the oxide film but also decrease the defect density in the film by a factor between 10^2 and 10^4 compared to films grown in aqueous environments (BSC 2003 [DIRS 161236], Section 6.3.7). It was found that the kinetics of passive corrosion of titanium in neutral solutions are controlled by the migration of the predominant defect in the oxide (an oxygen vacancy, O_V^{II}) across the passive film (BSC 2003 [DIRS 161236], Section 6.3.7). This increase in thickness and improvement in film properties would lead to a significant decrease in susceptibility to fluoride induced film breakdown and an independence of the passive corrosion rate on fluoride ion concentration. Thus, in the repository environment, the degradation of the titanium DS material will not be affected by fluoride exposure (BSC 2003 [DIRS 161236], Section 6.3.7).

6.3.4 Waste Package Outer Barrier General Corrosion Conceptual Model

Details of the general corrosion rate distributions used for the Alloy 22 Waste Package Outer Barrier (WPOB) are given in the report entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.3). Also see Section 4.1.3 for a discussion of the WPOB general corrosion inputs and Section 6.5.7 for discussion of implementation. The Alloy 22 general corrosion rate is considered a function of exposure temperature. The temperature dependence follows an Arrhenius relationship, i.e.,

$$R = \exp\left[C_o - \frac{C_1}{T}\right] \qquad \text{(Eq. 23)}$$

where

R = general-corrosion rate
T = temperature (Kelvin)
C_o = intercept term
C_1 = slope term (Kelvin)

as discussed in the report entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.3). Note that the sign of the slope term in this report is negative with respect to the slope term in the *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* report (BSC 2003 [DIRS 161235], Section 6.4.3) to be consistent with the input requirements of the WAPDEG software (BSC 2003 [DIRS 161240]). The slope term is determined from short-term polarization resistance data for Alloy 22 specimens tested for a range of sample configurations, metallurgical conditions, and exposure conditions (BSC 2003 [DIRS 161235], Section 6.4.3). From fitting the data to an Arrhenius relation of the form of Equation 23, the slope term, C_1, was found to be normally distributed with a mean of 3116.47 K and a standard deviation of 296.47 K (BSC 2003 [DIRS 161235], Section 6.4.3) (DTN: SN0308T0506303.004 [DIRS 164840]).

The intercept term, C_o, is determined from the general corrosion rate distribution derived from the weight loss of the 5-year crevice geometry samples exposed in the LTCTF (BSC 2003 [DIRS 161235], Section 6.4.3) and the value of the slope term, C_1. The general corrosion rate distribution derived from the weight loss of the 5-year crevice geometry samples exposed in the

LTCTF are considered to represent the distribution of long-term general corrosion rates of the WPOB at 60°C (333.15 K). Therefore,

$$\ln(R_o) = C_o - \frac{C_1}{333.15\text{K}} \qquad \text{(Eq. 24)}$$

or

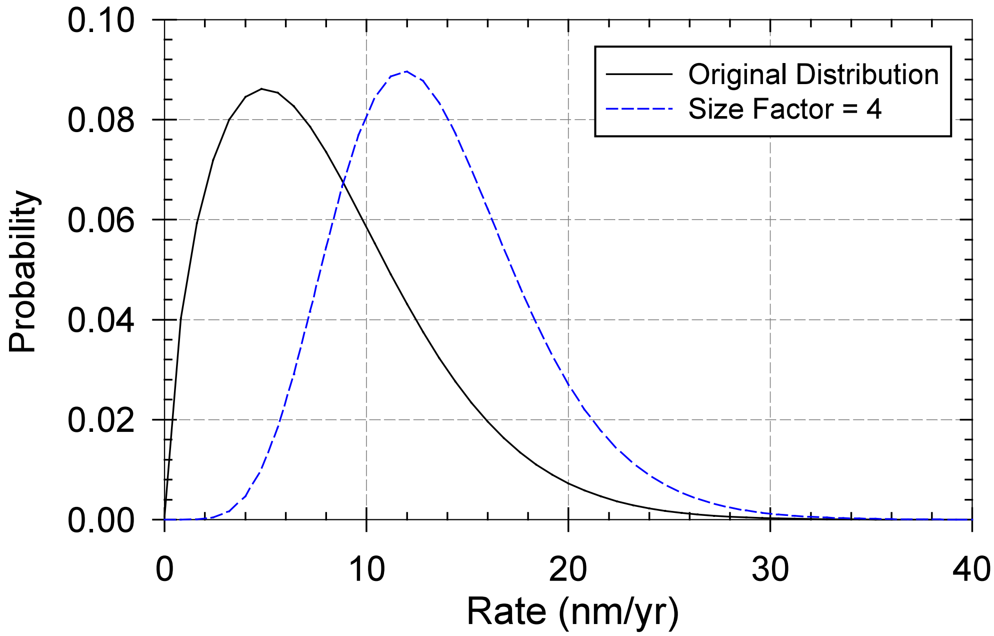
$$C_o = \ln(R_o) + \frac{C_1}{333.15\text{K}} \qquad \text{(Eq. 25)}$$

where R_o is the general corrosion rate distribution from the 5-year crevice geometry samples. Substituting for C_o in Equation 23,

$$R = \exp\left[\ln(R_o) + C_1\left(\frac{1}{333.15\text{K}} - \frac{1}{T}\right)\right] \qquad \text{(Eq. 26)}$$

The *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* report (BSC 2003 [DIRS 161235], Section 6.4.3) states that R_o is given by a Weibull distribution (Equation 1) (α = 8.88 nm/yr, β = 1.62, and θ = 0) (Table 6). This is a two-parameter Weibull distribution (since the location parameter, θ, is zero) with α being the scale parameter and β the shape parameter. As discussed in Section 6.3.2, the patch size used to model the WPs is four times the area of the crevice geometry sample size. Therefore, the general corrosion rates will be adjusted to account for the effects of this change of scale (Aziz 1956 [DIRS 159379]; Shibata 1996 [DIRS 119589]). Conceptually, the method employed corresponds to using the highest of four sampled corrosion rates (from the two-parameter Weibull distribution) to model general corrosion of the WP patch. This approach is conservative and appropriate for this application. The approach is conservative because it is probable that not all four samples from the Weibull distribution will have the highest rate, therefore, a more realistic representation of the overall general corrosion rate would be the average of the four sampled corrosion rates. However, this approach would not account for the fact that one fourth of the patch has the maximum of the four sampled corrosion rates. On this basis the proposed approach is conservative and appropriate for this application.

Mathematically stated, if *F(x)* is the cumulative probability distribution, then the probability that *x* will be the largest amongst *n* observations is $[F(x)]^n$ (Aziz 1956 [DIRS 159379]; Shibata 1996 [DIRS 119589]). In this context *n* can be called the *size factor*. The effect of this method is to shift the median general corrosion rate to higher values and to decrease the probability of sampling lower general corrosion rates. This can be seen in Figure 4 where the original distribution for R_o is plotted along with the distribution resulting from a size factor of 4.



Source DTN: SN0308T0506303.004 [DIRS 164840]
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 4. Effect of Scaling General Corrosion Distribution by a Size Factor of Four.

The variation in R_o, the general corrosion rate distribution determined from the 5-year crevice geometry samples, is considered to be entirely due to variability, i.e. a CDF for $\ln(R_o)$ is passed to the WAPDEG software used in the Integrated Waste Package Degradation Model (IWPD) Model. The *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* report (BSC 2003 [DIRS 161235], Section 6.4.3) states that C_1 is given by a truncated (at ±3 sds) normal distribution with a mean of 3116.47 and a sd of 296.47 (Table 7). The variation in the general corrosion rate slope term, C_1, is considered to be entirely due to uncertainty. For each realization of the IWPD Model, a single general corrosion rate slope term is sampled and applied to the Alloy 22 waste package outer barrier surfaces to model variation in the Alloy 22 general corrosion rate with exposure temperature. Spatial and temporal variability in the temperature of the repository lead to spatial and temporal variability in the general corrosion rates used to model general corrosion of Alloy 22.

6.3.5 Drip Shield Localized Corrosion Conceptual Model

The localized corrosion (LC) model for the DS is documented in the report entitled *General Corrosion and Localized Corrosion of the Drip Shield* (BSC 2003 [DIRS 161236], Section 6.4) and are tracked with DTN: MO0306SPAGLCDS.001 [DIRS 163912]. In the DS LC Model localized attack occurs if the open circuit corrosion potential (E_{corr}) exceeds or is equal to the threshold potential for breakdown of the passive film ($E_{critical}$), *i.e.*

$$E_{corr} \geq E_{critical} \qquad \text{(Eq. 27)}$$

The "threshold potential" is the potential below which localized corrosion will not initiate and beyond which the passive film breakdown occurs. Analyses presented in the *General Corrosion and Localized Corrosion of the Drip Shield* (BSC 2003 [DIRS 161236], Section 6.4.3) fit the difference (ΔE) between $E_{critical}$ and E_{corr} to a function of absolute temperature, T, solution pH, and the chloride ion concentration for a variety of solution compositions (not including $CaCl_2$-based solutions discussed later in this report), i.e.

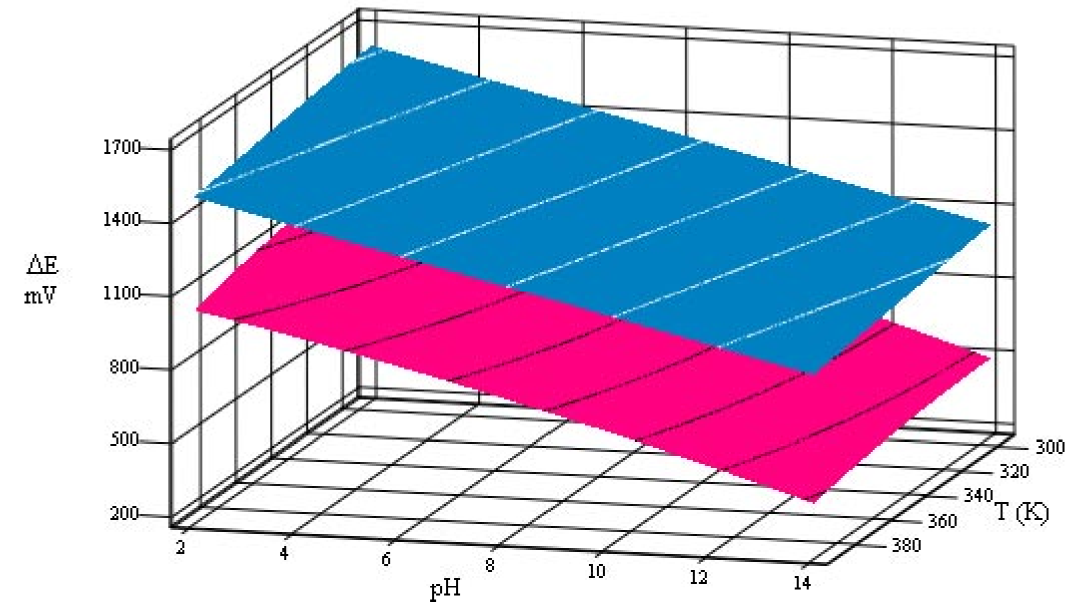
$$\Delta E = d_0 + d_1 \cdot T + d_2 \cdot log(Cl^-) + d_3 \cdot pH + \varepsilon \qquad \text{(Eq. 28)}$$

where the median values of the coefficients are $d_o = 2050$, $d_1 = -1.17$, $d_2 = 14.1$, and $d_3 = -48.9$, respectively. The covariance matrix resulting from the fitting procedure was determined to be (BSC 2003 [DIRS 161236], Section 6.4.3)

$$s = \begin{bmatrix} 56100 & -165 & 1150 & 66.1 \\ -165 & 0.506 & -4.36 & -1.07 \\ 1150 & -4.36 & 535 & 116 \\ 66.1 & -1.07 & 116 & 56.1 \end{bmatrix} \qquad \text{(Eq. 29)}$$

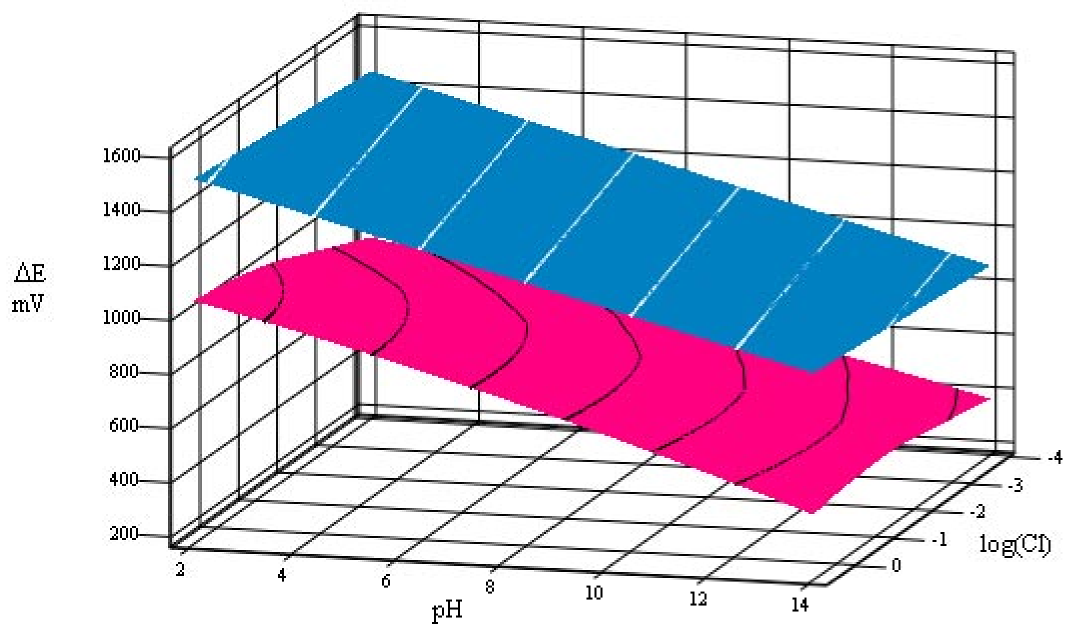
ε, the model error term, is a term representing data variance not explained by the fitting procedure and has a normal distribution with a mean of zero and variance of 10,500. Localized corrosion can initiate when E_{corr} exceeds or is equal to $E_{critical}$. This is equivalent to the condition that ΔE is equal to or less than zero.

Figure 5 shows the variation of ΔE with pH and temperature under a constant chloride concentration (3 mol/L Cl^-) and Figure 6 shows the effect of pH and chloride concentration under a constant temperature of 380 K. The figures taken together show that ΔE is significantly greater than zero over all ranges of pH, chloride concentration, and temperature. They also show that the median ΔE increases slightly with increasing chloride concentration and temperature but significantly decreases with increasing pH. Nevertheless, a gap between the corrosion potential and the threshold potential of several hundred millivolts is maintained even at very high pH. Also, a gap of the order of several hundred millivolts is maintained even at the -4σ confidence level. Truncation at the $\pm 4\sigma$ confidence level yields appropriate bounding values for use with this model. Localized corrosion of Titanium Grade 7 would not initiate in a repository-relevant environment even at pH values as high as 14 using these bounds (BSC 2003 [DIRS 161236], Section 6.4.3).



Source DTN: MO0003SPAPCC03.004 [DIRS 148992]

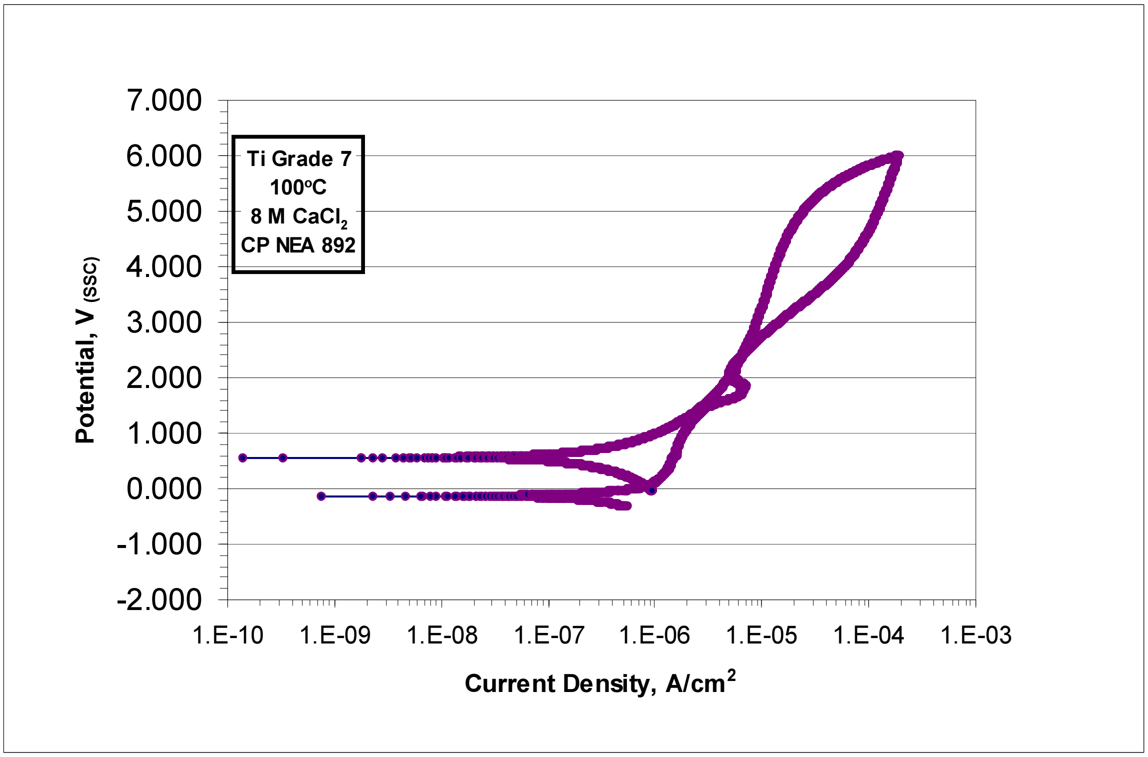
Figure 5. Plot of the Median *ΔE* and -4σ Confidence Interval Surface Versus *pH* and Absolute Temperature for Titanium Grade 7 Using a Chloride Ion Concentration of 3 mol/L



Source DTN: MO0003SPAPCC03.004 [DIRS 148992]

Figure 6. Plot of the Median *ΔE* and -4σ Confidence Interval Surface Versus *pH* and Base 10 Logarithm of Chloride Ion Concentration for Titanium Grade 7 Using an Absolute Temperature of 380 K

Analyses in the *General Corrosion and Localized Corrosion of the Drip Shield* (BSC 2003 [DIRS 161236], Section 6.4.5) report show that $CaCl_2$ containing environments do not result in localized corrosion of Titanium Grade 7 either. Figure 7 shows an example of a cyclic polarization curve obtained for Titanium Grade 7 in and environment containing high concentration of calcium chloride (8 M $CaCl_2$) at 100°C. ΔE (= $E_{20} - E_{corr}$ see discussion below) in Figure 7 is quite large (> 3.0V) indicating no possibility for localized corrosion to initiate.



Source DTN: MO0306SPAGLCDS.001 [DIRS 163912]

Figure 7. An Example of the Cyclic Polarization Curve of Titanium Grade 7 in 8 M $CaCl_2$ Water at 100°C, Showing a Very Large ΔE.

Table 18 summarizes results obtained for Titanium Grade 7 in environments containing high concentrations of $CaCl_2$. In Table 18, E_{corr} is the free corroding potential after 1 hour exposure in the given electrolyte, E_{20} is the potential in the forward scan of a cyclic polarization curve where the current density first reaches 20 µA/cm², E_{200} is the potential in the forward scan of a cyclic polarization curve where the current density first reaches 200 µA/cm². E_{R10} is the potential in the reverse polarization where the current density first reaches 10 µA/cm² and E_{R1} is the potential in the reverse polarization where the current density first reaches 1 µA/cm². The data were obtained in concentrated $CaCl_2$ solutions at 100 and 150°C in environments as indicated. In general (5 out of 6 tests), the ΔE (= $E_{20} - E_{corr}$) values are greater than 2 V, suggesting a significant margin of safety. The remaining specimen (NEA894) shows a ΔE value of 1.4 V, high enough to exclude the possibility of localized corrosion.

Table 18. Electrochemical Tests of Titanium Grade 7 in $CaCl_2$-Containing Environments.

Specimen ID	Specimen, Surface Finish	Environment	T (°C)	E_{corr} (mV, SSC)	E_{20} (mV, SSC)	E_{200} (mV, SSC)	E_{R10} (mV, SSC)	E_{R1} (mV, SSC)
NEA891	Disc, 600	8 M $CaCl_2$	100	-45	2,680	NA	NA	NA
NEA892	Disc, 600	8 M $CaCl_2$	100	-219	3,220	NA (~6,000)	3,260	986
NEA893	Disc, 600	8 M $CaCl_2$	100	-296	3,180	~4880	NA	NA
NEA894	Disc, 600	9 M $CaCl_2$	150	-176	1240	3,450	889	246
NEA895	Disc, 600	9 M $CaCl_2$	150	-205	2,180	3,630	1140	501
NEA896	Disc, 600	9 M $CaCl_2$ + 0.9 M $Ca(NO3)_2$	150	-108	2,410	3,400	NA	NA

Specimen I.D.	$\Delta E = E_{20} - E_{corr}$
NEA891	2,725
NEA892	3,439
NEA893	3,476
NEA894	1,416
NEA895	2,385
NEA896	2,518

E_{corr} is the free corroding potential after 1 h exposure in the given electrolyte; E_{20} is the potential in the forward scan of a cyclic polarization curve where the current density first reaches 20 μA/cm²; E_{200} is the potential in the forward scan of a cyclic polarization curve where the current density first reaches 200 μA/cm²; E_{R10} is the potential in the reverse polarization where the current density first reaches 10 μA/cm² and E_{R1} is the potential in the reverse polarization where the current density first reaches 1 μA/cm².

Source DTN: MO0306SPAGLCDS.001 [DIRS 163912]

The analyses summarized in this section clearly indicate that localized corrosion of the titanium drip shield material is not possible under the expected repository conditions. On this basis localized corrosion of the drip shield will not be considered further and should not be implemented within the TSPA-LA Model.

6.3.6 Waste Package Outer Barrier Localized Corrosion Conceptual Model

The localized corrosion (LC) model used in this report is documented in the report entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.4) (DTN: SN0308T0506303.003 [DIRS 164839]). Crevice corrosion is representative of localized corrosion of the WPOB under the exposure conditions expected in the post-closure repository (BSC 2003 [DIRS 161235], Section 6.4.4). This is a conservative and bounding modeling assumption because the initiation threshold for crevice corrosion in terms of water chemistry and temperature is lower than that for pitting corrosion, which is another form of localized corrosion attacking boldly exposed surfaces (BSC 2003 [DIRS 161235], Section 6.4.4).

When localized corrosion occurs, the localized corrosion of the WPOB propagates at a (time-independent) constant rate (BSC 2003 [DIRS 161235], Section 6.4.4). This modeling assumption is highly conservative because it is known that the localized corrosion rate decreases with time and this is particularly more likely under a thin water film condition that is expected to form on the waste package surface in the post-closure repository (BSC 2003 [DIRS 161235], Section 6.4.4). Also, in most cases, localized corrosion arrests or dies shortly after initiation.

The LC model for the waste package outer barrier (WPOB) consists of a LC initiation model and a LC propagation rate model. LC initiates when the open circuit potential, or corrosion potential (E_{corr}) is equal to or greater than a critical threshold potential (E_{rcrev}, the crevice repassivation potential), that is, ΔE (= E_{rcrev} - E_{corr}) ≤ 0.

The following limitations are identified for the application of the localized corrosion model for Alloy 22 (BSC 2003 [DIRS 161235], Section 1.2):

- Temperature from 20°C up to boiling temperature of $CaCl_2$-containing brines.
- Solution pH from 2 to 12.
- Chloride concentration from a very low non-zero value to 25 molal (*m*, moles/kg water). A value of 0.001 *m* is recommended for the chloride concentration for solutions with no chloride.
- Nitrate concentration from a very low non-zero value to 6 molal (*m*, moles/kg water). A value of 0.001 *m* is recommended for the nitrate concentration for solutions with no nitrate.
- The nitrate to chloride concentration ratio from zero to 1.0 for the crevice repassivation potential model. For solutions with the ratio greater than 1.0, the ratio is limited to 1.0. This ratio range is not applied to the corrosion potential model.

Note that no localized corrosion of the WPOB is expected for any water chemistries with the nitrate concentration greater than the upper bound (6 *m*). Because only nitrate ions are accounted for in the localized corrosion model for the inhibitive effect, the model results for solutions with significant amounts of other potentially inhibitive ions such as carbonate and sulfate (in addition to nitrate ions) are highly conservative. The model results for the beneficial effects of the inhibitive ions combined with the alkaline pH conditions of the typical carbonate waters in the repository are consistent with the experimental observations on the immunity of Alloy 22 to localized corrosion in those waters (BSC 2003 [DIRS 161235], Section 1.2).

6.3.6.1 Waste Package Outer Barrier Crevice Repassivation Potential for Localized Corrosion Initiation

The crevice repassivation potential (E_{rcrev}) is expressed as follows.

$$E_{rcrev} = E^{o}_{rcrev} + \Delta E^{NO_3^-}_{rcrev} \qquad \text{(Eq. 30)}$$

where E^{o}_{rcrev} is the crevice repassivation potential in the absence of nitrate ions (which tend to inhibit LC initiation), and $\Delta E^{NO_3^-}_{rcrev}$ is the crevice repassivation potential changes resulted from the inhibiting effect of nitrate ion in solution (BSC 2003 [DIRS 161235], Section 6.4.4).

The crevice repassivation potential of the mill-annealed and as-welded Alloy 22 in the absence of inhibitive nitrate ion is expressed as follows (BSC 2003 [DIRS 161235], Section 6.4.4).

$$E^{o}_{rcrev} = a_o + a_1 T + a_2 pH + a_3 \log([Cl^-]) + a_4 T \times \log([Cl^-]) \qquad \text{(Eq. 31)}$$

where E^{o}_{rcrev} is in mV vs. the Silver-Silver Chloride (SSC) reference electrode, a_o, a_1, a_2, a_3, and a_4 are constants, T is the temperature (°C), and $[Cl^-]$ is the chloride ion concentration. The median estimated regression coefficients are: a_o = 214.089, a_1 = -3.696, a_2 = 25.284, a_3 = -252.181, and a_4 = 1.414. The covariance matrix resulting from the least squares fitting was determined to be (BSC 2003 [DIRS 161235], Section 6.4.4) (DTN: SN0308T0506303.003 [DIRS 164839]):

$$CV = \begin{bmatrix} 2197.7 & -15.159 & -83.254 & -1805.2 & 15.897 \\ -15.159 & 0.22667 & -1.2402 & 18.767 & -0.19963 \\ -83.254 & -1.2402 & 31.826 & -32.372 & 0.74246 \\ -1805.2 & 18.767 & -32.372 & 2906.5 & -28.677 \\ 15.897 & -0.19963 & 0.74246 & -28.677 & 0.29946 \end{bmatrix} \quad \text{(Eq. 32)}$$

The entire variance of the model is due to uncertainty. It is recommended that the uncertainty of the parameter coefficients of the above model be limited to ±2 sd (BSC 2003 [DIRS 161235], Section 6.4.4). The lower triangular Cholesky factorization, T, of the covariance matrix (such that $T \cdot T^T = CV$) is given below.

$$T = \begin{bmatrix} 46.8796331 & 0 & 0 & 0 & 0 \\ -0.32336004 & 0.34943996 & 0 & 0 & 0 \\ -1.7759098 & -5.19247503 & 1.3078025 & 0 & 0 \\ -38.50712731 & 18.07272935 & -5.28748716 & 32.69740173 & 0 \\ 0.33910248 & -0.25749147 & 0.00585517 & -0.33441816 & 0.07935909 \end{bmatrix} \quad \text{(Eq. 33)}$$

The Cholesky factorization can be used as a direct way of generating coefficient vectors with the proper covariance structure (Iman and Conover 1982 [DIRS 124158], p. 315).

The effect of nitrate ions on the crevice repassivation potential is represented as follows.

$$\Delta E_{rcrev}^{NO_3^-} = b_o + b_1[NO_3^-] + b_2 \frac{[NO_3^-]}{[Cl^-]} \quad \text{(Eq. 34)}$$

where $\Delta E_{rcrev}^{NO_3^-}$ is in mV vs. SSC, b_o, b_1 and b_2 are constants and other parameters are defined as before. The parameter coefficients resulting from the fitting procedure were determined to be: $b_0 = -50.959$, $b_1 = 115.867$, and $b_2 = 1045$. The effect of the interaction of the competing aggressive ions (e.g., chloride ions) and inhibitive nitrate ions on the crevice repassivation potential is represented with the ratio of the concentrations of the two competing ions and the concentration of nitrate ion. The linear relationship between $\Delta E_{rcrev}^{NO_3^-}$ and the concentration ratio is applicable for concentration ratios between 0.1 and 1.0 (BSC 2003 [DIRS 161235], Section 6.4.4). Because the effect of the measurement uncertainty has already been captured in the crevice repassivation potential model with no nitrate ion present, only the mean value of the $\Delta E_{rcrev}^{NO_3^-}$ is used to determine the crevice repassivation potential (E_{rcrev}.) (BSC 2003 [DIRS 161235], Section 6.4.4).

Variability in the crevice repassivation potential among waste packages is included through the temporally and spatially varying waste package temperature and chemistry exposure conditions.

6.3.6.2 Waste Package Outer Barrier Long-Term Corrosion Potential for Localized Corrosion Initiation

The long-term corrosion potential model (E_{corr}) for the WPOB is expressed as follows (BSC 2003 [DIRS 161235], Section 6.4.4):

$$E_{corr} = c_o + c_1 T + c_2 pH + c_3 [Cl^-] + c_4 \log(\frac{[NO_3^-]}{[Cl^-]}) \quad \text{(Eq. 35)}$$

where E_{corr} is the long-term corrosion potential in mV vs. SSC, c_o, c_1, c_2, c_3, and c_4 are coefficients of the model parameters, and other parameters are defined as before. The median estimated regression coefficients are: $c_0 =$ 365.511, $c_1 =$ 1.853, $c_2 =$-48.091, $c_3 =$-29.641, and $c_4 =$ -4.263. The covariance matrix resulting from the least squares fitting was determined to be (BSC 2003 [DIRS 161235], Section 6.4.4) (DTN: SN0308T0506303.003 [DIRS 164839]):

$$CV = \begin{bmatrix} 1082.5 & -10.818 & -31.492 & 0.77527 & -37.167 \\ -10.818 & 0.13976 & -0.029431 & -0.1269 & 0.37478 \\ -31.492 & -0.029431 & 6.3919 & 0.42229 & 0.59728 \\ 0.77527 & -0.1269 & 0.42229 & 3.7299 & 6.1905 \\ -37.167 & 0.37478 & 0.59728 & 6.1905 & 18.711 \end{bmatrix} \quad \text{(Eq. 36)}$$

The lower triangular Cholesky factorization, T, of the covariance matrix (such that $T \cdot T^T = CV$) is given below.

$$T = \begin{bmatrix} 32.90136775 & 0 & 0 & 0 & 0 \\ -0.32880092 & 0.17790434 & 0 & 0 & 0 \\ -0.95716386 & -1.9344517 & 1.31667534 & 0 & 0 \\ 0.02356346 & -0.66975495 & -0.646146 & 1.6921195 & 0 \\ -1.12964909 & 0.01883226 & -0.33990853 & 3.55181823 & 2.16877563 \end{bmatrix} \quad \text{(Eq. 37)}$$

The purpose of this corrosion potential model is *to estimate the long-term steady-state open-circuit corrosion potential of Alloy 22* for a range of exposure conditions related to the repository. The model *should not be used for short-term transient conditions* (BSC 2003 [DIRS 161235], Section 6.4.4). The entire variance of the model is due to uncertainty. As with the crevice repassivation potential model, it is recommended that the uncertainty of the parameter coefficients of the corrosion potential model be limited to ±2 sd. Note that the above corrosion potential model, in conjunction with the crevice repassivation potential model, is to be used to evaluate *the long-term localized corrosion susceptibility of the WPOB* and is not intended for modeling of short-term transient behavior (BSC 2003 [DIRS 161235], Section 6.4.4).

Variability in the corrosion potential among waste packages is included through the temporally and spatially varying waste package temperature and chemistry exposure conditions.

6.3.6.3 Conservatism in the Critical Potential for Crevice Corrosion Initiation

The crevice repassivation potentials from the short-term cyclic potentiodynamic polarization (CPP) tests are a highly conservative measure for the critical potential for localized corrosion initiation of the WPOB. The approach conservatively ignores the fundamental aspects of the localized corrosion processes: localized corrosion initiation (i.e. initial local passive film breakdown), stabilization, and propagation. A better representation of the localized corrosion initiation would be the use of the passive film breakdown potentials (obtained from the forward scan curves of the CPP test), coupled with the stabilization and propagation processes of localized corrosion. The more realistic measure of the critical potentials can be obtained using a modified potentiostatic polarization technique (also referred to as a potential step technique). In this technique, the sample is potentiostatically held at a potential and monitored for the corrosion current changes with time.

In addition, discontinued tortuous thin water films are expected to form on the waste package surface in the nominal-case post-closure repository. The fully immersed condition used to measure the crevice repassivation potentials in the current investigation is considered conservative because, for the same water chemistry, a fully immersed condition is generally more aggressive than a thin water film condition. Kinetics of the cathodic reactions involved in localized corrosion under discontinued tortuous thin water films is expected to be slower than a fully immersed condition. Such reduced cathodic reaction kinetics are likely to constrain the corresponding anodic reactions at the crevice corrosion site, and to limit stabilization of crevice corrosion and slow down the propagation rate. Mode details of the above conservatism are discussed in the *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* report (BSC 2003 [DIRS 161235], Section 5).

6.3.6.4 Waste Package Outer Barrier Localized Corrosion Penetration Rate

In the localized corrosion penetration rate model, localized corrosion propagates at a (time-independent) constant rate (BSC 2003 [DIRS 161235], Section 6.4.4). The localized corrosion penetration rates for the WPOB range from 12.7 to 1270 μm/yr with the median value of 127 μm/yr, as shown in Table 8 (converted to mm/yr). The LC penetration rate follows a log-uniform distribution between the bounds (BSC 2003 [DIRS 161235], Section 6.4.4). The entire variance in the penetration rate is due to uncertainty.

Table 19. Distribution of Localized Corrosion Rates for Alloy 22 (DTN: SN0308T0506303.003 [DIRS 164839]).

Input Name	Input Source	Input Value	Units
LogUniform lower bound	BSC 2003 [DIRS 161235], Section 6.4.4 DTN: SN0308T0506303.003 [DIRS 164839]	1.27E-2	mm/yr
LogUniform upper bound	BSC 2003 [DIRS 161235], Section 6.4.4 DTN: SN0308T0506303.003 [DIRS 164839]	1.270	mm/yr

The current crevice corrosion penetration model for the WPOB assumes that the crevice corrosion propagates at a (time-independent) constant rate. This assumption is highly conservative because it is known that the localized corrosion rate decreases with time (CRWMS M&O 1998 [DIRS 100349], Table 3-2; Hunkeler and Boehni 1983 [DIRS 162221]; McGuire et al. 1998 [DIRS 152193], Section 5.2.8, EPRI 2002 [DIRS 158069], Section 5.3.1; Frankel 1998 [DIRS 162216]; Newman and Franz 1984 [DIRS 162250]). Decrease of the crevice corrosion propagation rate with the penetration depth is particularly more likely under the condition of discontinued tortuous thin water films that are expected to form on the waste package surface in the post-closure repository. Under the condition of such discontinued tortuous thin water films on the waste package surface, the cathodic currents from the interior of the corroding crevice to the outside surrounding the crevice mouth would be limited and not be able to support sustained penetration rates as the crevice grows deeper. This would result in a rapid decrease of the propagation rate and, for many cases, stifle or arrest of crevice corrosion.

A more realistic conceptual representation of the time-dependent (or depth-dependent) localized corrosion is discussed in the *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* report (BSC 2003 [DIRS 161235], Section 6.4.4.8). As discussed in the report, there is abundant literature data that demonstrate the time-dependent growth behavior of localized corrosion of many metals and alloys.

6.3.7 Drip Shield Stress Corrosion Cracking Conceptual Model

Although the drip shield (DS) is subject to stress corrosion cracking (SCC), this process is not modeled in the Integrated Waste Package Degradation (IWPD) Model. Possible sources of stress in the DS include (1) weld induced residual stresses; (2) plasticity induced residual stresses caused by seismic events; and (3) residual stresses produced by rock falls (BSC 2003 [DIRS 161234], Section 6.3.7). All the drip shield fabrication welds will be fully stress-relief annealed before placement in the drifts (Plinski 2001 [DIRS 156800], Section 8.3.17). The weld induced residual stresses for the DS will be mitigated by the annealing process (BSC 2003 [DIRS 161234], Section 6.3.7), therefore the DS is not subject to SCC upon emplacement in the repository. However, the drip shields are potentially subject to SCC under the action of seismic-induced loading and rockfalls. The effects of seismicity are discussed in Section 6.3.16.

An analysis of the consequence of SCC of the DS (e.g., due to residual stresses produced by rock falls) is presented in the report entitled *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234], Section 6.3.7) and summarized in this section. Stress corrosion cracks in passive alloys such as Titanium Grade 7 tend to be very tight (small crack opening displacement) by nature because the crack tip stress induced passive film rupture, repassivation and re-rupture repetitive process results in a relatively high effective crack tip corrosion rate as compared to the unstressed sides of the crack. As the crack grows through-wall, the tensile stresses normal to the crack walls are relieved, and the resulting crack faces continue to corrode by general corrosion at a very low passive corrosion rate. In the *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234], Section 6.3.7) report, it is estimated that it would take ~3400 years for the crack to fill with corrosion products. In the interim, while the crack faces are passively corroding but before the corrosion film grows to a thickness where it will completely fill the crack, there could be a small amount of water transport by surface diffusion (film flow) into the crack and through the drip shield. However, the small heat flux present across the drip shield wall will result in evaporation of the slowly flowing water and a resultant scale deposit (principally calcium carbonate - [calcite]) will form over the crack where it intersect the upper drip shield surface as well as within the crack.

A detailed calculation of the expected rate of SCC plugging due to mineral precipitation resulting from evaporation of a pore water of typical composition dripping onto a drip shield at the crack location has been performed (BSC 2001 [DIRS 156807]). SCC cracks are sealed in a few hundred years at most when water is allowed to flow through the cracks at the expected very low film flow rate (BSC 2001 [DIRS 156807], Section 6.3). When the cracks are bridged by water, the sealing process may take thousands of years, but no flow occurs since the water is held by capillary forces. Because of the high density of the mineral deposits and lack of pressure gradient to drive water through the crack, the probability of solution flow through the crack would approach zero (BSC 2003 [DIRS 161234], Section 6.3.7). Therefore, since the primary role of the drip shield is to keep water from contacting the waste package, SCC of the drip shield does not compromise its intended design purpose. On this basis, SCC of the drip shield is not modeled in the IWPD Model.

6.3.8 Waste Package Stress Corrosion Cracking Conceptual Model

Similar to the DS, all regions of the waste package (including fabrication welds), except the waste package closure lid welds, are stress relief annealed before the waste packages are loaded with waste (Plinski 2001 [DIRS 156800], Section 8.1.7), and thus do not develop residual stress/stress intensity factors high enough for SCC to occur (BSC 2003 [DIRS 161234], Section 6.4.2). However, the waste packages are potentially subject to SCC under the action of seismic-induced loading and rockfalls. The effects of seismicity are discussed in Section 6.3.16.

According to the *Drip Shield Structural Response to Rock Fall* calculation (BSC 2003 [DIRS 162598], Section 6), LS-DYNA analysis shows that the deflection of the drip shield due to rockfall is not large enough to contact the waste package. The drip shield will withstand a 11.5 MT rockfall without contacting the waste package. The maximum displacement from the 11.5 MT rockfall event is 254 mm (BSC 2003 [DIRS 165304]) and The minimum gap between the DS and waste package outer barrier was calculated to be about 380 mm based on the following equation:

$$Gap = h_{int\ ds} - dist_{inv} - \frac{d_{wp}}{2} \qquad \text{(Eq. 38)}$$

where

$h_{int\ ds}$ = interior height of drip shield (BSC 2003 [DIRS 165304], Table 1) (2715.62 mm)

$dist_{inv}$ = distance from top of invert to centerline of WP for 5 DHLW (BSC 2003 [DIRS 164069]) (1282 mm)

d_{wp} = nominal diameter of WP (5 HLW/1 DOE SNF – Short) (BSC 2003 [DIRS 157817]) (2110 mm)

Thus, the drip shield provides adequate protection to the waste package from rockfall during the regulatory time period. On this basis, SCC due to rockfall is not considered further in the Integrated Waste Package Degradation Model.

A dual closure-lid design (Figure 8) for the Alloy 22 waste package outer barrier (or outer shell) has been proposed for LA (Bokhari 2003 [DIRS 162429]). The outer closure lid is 25-mm thick and the middle closure lid is 10-mm thick (Bokhari 2003 [DIRS 162429]). The primary differences in closure lid design to be used for LA with respect to the closure lid design used in SR are (a) the full penetration stainless steel lid weld will be replaced with a spread ring and seal weld; (b) the outer closure lid extension is eliminated; (c) the outer closure lid mitigation method will be laser peening instead of induction annealing; and (d) no laser peening will be applied to the middle closure lid (Bokhari 2003 [DIRS 162429]). The effects of the peening method applied to the outer closure lid are accounted for in the stress and stress intensity factor profiles discussed in the next section.

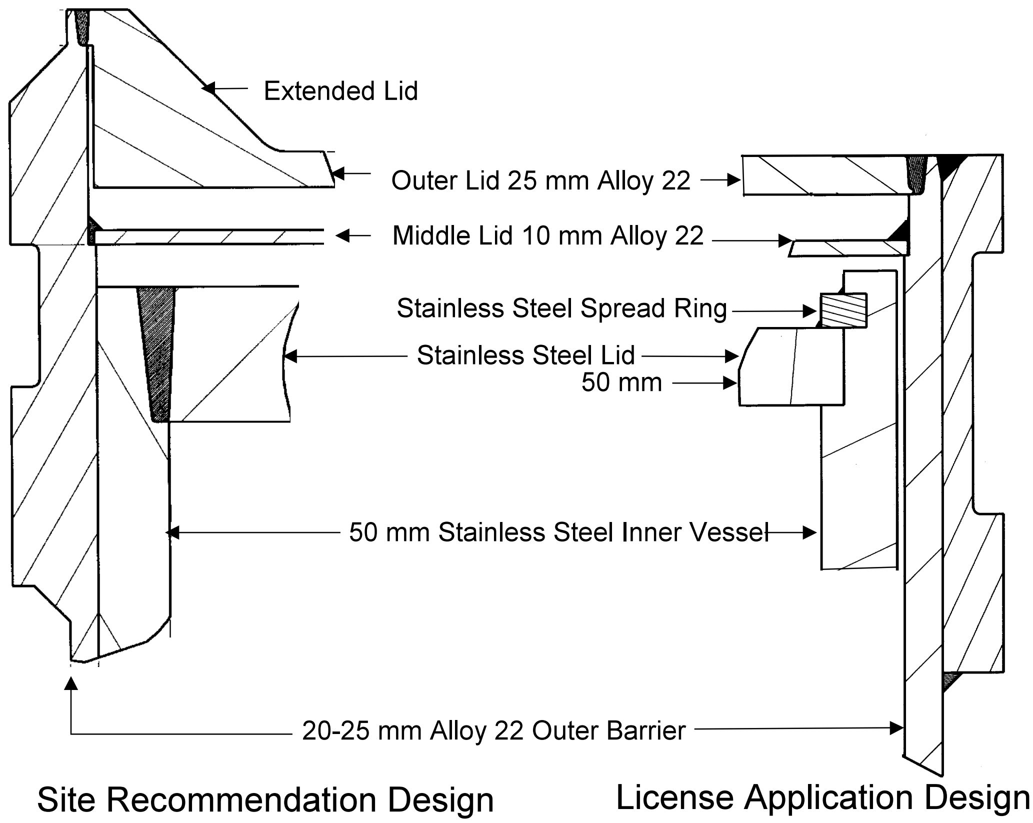


Figure 8. Schematic of the Dual Closure Lids of Waste Package Outer Barrier.

One can see in Figure 8 that there is a physical separation between the two lids. Thus, any SCC cracks initiated in the outer closure-lid stop after penetrating it, and then the middle closure-lid welds are subject to the external environment and the potential for SCC crack initiation and growth.

6.3.8.1 Stress and Stress Intensity Factor Profile Conceptual Model

Inputs to this analysis include stress and stress intensity factor profiles (stress or stress intensity factor versus depth) and slip dissolution model parameters appropriate for both the outer closure and middle closure lids of the waste package outer barrier. Table 11 summarizes these inputs and their sources. These inputs can be found in the report entitled *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234]).

In the report entitled *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234], Section 6.2.2), it is concluded that the hoop stress, which promotes radially oriented crack growth, is the dominant component of stress in the waste package outer barrier closure lid weld regions (see also BSC 2003 [DIRS 161234], Table 4.1-3). On this basis, only the hoop stress profiles are considered further in this report.

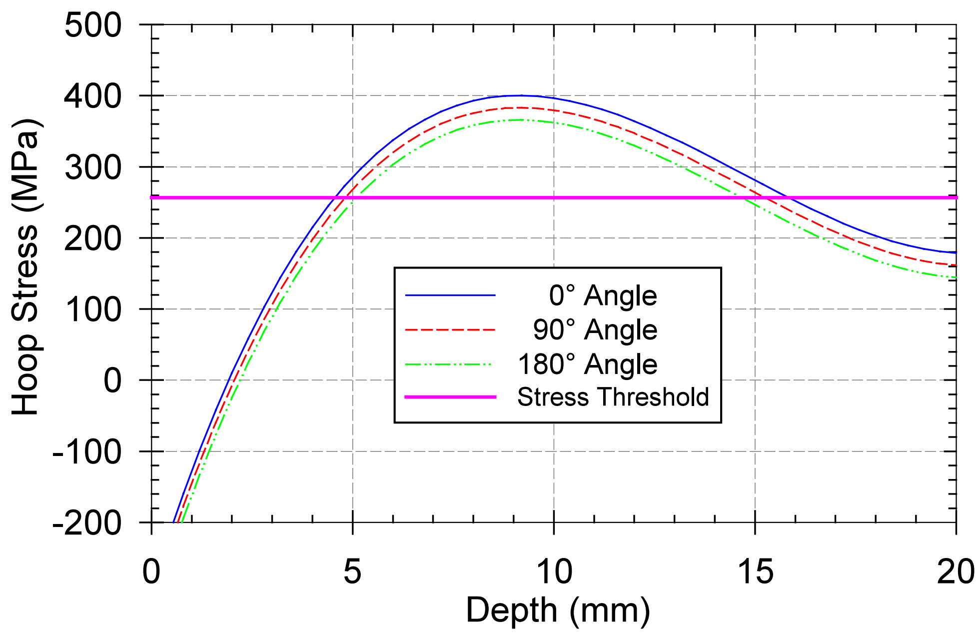
The hoop stress (σ in MPa) as a function of depth (x in mm) in the closure weld regions of the Alloy 22 waste package outer barrier is given by a third order polynomial equation of the form (BSC 2003 [DIRS 161234], DTN: LL030607012251.065 [DIRS 163968]):

$$\sigma(x,0) = A_0 + A_1 \cdot x + A_2 \cdot x^2 + A_3 \cdot x^3 \quad \text{(Eq. 39)}$$

where the values of the coefficients (A_i's) used in the Integrated Waste Package Degradation (IWPD) Model are given in Table 12. The second argument in the stress function is used to represent angular variation (θ = 0 arbitrarily chosen) around the circumference of the Alloy 22 waste package outer and middle closure-lid welds. The angular variation is included using the following functional form (BSC 2003 [DIRS 161234], Section 6.4.5, DTN: LL030607012251.065 [DIRS 163968]):

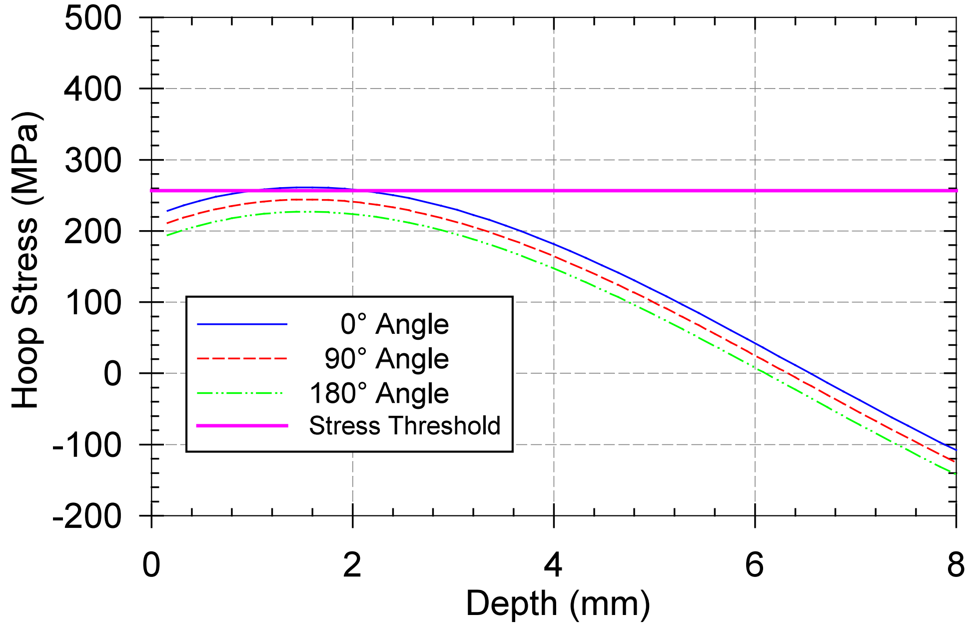
$$\sigma(x,\theta) = \sigma(x,0) - (17.236893) \cdot (1 - \cos(\theta)) \quad \text{(Eq. 40)}$$

Note that $\sigma(x, 0)$ (defined in Equation 39) uses the stress coefficients (A_i) defined in Table 12 with x in units of mm. Figure 9 shows the median (not accounting for uncertainty, which is discussed below) stress variation with angle for the WPOB outer closure lid weld region and Figure 10 shows the median stress variation with angle for the WPOB middle closure lid weld region. Also included on the graphs is the stress threshold for nucleation of incipient flaws (discussed further in the next section). One should note that the depth on these graphs do not start at zero thickness nor extend to the full lid thickness. For consistency stress values were calculated at the same depth values as the stress intensity factor profiles given in Table 13.



Source DTN: LL030607012251.065 [DIRS 163968]
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 9. Variation of Hoop Stress Versus Depth for WPOB Outer Closure Lid



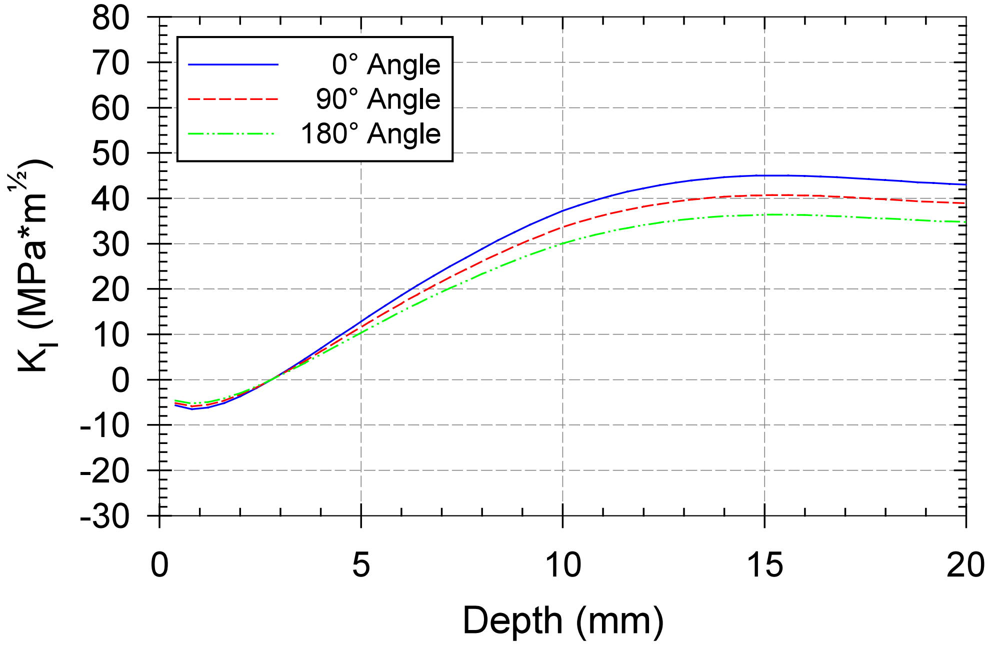
Source DTN: LL030607012251.065 [DIRS 163968]
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 10. Variation of Hoop Stress Versus Depth for WPOB Middle Closure Lid

Based on the angular stress variation in Equation 40, the stress intensity factor variation with angle is given by (BSC 2003 [DIRS 161234], Section 6.4.5, DTN: LL030607012251.065 [DIRS 163968]):

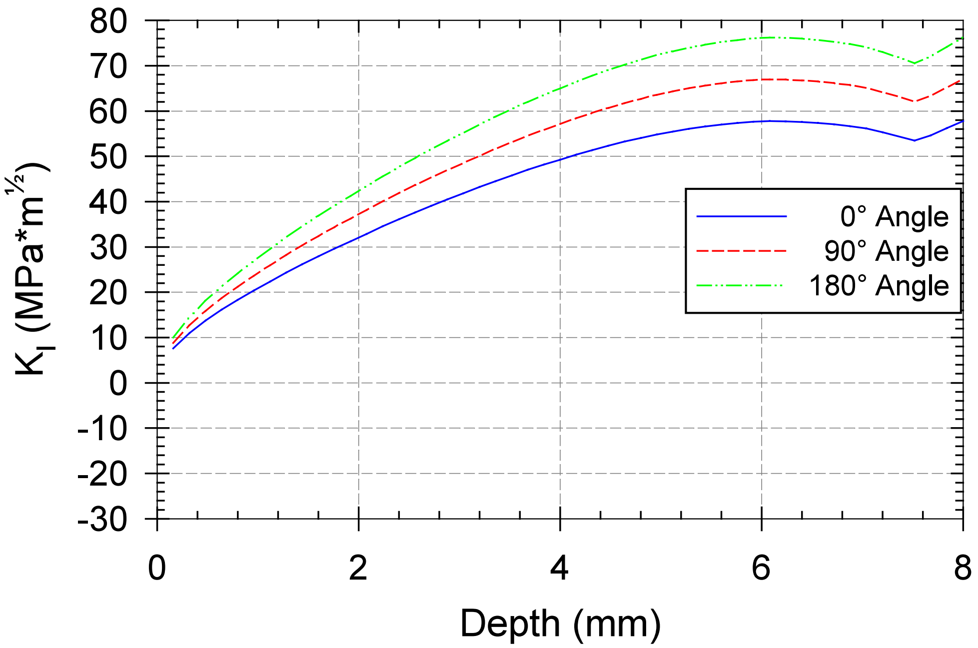
$$K_I(x,\theta) = K_I(x) \cdot \left(\frac{\sigma(Thck,\theta)}{\sigma(Thck,0)} \right) \quad \text{(Eq. 41)}$$

where *Thck* is taken to be the maximum depth value given in Table 13 and $K_I(x)$ is given by the values in Table 13. The variation of the stress and stress intensity factor profiles with angle is due to variability (BSC 2003 [DIRS 161234], Section 6.4.5). Figure 11 shows the stress intensity factor variation with angle for the WPOB outer closure lid weld region and Figure 12 shows the stress intensity factor variation with angle for the WPOB middle closure lid weld region.



Source DTN: LL030607012251.065 [DIRS 163968]
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 11. Variation of Stress Intensity Factor Versus Depth for WPOB Outer Closure Lid



Source DTN: LL030607012251.065 [DIRS 163968]
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 12. Variation of Stress Intensity Factor Versus Depth for WPOB Middle Closure Lid

The uncertainty in the stress and stress intensity factor profiles is introduced through a scaling factor, z. The scaling factor, z, which is sampled from a normal distribution with a mean of zero and a standard deviation of 5 percent of the yield strength, YS, with an upper bound of 15 percent of the YS and a lower bound of –15 percent of the YS (BSC 2003 [DIRS 161234], Section 6.4.5). The numerical value of the yield strength, YS, used in these calculations is the yield strength at 473 K (see Table 14). The value of YS (285 MPa) is obtained by linear interpolation between the values of the yield strength at 366 K (338 MPa) and 477 K (283 MPa) (see Table 11) i.e.,

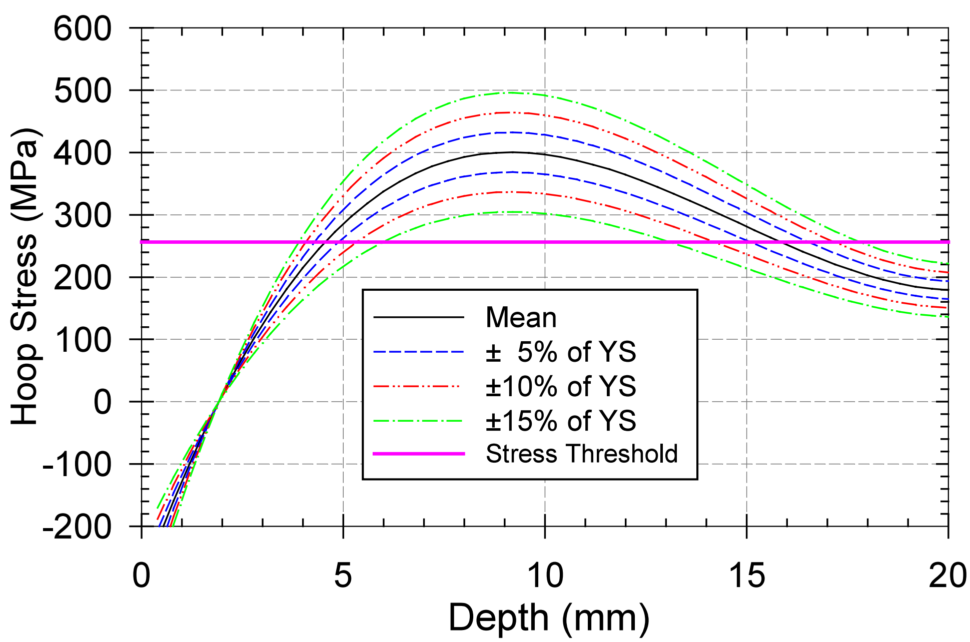
$$\mathrm{YS} = 338 + \left(\frac{473-366}{477-366}\right)\cdot(283-338) = 285\,\mathrm{MPa} \qquad \text{(Eq. 42)}$$

The stress relation, accounting for uncertainty, is given by

$$\sigma_u(x,\theta,z) = \sigma(x,\theta)\cdot\left(\frac{\sigma(Thck,\theta)+z}{\sigma(Thck,\theta)}\right) \qquad \text{(Eq. 43)}$$

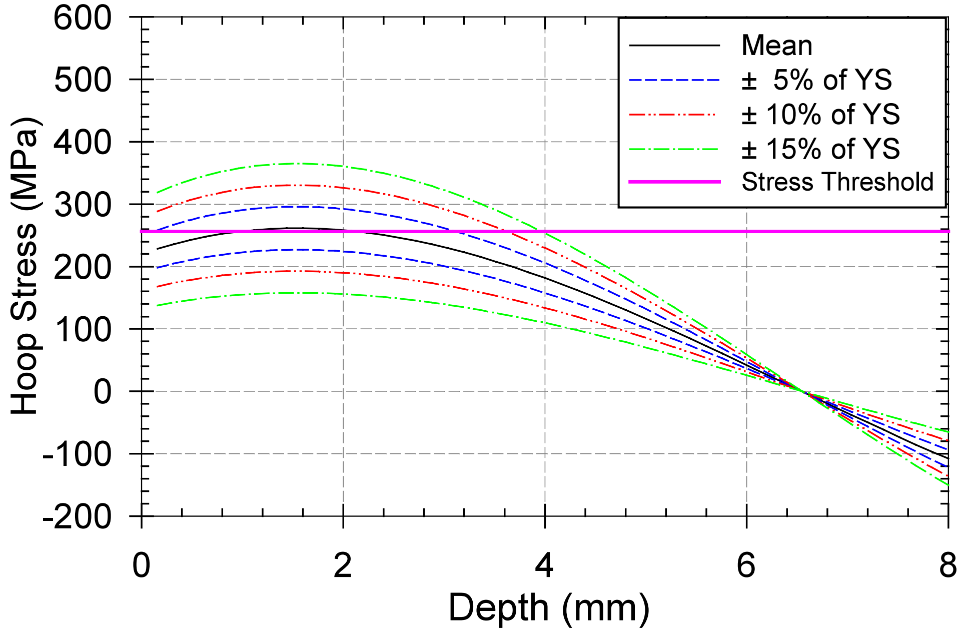
and the stress intensity factor relation is given by

$$K_{I\,u}(x,\theta,z) = K_I(x,\theta)\cdot\left(\frac{\sigma(Thck,\theta)+z}{\sigma(Thck,\theta)}\right) = K_I(x,0)\cdot\left(\frac{\sigma(Thck,\theta)+z}{\sigma(Thck,0)}\right) \qquad \text{(Eq. 44)}$$



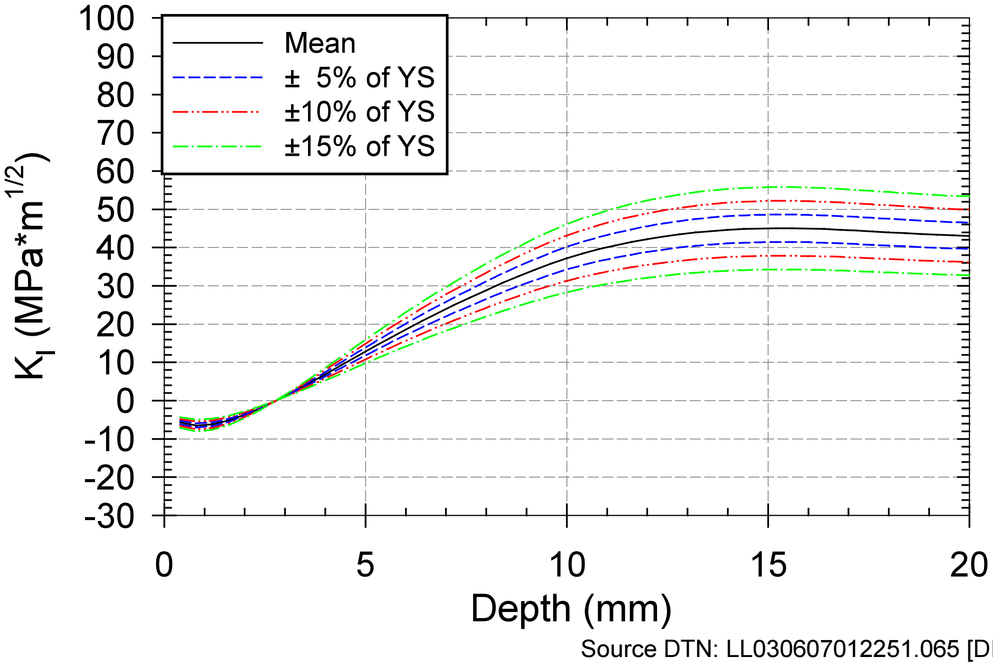
Source DTN: LL030607012251.065 [DIRS 163968]
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 13. Variation of Hoop Stress (θ = 0) Versus Depth for WPOB Outer Closure Lid



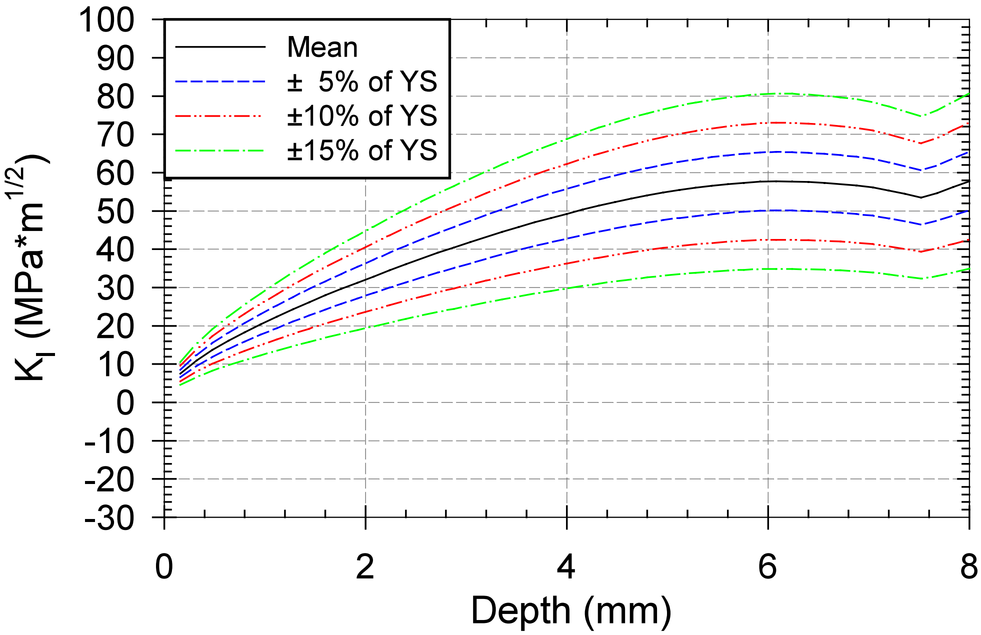
Source DTN: LL030607012251.065 [DIRS 163968]
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 14. Variation of Hoop Stress (θ = 0) Versus Depth for WPOB Middle Closure Lid



Source DTN: LL030607012251.065 [DIRS 163968]
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 15. Variation of Stress Intensity Factor (θ = 0) Versus Depth for WPOB Outer Closure Lid



Source DTN: LL030607012251.065 [DIRS 163968]
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 16. Variation of Stress Intensity Factor (θ = 0) Versus Depth for WPOB Middle Closure Lid

The uncertainty treatment of these inputs is encompassed in the parameter *z* which is sampled once per realization of the Integrated Waste Package Degradation Model for each closure lid (i.e. a different value of *z* may be sampled for each lid in a given realization).

6.3.8.2 Weld Flaw Conceptual Model

Flaws in the closure-lid welds are likely sites for SCC. Weld flaws are generally larger than other surface defects and are conservatively modeled as maintaining their depth relative to the advancing general corrosion front (i.e. they are not removed by general corrosion processes). Therefore, the characteristics of flaws in the closure welds are important inputs to the waste package SCC analysis. As discussed earlier, residual stress analyses showed that the hoop stress is the dominant stress driving crack growth; thus, only radial-oriented flaws are potential sites for SCC.

This section lists the design information inputs to the Integrated Waste Package Degradation (IWPD) Model weld flaw analysis for the Alloy 22 waste package outer barrier (or outer shell) closure-lid welds.

The probability of non-detection, P_{ND}, of weld flaws of length x using an ultrasonic testing inspection technique is (BSC 2003 [DIRS 164475], Section 6.2.1.2.1, Equation 21)

$$P_{ND}(x) = \varepsilon + \frac{1}{2}(1-\varepsilon)erfc\left(v \cdot \ln\left(\frac{x}{b}\right)\right) = \frac{\varepsilon+1}{2} + \frac{\varepsilon-1}{2} erf\left(v \cdot \ln\left(\frac{x}{b}\right)\right) \quad \text{(Eq. 45)}$$

The parameters in Equation 45 are identified in Table 20 and correspond to inputs in Table 9.

Table 20. Probability of Non-Detection Inputs Used in the IWPD Model and Their Sources

Input Name	Input Source	Input Value	Units
Lower limit of probability of non-detection, ε	BSC 2003 [DIRS 164475], Table 11	0.005	N/A
Characteristic flaw size, *b*	BSC 2003 [DIRS 164475], Table 11	2.5	mm
Shape factor, ν	BSC 2003 [DIRS 164475], Table 11	3	N/A

Table 21 lists the inputs to the IWPD Model weld flaws analysis for the Alloy 22 waste package outer barrier closure-lid welds.

Table 21. Weld Flaw Analysis Inputs Used in the IWPD Model and Their Sources

Input Name	Input Source	Input Value	Units
CSNF WP outer closure lid weld volume (V)	BSC 2003 [DIRS 164610], Table 19	1350189	mm^3
CSNF WP middle closure lid weld volume (V)	BSC 2003 [DIRS 164610], Table 18	490478	mm^3
CDSP WP outer closure lid weld volume (V)	BSC 2003 [DIRS 164610], Table 19	1753091	mm^3
CDSP WP middle closure lid weld volume (V)	BSC 2003 [DIRS 164610], Table 18	639901	mm^3
Weld Thickness (*th*)	BSC 2001 [DIRS 157812], BSC 2001 [DIRS 157817], and BSC 2001 [DIRS 157818], Sheet 3 of 3	25 for outer closure lid 10 for middle closure lid	mm
Number of sample welds	BSC 2003 [DIRS 164475], Section 6.2.1.1.2	16	N/A
Number of sample flaws (n_f)	BSC 2003 [DIRS 164475], Table 11	7	N/A
Cumulative size of sample flaws (S_f)	BSC 2003 [DIRS 164475], Attachment I, p. I-3	31.75	mm
Sample weld diameter, D	BSC 2003 [DIRS 164475], Section 6.2.1.1.2	60.765	in
Flaw size distribution parameter(λ_s)	BSC 2003 [DIRS 164475], Equation 2	Gamma distribution with a mean of n_f /S_f and a standard deviation of sqrt(n_f)/S_f	mm^{-1}
Flaw count distribution parameter (λ_c)	BSC 2003 [DIRS 164475], Equation 12	Gamma distribution with a mean of (n_f + ½)/ V_f and a standard deviation of sqrt(n_f + ½)/ V_f	mm^{-3}
Fraction of radial-oriented flaws (F_r)	BSC 2003 [DIRS 164475], Table 12	0.008	N/A
Fraction of plate to be included for propagating embedded flaws (F_ψ)	BSC 2003 [DIRS 161234], Table 8-1	0.25	N/A

The cumulative volume of sample welds, V_f, is calculated as

$$V_f = \pi D \cdot 16 \cdot CS \quad \text{(Eq. 46)}$$

where D is the sample weld diameter for the sixteen weld samples and CS is the sample weld cross section. The sample weld cross section is calculated from the values in Table 10 as (where $d_{AB} = d_{OC} - d_{AO} - d_{BC}$),

$$CS = \frac{\pi d_{AO}^2}{2} + 2d_{AO}\left(d_{BC} + d_{AB}\right) + \left(\tan\theta_3 + \tan\theta_2\right)\left[\frac{d_{AB}^2}{2} + d_{BC}d_{AB}\right] + \frac{d_{BC}^2}{2}\left(\tan\theta_4 + \tan\theta_1\right) \quad \text{(Eq. 47)}$$

The calculated value for cumulative volume of sample welds, V_f, equals 18610540.33 mm^3. A detailed derivation of this calculation may be found in the *Analysis of Mechanisms for Early Waste Package/Drip Shield Failure* (BSC 2003 [DIRS 164475], pp. I-24 through I-26).

Weld flaw sizes follow an exponential distribution of parameter λ_s normalized to the weld thickness (BSC 2003 [DIRS 164475], Attachment I). The flaw size probability density function is represented below:

$$f_s(x) = \frac{\lambda_s \exp(-\lambda_s \cdot x)}{1 - \exp(-\lambda_s th)} \quad \text{(Eq. 48)}$$

The flaw size distribution parameter (representing epistemic uncertainty), λ_s, is gamma distributed with shape parameter n_f, and scale parameter, $1/S_f$.

The fraction of non-detected defects remaining in the weld after inspection is given by the integration of the two functions above (Equation 45 and Equation 48):

$$F_{nr}(th) = \int_0^{th} P_{ND}(u) f_s(u)\,du \quad \text{(Eq. 49)}$$

While the post-inspection weld flaw sizes is given by the cumulative distribution function:

$$G(x) = \frac{\int_0^{x} P_{ND}(u) f_s(u)\,du}{F_{nr}(th)} \quad \text{(Eq. 50)}$$

The distribution for the number of defects before any inspection or repair follows a Poisson distribution with parameter λ_c. The flaw count distribution parameter (representing epistemic uncertainty), λ_c, is gamma distributed with shape parameter, (n_f + ½), and scale parameter, $1/V_f$.

The distribution for the number of defects that remain after inspection is Poisson distributed with parameter λ (count per closure weld given volume, V, and thickness, th), given by the product below (Equation 51). This expression contains the fraction of weld flaws that are radially-oriented, F_r, the fraction of embedded weld flaws able to propagate, F_ψ, and the fraction of non-detected defects, $F_{nr}(th)$:

$$\lambda = F_r \cdot F_\psi \cdot F_{nr}(th) \cdot (V \cdot \lambda_c) \quad \text{(Eq. 51)}$$

The various weld volumes, V, and thicknesses, th, are as given for each of the four closure lid types (see Table 21).

In summary, variation for weld flaw sizes is expressed as variability at the WP level given by the truncated exponential pdf in Equation 48, with an uncertain parameter, λ_s, sampled for each realization. The variation in the number of weld defects is expressed as variability at the WP level given by a Poisson distribution, with an uncertain parameter λ (count per closure weld) given by Equation 51. This parameter in turn is a function of parameters, λ_s (from the fraction of non-detected defects, $F_{nr}(th)$ term), and λ_c, which are sampled as uncertain for each realization.

6.3.8.3 Slip Dissolution Conceptual Model

The Slip Dissolution Model for stress corrosion cracking (BSC 2003 [DIRS 161234], Section 6.3) requires a threshold stress, a stress intensity factor threshold, an incipient crack size, and crack growth rate parameters (which are functions of n, the repassivation slope). These inputs and their sources are listed in Table 14 of this report.

The threshold stress is defined as the minimum stress at which cracks initiate on a "smooth" surface. These cracks are referred to in this analysis as incipient cracks (to distinguish them from weld flaws) and typically form at local surface defects such as grain boundary junctions and surface roughness. Incipient cracks are considered to be 0.05 mm in length at the time of their nucleation (BSC 2003 [DIRS 161234], Section 6.2.1 and Table 8-1). In this report, the threshold stress is taken to be 90% of the yield strength (Table 14). Incipient cracks initiate when general corrosion has penetrated to the depth at which the stress profile (Section 6.3.8.1) exceeds the threshold stress.

Weld flaws are already nucleated and thus do not require a stress threshold to nucleate. However, most weld flaws are embedded within the material and therefore not exposed to the environment. As general corrosion proceeds, some initially embedded weld flaws may be exposed to the environment (BSC 2003 [DIRS 161234], Section 6.2.2) while others are "corroded away." This evolution of the number of defects is not considered in detail. It has been recommended that a conservative approach would be to consider the fraction of weld flaws embedded within the outer ¼ of the weld thickness (BSC 2003 [DIRS 161234], Section 6.2.2) to be capable of propagation by the slip-dissolution model. As discussed in Section 6.3.8.2 of this report, only 0.8% of weld flaws are capable of propagation based on their orientation with respect to the dominant stress components.

Stress corrosion crack growth can occur when the stress intensity factor at the tip of the incipient crack or weld flaw exceeds or is equal to a threshold stress intensity factor. The depth of the tip is the sum of the general corrosion depth and the crack or weld flaw depth. The stress intensity factor at this depth is determined from the stress intensity factor profile (Section 6.3.8.1). The threshold stress intensity factor, K_{ISCC}, is given as a function of the repassivation slope, n and V_{gc} (which equals 7.23 nm/yr or 7.23x10^{-6} mm/yr) (BSC 2003 [DIRS 161234], Section 6.3.5):

$$K_{ISCC} = \left(\frac{7.23 \cdot 10^{-6} \ \frac{\text{mm}}{\text{yr}}}{\overline{A}} \right)^{1/\overline{n}} \qquad \text{(Eq. 52)}$$

$\overline{A}$ and $\overline{n}$ are functions of n, as discussed below. The threshold stress intensity factor is applied to both incipient cracks and weld flaws. It should be noted that parameter $\overline{A}$, and the equations using $\overline{A}$ are converted from units of mm/s (as expressed in Section 4.1.7) to mm/yr in this Section in order to be consistent with their use in the IWPD Model.

Once crack growth initiates the crack(s) grow at a velocity given by (BSC 2003 [DIRS 161234], Table 8-1, DTN: LL030607012251.065 [DIRS 163968]):

$$V_t = \overline{A}(K_I)^{\overline{n}} \qquad \text{(Eq. 53)}$$

where V_t is the crack growth rate in mm/yr, and K_I is the stress intensity factor in MPa(m)$^{1/2}$. Parameters, $\overline{A}$ and $\overline{n}$, in the above equation are expressed in terms of the repassivation slope, *n*, as follows.

$$\overline{A} = 7.8x10^{-2} n^{3.6} \left(4.1x10^{-14}\right)^{n} \cdot \left[\left(60\frac{\text{s}}{\text{min}}\right)\left(60\frac{\text{min}}{\text{hr}}\right)\left(24\frac{\text{hr}}{\text{day}}\right)\left(365.25\frac{\text{day}}{\text{yr}}\right)\right] \qquad \text{(Eq. 54)}$$

$$\overline{n} = 4n \qquad \text{(Eq. 55)}$$

In the IWPD Model, the parameter *n* is represented by a truncated normal distribution (at ±2 standard deviations (sds)) with a mean of 1.304, a sd of 0.16 (Table 14). The variation in the repassivation slope, *n*, is entirely due to uncertainty. The repassivation slope is sampled once per realization of the IWPD Model (i.e. the same value of *n* is used for each lid in a given realization).

The variations in the threshold stress and threshold stress intensity factor (through its dependence on *n*) distributions are entirely due to uncertainty. The thresholds are sampled once per realization of the IWPD Model (i.e. the same value of these thresholds are used for each lid in a given realization).

6.3.9 Microbially Influenced Corrosion Conceptual Model

Microbially influenced corrosion (MIC) is the change in the corrosion rate of an industrial alloy by the presence or activity, or both, of microorganisms. MIC most often occurs due to the increase in anodic or cathodic reactions due to the direct impact of microorganisms on the alloy, or by indirect chemical effects on the surrounding solution. Microorganisms can affect the corrosion behavior of an alloy either by acting directly on the metal or through their metabolic products. For example, some types of aerobic bacteria may produce sulfuric acid by oxidizing reduced forms of sulfur (e.g., elemental, sulfide, sulfite), and certain fungi transform organic matter into organic acids (Fontana 1986 [DIRS 100890], Section 8-10).

6.3.9.1 Drip Shield Microbially Influenced Corrosion Conceptual Model

Corrosion handbooks and literature reviews generally state that titanium alloys are immune to MIC (Revie 2000 [DIRS 159370], Chapter 47; Little and Wagner 1996 [DIRS 131533]; Brossia, et al. 2001 [DIRS 159836], Section 4.1.3). It is the remarkable stability of the TiO_2 passive film formed on titanium alloys which confers this immunity. While titanium is susceptible to biofouling in seawater solutions, the biofilm does not compromise the integrity of the passive film and therefore, biofouled titanium maintains its resistance to localized corrosion processes (Revie 2000 [DIRS 159370], Chapter 47). It has been reported that production of nitrates, polythionates, thiosulfates, and oxygen associated with aerobic biologic activity does not significantly increase the corrosion rate of titanium alloys (Brossia et al. 2001 [DIRS 159836], Section 4.1.3).

Steep gradients in O_2 and pH can exist within biofilms; typically aerobic and near neutral in the outer layers becoming acidic and low in O_2 close to the metal surface (Shoesmith and Ikeda 1997 [DIRS 151179], Section 6). Hydrogen peroxide has been detected in biofilms at millimolar levels, the amount of which is thought to be controlled by bacteria enzymes during the aerobic respiration process (Shoesmith and Ikeda 1997 [DIRS 151179]). Hydrogen peroxide maintains a low pH (< 3) near the metal by oxidizing metal cations which then undergo hydrolysis. These chemical changes can lead to enoblement (a shift of the corrosion potential to more positive values) of titanium by up to 500 mV (Shoesmith and Ikeda 1997 [DIRS 151179], Section 6). It is clear from Figure 10 and Figure 11 of the *General Corrosion and Localized Corrosion of the Drip Shield* (BSC 2003 [DIRS 161236], Section 6.5.2) that ΔE far exceeds 500 mV at low pH values (i.e. localized corrosion will not initiate even if the corrosion potential is increased by 500 mV). Enoblement can also lead to several beneficial effects including thickening of the passive film and a decrease in the number density of defects (Shoesmith and Ikeda 1997 [DIRS 151179], Section 3 and 6). According to Shoesmith et al. (1995 [DIRS 117892]), the initiation of crevice corrosion under biofilms has never been observed for titanium. Lastly, microbial growth in the repository will likely be limited by the availability of nutrients (BSC 2003 [DIRS 161235], Section 6.4.5).

6.3.9.2 Waste Package Microbially Influenced Corrosion Conceptual Model

It has been observed that nickel-based alloys such as Alloy 22 are relatively resistant to microbial influenced corrosion (Lian et al. 1999 [DIRS 110238]). Furthermore, it is believed that microbial growth in the repository will be limited by the availability of nutrients (BSC 2003 [DIRS 161235], Section 6.4.5). H^+ is known to be generated by bacterial isolates from Yucca Mountain. Also thiobaccilus ferro-oxidans oxidize Fe^{2+}, while geobacter metallireducens reduce Fe^{3+}. Other microbes can reduce SO_4^{2-} and produce S^{2-}.

There are no standard tests designed specifically to investigate the susceptibility of an engineering alloy to MIC (Stoecker 1987 [DIRS 162243]). One commonly used type of evaluation to determine the MIC factor is to test the alloy of interest in-situ (field) using the same variables as for the intended application. However, testing in the laboratory with live organisms can provide more controlled conditions of various environmental variables, and sterile controls can be incorporated to better assess MIC-specific effects (Horn and Jones 2002 [DIRS 162220]). Analyses conducted in the report entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.5) utilized data of this type to evaluate the microbiological processes on general corrosion of the WPOB (Horn et al. 1998 [DIRS 100457]). For general corrosion of the WPOB, the effect of MIC can be described as follows (BSC 2003 [DIRS 161235], Section 6.4.5)

$$CR_{MIC} = CR_{st} \cdot f_{MIC} \quad \text{(Eq. 56)}$$

where CR_{MIC} is the general corrosion rate in presence of microorganisms, CR_{st} is the general corrosion rate of the alloy in absence of MIC, and f_{MIC} is the MIC factor. It was found that the value of f_{MIC} for Alloy 22 in sterile media (no microbes) is one (f_{MIC} = 1), whereas the value of f_{MIC} for Alloy 22 in inoculated media (with microbes) is larger (f_{MIC} = 2). Therefore, the MIC factor, f_{MIC}, is taken to be uniformly distributed between 1 and 2. The variation in f_{MIC}, is entirely due to uncertainty (BSC 2003 [DIRS 161235], Section 6.4.5) (DTN:

SN0308T0506303.004 [DIRS 164840]). The MIC factor is applied to the WPOB general corrosion rate when the relative humidity at the WPOB surface is above 90%.

6.3.10 Aging and Phase Instability Conceptual Model

6.3.10.1 Drip Shield Aging and Phase Instability Conceptual Model

Aging and Phase instability of the DS is considered in Section 6.5.3 of the report entitled *General Corrosion and Localized Corrosion of the Drip Shield* (BSC 2003 [DIRS 161236]). In the report, it is observed that Titanium Grade 7 is a stabilized alpha (α) phase alloy and possesses outstanding phase stability. While Titanium Grade 7 does contain small amounts of alloying elements (DTN: MO0003RIB00073.000 [DIRS 152926]), most notably palladium (Pd), it is essentially a pure titanium alloy which has little capability to form intermetallic compounds under the thermal exposure conditions in the repository.

The solubility of Pd in Titanium Grade 7 is about 1 weight percent at 400°C. The nominal concentration of Pd in Titanium Grade 7 is well below the solubility limit at this temperature (Gdowski 1997 [DIRS 102789], pp. 1-8). Titanium-palladium intermetallic compounds capable of being formed in this system have not been reported to occur in Titanium Grade 7 with normal heat treatments.

Hua *et al*. (2002 [DIRS 160670]) tested both the base metal and welded metal of Titanium Grade 7 in a concentrated basic environment at 60, 70, 80, 90, 100 and 105^{o}C for up to eight weeks (Hua *et al* 2002 [DIRS 160670]; Hua and Gordon 2003 [DIRS 163111]). No difference in weight loss and, therefore, in corrosion rate was observed between the base metal and welds. The boundaries between the welds and heat-affected zone (HAZ) and between the HAZ and base metal were not visibly attacked. Therefore, the effects of phase instability on the degradation of Titanium Grade 7 and welded Titanium Grade 7 will be insignificant (BSC 2003 [DIRS 161236], Section 6.5.3).

6.3.10.2 Waste Package Aging and Phase Instability Conceptual Model

Before waste loading, the waste containers (base metal and fabrication welds) are fully annealed (Plinski 2001 [DIRS 156800], Section 8.1.7). After waste loading the closure lids are welded onto the waste container (Plinski 2001 [DIRS 156800], Section 8.1.8). The corrosion performance of Alloy 22 base metal is not affected by aging and phase instability as long as the waste package surface temperature is kept below 200°C under the exposure conditions expected in the repository (BSC 2003 [DIRS 161235], Section 6.4.6). Comparison of the anodic passive current densities of as-welded Alloy 22 samples to those of the Alloy 22 base metal samples show no significant effect of welds on the passive corrosion behavior of the alloy (BSC 2003 [DIRS 161235], Section 6.4.6).

The fabrication welds including the closure welds of the WPOB can be subject to thermal aging and phase instability under long-term thermal exposure in the repository (BSC 2003 [DIRS 161235], Section 6.4.6). Analyses conducted in the report entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235], Section 6.4.6) studied the effect of thermal aging on corrosion of Alloy 22. Three metallurgical conditions of

Alloy 22 were studied using the multiple crevice assembly samples: mill annealed, as-welded, and as-welded plus thermally aged (at 700°C for 173 hours). The samples were tested in 5 M $CaCl_2$ solutions with the test temperatures varying from 45 to 120°C. Comparison of the calculated corrosion rates of the mill annealed, as-welded, and as-welded plus thermally aged samples showed no apparent enhancement of the corrosion rate due to welding or thermal aging of the welded samples for the tested conditions.

On this basis neither Alloy 22 base metal nor weld metal are subject to enhanced corrosion due to the effects of thermal aging (BSC 2003 [DIRS 161235], Section 6.4.6).

6.3.11 Inside-Out Degradation

When the waste package fails, the waste package degradation analysis also considers corrosion degradation of the waste package on its inner surface (inside-out corrosion). The inside-out corrosion analysis includes general corrosion of the Alloy 22 waste-package outer barrier. The inside-out corrosion could cause penetrations by general corrosion in addition to those by outside-in corrosion only. In the WAPDEG software (BSC 2002 [DIRS 162606], Section 3.1) inside-out general corrosion initiates on the next time step at the time of the waste package failure. The in-package water condition is considered the same as the water condition initially on the outside of the drip shield. Since the drip shields life span is shorter than the waste packages (Section 6.6), the water condition initially on the outside of the drip shield is employed for the water condition contacting the waste package inner and outer surfaces at the time of waste package failure. Similar to the outside-in general corrosion rates, the inside-out corrosion rates are modified for the modeled waste package configuration (Figure 3) and for patch scaling effects (Section 6.3.4). Inside-out stress corrosion cracking is not simulated since it would be of negligible consequence to waste package performance either because the waste package has already been breached by the much larger patch penetrations (due to general corrosion) or because the patches susceptible to stress corrosion cracking (SCC) have already breached by SCC.

6.3.12 Early Failure Conceptual Model

In the *Analysis of Mechanisms for Early Waste Package/Drip Shield Failure* (BSC 2003 [DIRS 164475], Section 6.1.6), several general types of manufacturing defects were identified including weld flaws, base metal flaws, improper weld material, improper base metal, improper heat treatment, improper weld-flux material, poor weld-joint design, contamination, mislocated welds, missing welds, handling damage, and administrative or operational error. Weld flaws in waste package welds have been discussed in detail in Section 4.1.5 and Section 6.3.8 in relation to their effect on stress corrosion cracking (SCC).

6.3.12.1 Drip Shield Early Failure

Of the general types of manufacturing defects identified above, only weld flaws, base metal flaws, improper weld or base metal material, improper heat treatment, contamination, handling damage, and administrative or operational error are considered applicable to the drip shield (DS) (BSC 2003 [DIRS 164475], Section 6.3).

Although weld and base metal flaws in the DS materials do have a probability of occurrence in the repository (BSC 2003 [DIRS 164475], Sections 6.3.1 and 6.3.2), the consequence of their occurrence is stress corrosion cracking (SCC) (BSC 2003 [DIRS 164475], Section 6.4.1). As discussed in Section 6.3.7 of this report, SCC of the DS is of no consequence to performance. On this basis, weld and base metal flaws in the DS materials are of no consequence to performance and will not be considered further.

The use of improper weld or base metal material is possible in the repository (BSC 2003 [DIRS 164475], Section 6.3.3), however, due to the strict controls that will govern the fabrication of the DS, it is expected that the material composition of the improper weld or base metal material will differ only slightly from the intended composition (BSC 2003 [DIRS 164475], Section 6.4.2). In view of the high corrosion resistance of the materials in question, the consequences of improper weld or base metal is expected to be insignificant (BSC 2003 [DIRS 164475], Section 6.4.2).

Similar to the case of weld and base metal flaws in the DS materials, although improper heat treatment of DS materials is possible in the repository (BSC 2003 [DIRS 164475], Section 6.3.4), the consequence of improper heat treatment is stress corrosion cracking (SCC) (BSC 2003 [DIRS 164475], Section 6.4.3). As discussed in Section 6.3.7 of this report, SCC of the DS is of no consequence to performance. On this basis, improper heat treatment of DS materials is of no consequence to performance and will not be considered further.

The probability of DS surface contamination is also evaluated in the *Analysis of Mechanisms for Early Waste Package/Drip Shield Failure* (BSC 2003 [DIRS 164475], Section 6.3.5). It is found that the consequence of DS surface contamination is not significant from a corrosion standpoint (BSC 2003 [DIRS 164475], Section 6.4.5). On this basis, DS surface contamination is not considered further.

Similar to the case of improper heat treatment of DS materials, although handling damage of DS materials is possible in the repository (BSC 2003 [DIRS 164475], Section 6.3.6), the consequence of handling damage is stress corrosion cracking (SCC) (BSC 2003 [DIRS 164475], Section 6.4.5). As discussed in Section 6.3.7 of this report, SCC of the DS is of no consequence to performance. On this basis, improper heat treatment of DS materials is of no consequence to performance and will not be considered further.

It is extremely unlikely that a gap between adjacent drip shield segments, due to the administrative/operational error of improper DS emplacement, would go unnoticed (BSC 2003 [DIRS 164475], Section 6.3.7).

Overall, the types of manufacturing defects considered applicable to the drip shield (DS) (BSC 2003 [DIRS 164475], Section 6.3) have no consequence on DS performance and are not considered further in this analysis.

6.3.12.2 Waste Package Early Failure

Of the general types of manufacturing defects identified in Section 6.3.12, improper weld flux material (the welding method will not use weld-flux material), poor joint design (a significant development and testing effort renders poor design extremely unlikely), missing welds (the probability of missing welds is less than 8.9×10^{-9} per waste package), and mislocated welds (extremely unlikely for the large multi-pass welds on the waste packages) (BSC 2003 [DIRS 164475], Section 6.2) are not considered further.

Weld flaws in waste package welds have been discussed in detail in Section 4.1.5 and Section 6.3.8 in relation to their effect on stress corrosion cracking (SCC).

Although base metal flaws in the WPOB material do have a probability of occurrence in the repository (BSC 2003 [DIRS 164475], Section 6.2.2), the consequence of their occurrence is stress corrosion cracking (SCC) (BSC 2003 [DIRS 164475], Section 6.4.1). As discussed in Section 6.3.8, all regions of the waste package (including fabrication welds), except the waste package closure lid welds, are stress relief annealed before the waste packages are loaded with waste (Plinski 2001 [DIRS 156800], Section 8.1.7), and thus do not develop residual stress/stress intensity factors high enough for SCC to occur (in the absence of seismic activity) (BSC 2003 [DIRS 161234], Section 6.4.2).

The use of improper weld or base metal material for the WP is possible in the repository (BSC 2003 [DIRS 164475], Section 6.2.3), however, due to the strict controls that will govern the fabrication of the WP, it is expected that the material composition of the improper weld or base metal material will differ only slightly from the intended composition (BSC 2003 [DIRS 164475], Section 6.4.2). In view of the high corrosion resistance of the materials in question, the consequences of improper weld or base metal is expected to be insignificant (BSC 2003 [DIRS 164475], Section 6.4.2).

The probability of WP surface contamination is also evaluated in the *Analysis of Mechanisms for Early Waste Package/Drip Shield Failure* (BSC 2003 [DIRS 164475], Section 6.2.6). It is found that the consequence of WP surface contamination is not significant from a corrosion standpoint (BSC 2003 [DIRS 164475], Section 6.4.5). On this basis, WP surface contamination is not considered further.

The type of administrative or operational errors that could lead to unanticipated operating conditions are those which could affect the exposure conditions (e.g., T, RH, chemistry) and impact the corrosion rates, result in placement in prohibited areas, or allow water contact at times earlier than expected (BSC 2003 [DIRS 164475], Section 6.2.8).

A thermally overloaded WP would result in an increase in heat output (which can be expected not to exceed a few kilowatts) (BSC 2003 [DIRS 164475], Section 6.2.8). Since the WP is a metallic container with a large heat transfer area, the temperature at the surface of the WP is mainly governed by the temperature in the drift where the WP is located, rather than the heat output within the WP (BSC 2003 [DIRS 164475], Section 6.2.8). Therefore, the increase in heat output generated by a thermally overloaded WP would be effectively dissipated into the drift, and is not expected to alter the WP surface temperature to an extent significant enough to jeopardize its postclosure performance. Therefore this event will not be considered further.

For improper WP placement, the only current prohibition relates to placement across faults. Since only a small fraction of the WPs could be subjected to such an error, and the mean fault displacement with an annual return probability of 10^{-4} is less than 1 mm (BSC 2003 [DIRS

164475], Section 6.2.8), no consequence is expected for postclosure performance. Therefore this event will not be considered further.

The remaining types of manufacturing defects (improper heat treatment and handling damage (including improper laser peening)) were grouped together, because they share the same consequence of increasing the susceptibility of the WP to stress corrosion cracking (BSC 2003 [DIRS 164475], Section 7). Among these defects, improper heat treatment is, by far, the dominant process in terms of probability (BSC 2003 [DIRS 164475], Section 7). Therefore, improper heat treatment, improper laser peening, and handling damage shall be collectively referred to as "WP early failure" for the remainder of this report.

In this representation, variation in the number of early failed WPs is expressed as variability deriving from a discrete Poisson distribution with an uncertain intensity parameter. The uncertain intensity parameter is the product of the uncertain rate of WP failures (log normally distributed) and the number of WPs in a realization. As summarized in Table 16 in Section 4.1.9 of this report, the Poisson intensity is sampled from a log normal distribution with a median of 7.2×10^{-6} and an error factor of 15 (BSC 2003 [DIRS 164475], Section 7, Table 20]. These inputs need to be adjusted to conform to the input requirements of the GoldSim software (GoldSim Technology Group. 2002 [DIRS 160643], Appendix B) for log normal distributions. First, note that the median is equal to the geometric mean for log normal distributions (Evans, et al. [DIRS 112115], Chapter 25). Second, according to the *Analysis of Mechanisms for Early Waste Package/Drip Shield Failure* (BSC 2003 [DIRS 164475], Section 6.2.2), the shape parameter, σ_k, is related to the error factor by

$$\sigma_k = \frac{\ln(EF)}{1.645} = \ln\left(EF^{1/1.645}\right) \qquad \text{(Eq. 57)}$$

The shape parameter is the standard deviation in log space (Evans, et al. [DIRS 112115], Chapter 25). Therefore, the geometric standard deviation of the log normal distribution is given by (GoldSim Technology Group. 2002 [DIRS 160643], Appendix B)

$$e^{\sigma_k} = EF^{1/1.645} \qquad \text{(Eq. 58)}$$

The input parameters for the GoldSim software are as summarized in Table 22.

Table 22. Waste Package Early Failure Inputs to the GoldSim Software

Input Name	Input Source	Input Value	Units
Evaluation probability per WP (Uncertain Poisson intensity)	This report	Log normal distribution with a geometric mean of 7.2×10^{-6} and geometric sd of 15^(1/1.645) truncated at 7.44213E-3	per WP
Number of Early Failed WP per realization	This report	Poisson Distribution with intensity given above.	# WP/realization

Since an improperly heat treated WP might be susceptible to aging and phase instability, it is not possible to identify a single and specific mechanism of degradation. For these reasons, the following recommendations are made in the *Analysis of Mechanisms for Early Waste*

Package/Drip Shield Failure (BSC 2003 [DIRS 164475], Section 6.4.8) for evaluating WP early failure

- A failure of the WP outer barrier shell and outer and middle closure lids should be assumed as well as the failure of the stainless steel structural inner vessel and its' lid.
- The affected WPs should be assumed to fail immediately upon initiation of degradation processes.
- The entire WP surface area should be considered affected by WP early failure.
- The materials of the entire affected area should be assumed lost upon failure of the WPs because the affected area could be subjected to stress corrosion cracking and enhanced localized and general corrosion.

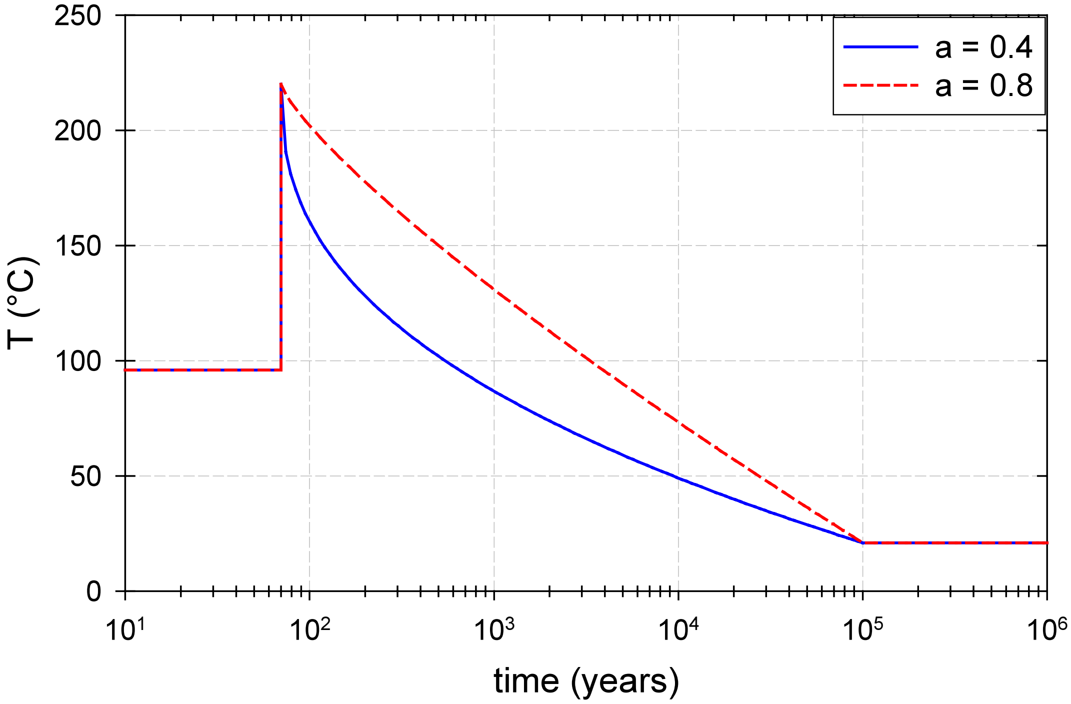
6.3.13 Representative Waste Package and Drip Shield Exposure Conditions

An abstraction of temperature and relative humidity behavior will be used to give simple parameterized inputs for waste package and drip shield to exposure conditions. The representative thermal hydrologic history files produced in this Section are used in this document only for demonstration of model application to generate example outputs.

Temperature response will be interpolated (on a logarithmic time scale) from a peak temperature at 70 years to a background temperature of 21°C at one hundred thousand years. To study the system response to differing decay rates, a power term in the interpolation is used. The temperature as a function of time abstraction is given by:

$$T(t) = T_o + (21°\text{C} - T_o)\left(\frac{\ln\left(\frac{t}{70\text{yr}}\right)}{\ln\left(\frac{10^5\,\text{yr}}{70\text{yr}}\right)}\right)^a, \quad 70\text{yr} \le t \le 10^5\,\text{yr} \qquad \text{(Eq. 59)}$$

The peak temperature is given by T_o and the decay term is a. Peak temperature values of 160 and 220°C and decay term values of 0.4 and 0.8 will be evaluated. Schematic temperature versus time profiles using a peak temperature of 220°C are shown in Figure 17.



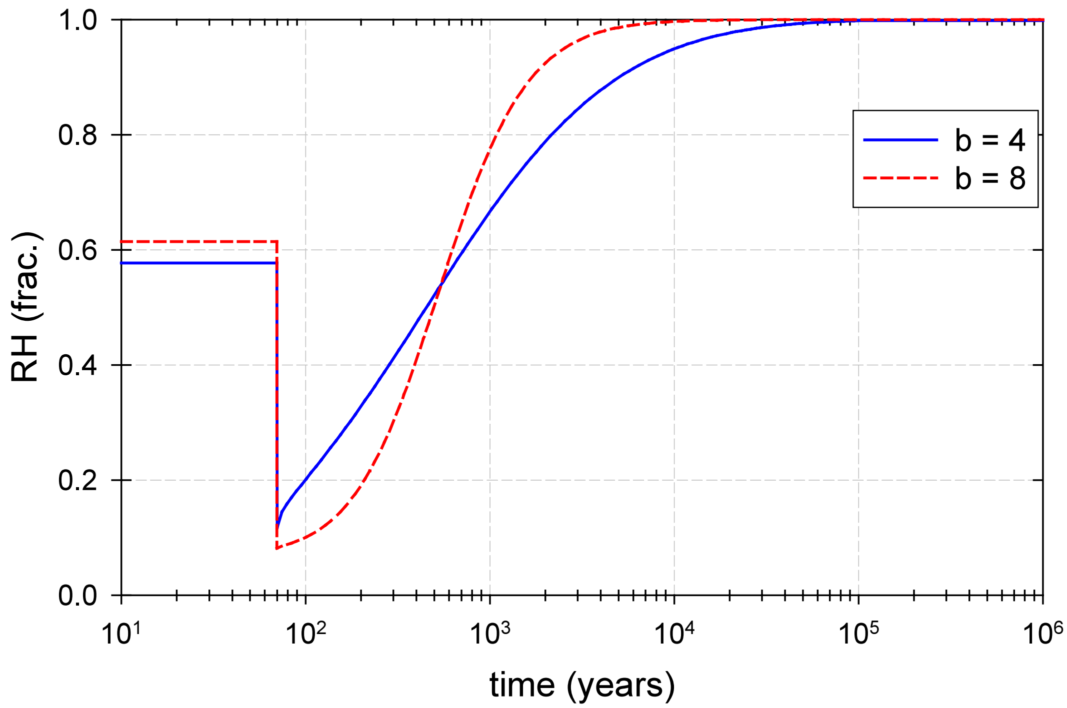
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 17. Schematic Temperature Versus Time Profiles for a Peak Temperature of 220°C and Decay Terms of 0.4 and 0.8

The relative humidity (RH) will be modeled by a logistic function of temperature. At low temperature, the RH will reach a limit of one and at high temperatures, the RH limit will be set at 0.08. The midpoint transition temperature between these limits is set at a temperature of 100°C. The RH as a function of temperature is given by:

$$\mathrm{RH}(T) = 0.08 + \frac{(1.00 - 0.08)}{1 + \left(\frac{T}{100.0°C}\right)^{b}} \qquad \text{(Eq. 60)}$$

The scaling term, b, is varied to change the rate at which RH varies with temperature. Scaling term values of 4 and 8 will be evaluated. Schematic RH versus time profiles using a peak temperature of 220°C, a decay term of 0.4, and scale terms of 4 and 8 are shown in Figure 18.



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 18. Schematic Relative Humidity Versus Time Profiles for a Peak Temperature of 220°C, Decay Term of 0.4, and Scale Terms of 4 and 8.

In this way a total of eight different thermal hydrologic histories were created; one for each unique combination of the three factors T_o, a, and b. These combinations are summarized in Table 23.

Table 23. Combinations of Peak Temperature, T_o, Decay Term, *a*, and Scaling Term, *b*, Used to Create Representative Thermal Hydrologic Histories

T_o °C	a	b
160	0.4	4
160	0.4	8
160	0.8	4
160	0.8	8
220	0.4	4
220	0.4	8
220	0.8	4
220	0.8	8

All eight thermal hydrologic histories were copied to one exposure file used in the IWPD Model simulations documented in this report. Each thermal hydrologic history is considered to represent the behavior of 1/8 (0.125) of the drip shields and waste packages simulated.

6.3.14 Radiation Enhanced Corrosion

Gamma radiation is the dominant contributor to dose rate at the waste package surface (BSC 2003 [DIRS 165269], Table 60). The effects of radiation on waste package materials corrosion differ depending on the amount of liquid present on their surfaces (i.e. humid air or aqueous conditions). Under humid air conditions, a thin film of liquid forms that may contain trace constituents (e.g., dissolved gases). Irradiation of these films could lead to acidic conditions and to enhanced corrosion rates. Under aqueous conditions (bulk solutions), anodic shifts in the open circuit potential of stainless steel in gamma irradiated solutions have been experimentally observed. These shifts in potential have been shown to be due to the formation of hydrogen peroxide (BSC 2003 [DIRS 161236], Section 6.5.1).

Calculations of the expected radiation levels at the surface of the waste package have been performed. For a bounding case waste package containing 21 PWR spent fuel assemblies (75 GWd/MTU burnup, and 5 year decay), the maximum surface radiation level was calculated to be about 1100 rem/hour (1100 rad/hr) (BSC 2003 [DIRS 165269], Table 60). This value is an upper bound at the time of emplacement. During the ventilation period of 50 years, no aqueous or humid air environment is capable of forming. After 50 years, the maximum surface radiation level decreases to levels in the range of 25-85 rad/hour (BSC 2003 [DIRS 165269], Figure 6). One hundred years after emplacement, the calculated levels reduce to about 12 to 26 rad/hour. Although there is little information available in the literature on the effects of radiation on Alloy 22 and in specific, some data are available on the corrosion of Alloy C-4, which is compositionally similar to Alloy 22. Gamma irradiation in aggressive $MgCl_2$ brines showed that below ~100 rad/hour (Shoesmith and King 1998 [DIRS 112178], p. 29) irradiation has no observable influence on the corrosion behavior of Alloy C-4. In this same environment, it was found that at dose rates above 1,000 rad/hr (up to 10^4 rad/hr) only a minor enhancement of film growth rates on Titanium Grade 7 was observed and passivity was not threatened (Shoesmith and King [DIRS 112178], p. 30). Based on this data it is concluded that, even in aggressive $MgCl_2$ brines, the radiation levels in the repository are not high enough to result in an enhancement of corrosion processes on Alloy 22 or Titanium Grade 7.

6.3.15 Igneous Induced Drip Shield and Waste Package Degradation

Igneous activity is a disruptive event that is included in the Total System Performance Assessment for the License Application (TSPA-LA) analyses. Igneous induced waste package and drip shield degradation is discussed in further detail in the reports entitled *Number of Waste Packages Hit by Igneous Intrusion* (BSC 2003 [DIRS 161851]) and *Igneous Intrusion Impact on Waste Packages and Waste Forms* (BSC 2003 [DIRS 165002]). Two igneous activity scenarios are considered: (1) The Igneous Intrusion Groundwater Release Scenario ("Igneous Intrusion" Scenario, for short) considers the in-situ damage to waste packages that occurs if they are encapsulated or otherwise affected by magma as a result of an igneous intrusion, and (2) The Volcanic Eruption Scenario is the direct release of radioactive waste due to a volcanic eruption that intersects the repository. An igneous intrusion is defined as magmatic activity that does not reach the earth's surface. Magma that does reach the surface from igneous activity is an eruption (or extrusive activity). The objective of the report entitled *Number of Waste Packages Hit by Igneous Intrusion* (BSC 2003 [DIRS 161851]) is to develop a probabilistic measure of the number of waste packages that could be affected by each of the two scenarios. The analysis evaluates geometric relationships between dike intersection area and conduit geometry and the number of waste packages impacted by dikes and conduits. The objective of the report entitled *Igneous Intrusion Impact on Waste Packages and Waste Forms* (BSC 2003 [DIRS 165002]) is to assess the potential impacts of igneous intrusion on waste packages and waste forms in the emplacement drifts. The analysis includes an assessment of deleterious dynamic, thermal, hydrologic, and chemical impacts on the waste packages and waste forms.

It was assumed, for the purposes of modeling, that the main section of each drift, which contains the waste packages, will not be backfilled. Therefore, it is assumed, for the purposes of modeling, in the report entitled *Number of Waste Packages Hit by Igneous Intrusion* (BSC 2003 [DIRS 161851], Assumption 5.2) that for any drift intersected by a dike, all waste packages therein will be destroyed.

Key results from the *Igneous Intrusion Impact on Waste Packages and Waste Forms* (BSC 2003 [DIRS 165002], Section 6.7) include:

- For any drift that is intersected by a dike, all of the drip shields and waste packages located in that drift would be destroyed and would provide no protection to the waste forms.

- For any drift not intersected by a dike, the effects of igneous intrusions would be negligible, i.e. drip shield and waste package degradation should be modeled using nominal exposure conditions.

The bases for the dike intersection case are:

- Pressures would develop within waste packages, as a result of high temperatures (estimated to be ~ 1200°C), which would be on the order of the yield strength of the waste package materials. If, as is likely prior to igneous intrusion, the waste packages had undergone some degradation (e.g., general corrosion), failure would require less pressure than for non-degraded waste packages (BSC 2003 [DIRS 165002], Section 6.5.1).
- Literature reviews (e.g., Gordon 2003) suggest that the structural integrity of waste package and drip shield materials could be severely compromised (BSC 2003 [DIRS 165002], Section 6.5.1).
- Furthermore, as discussed in Section 6.3.10, aging and phase instability can affect waste package degradation if the exposure temperature is significantly above 200°C. During igneous intrusions, the waste package surface temperature will be very high for extended periods.
- Also, since the drifts will not be backfilled, there are no credible mechanisms to block or mitigate the resulting effects from the dike intrusion upon the drip shields and waste packages (BSC 2003 [DIRS 161851], Section 5.2).

The bases for the non-intrusive case are:

- The maximum temperature rise in drifts adjacent to those which have experienced igneous intrusion is 10°C and the thermal perturbation lasts on the order of tens of years (i.e. the host rock provides an effective thermal insulation barrier to the impacts of adjacent drift magma intrusions) (BSC 2003 [DIRS 16450], Section 6.5.2).
- Analyses of volatile gas flow presented in the *Igneous Intrusion Impact on Waste Packages and Waste Forms* report (BSC 2003 [DIRS 165002], Section 6.5.2) indicate that volatile gas concentrations, entering drifts adjacent to those which have experienced igneous intrusion, would be low and significantly reduce after two years. Furthermore,

gases released from magma would tend to react with the surrounding host rock before reaching the adjacent drift greatly reducing their aggressiveness (BSC 2003 [DIRS 165002, Section 6.5.2).

- Also, the presence of backfill in ventilation drifts, access drifts, and turnouts will serve as credible mechanisms to protect waste packages in drifts which are not exposed directly to magma (i.e. drifts which are not intersected by a dike) (BSC 2003 [DIRS 161851], Section 5.2).

It was concluded in the report entitled *Number of Waste Packages Hit by Igneous Intrusion* (BSC 2003 [DIRS 161851], Section 7.2) that the Igneous Intrusion Scenario shows a range of consequences, extending from virtually no impact up to an impact upon all waste packages in the repository. The 50^{th} percentile value indicates approximately 3160 waste packages impacted, out of over 11,000.

Primary outputs from the report entitled *Number of Waste Packages Hit by Igneous Intrusion* (BSC 2003 [DIRS 161851]) are a cumulative distribution function (CDF) for the number of waste packages hit by an igneous intrusion for use in TSPA analyses of the Igneous Intrusion Scenario and a CDF for the number of waste packages hit by an eruptive conduit for use in the eruptive scenario.

6.3.16 Seismic Induced Drip Shield and Waste Package Degradation

The seismic induced drip shield and waste package degradation models, analyses and conclusions described in this section are taken from the report entitled *Seismic Consequence Abstraction* (BSC 2003 [DIRS 161812]). The scope is limited to abstracting the mechanical response of Engineered Barrier System (EBS) components (including the DS and WP) to seismic hazards during the postclosure period and defining algorithms for the seismic scenario. The abstractions are based on the results from design structural response calculations of EBS components to vibratory ground motion, from analyses for fault displacement, and from analyses of rockfall induced by vibratory ground motion. The structural response calculations and rockfall calculations from these design calculations and scientific analyses that provide the model and analyses inputs are described in the *Seismic Consequences Abstraction* (BSC 2003 [DIRS 161812], Section 4.1). The structural response calculations describe degradation of the waste package and drip shield over a 20,000-year time frame, which includes the initial 10,000-year regulatory period.

The abstraction for damage to the waste package from vibratory ground motions is based on engineering calculations that cover a range of peak ground velocity (PGV) of 1 m/s to 6 m/s and have a maximum damage of less than 2 percent of the surface area of the waste package. Similarly, the abstraction for damage to the drip shield from vibratory ground motions is valid within a range of PGV from 1 m/s to 6 m/s. These vibratory ground motion abstractions as well those for the drip shield response to rockfall are stochastic distributions whose parameters (i.e. the upper and lower bounds for a uniform distribution or the mode and bounds of a log-triangular distribution) are a function of the amplitude of the ground motion.

The seismic failure criteria for Alloy 22 and Titanium Grade 7 have generally been selected in a conservative manner. Note that the failure criteria are based on considerations of accelerated stress corrosion cracking (SCC) related corrosion degradation due to residual stress, rather than mechanical failure from exceeding the ultimate tensile stress of Alloy 22 or Titanium Grade 7. In fact, none of the structures reached ultimate tensile failure in any of the structural calculations to date. The rationale for selection of the SCC stress thresholds for failure is based on information in the report entitled *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234], Section 6.2.1). The conservative approach to defining the stress thresholds for failure provides ample safety margin, helping to enhance confidence in the seismic failure criteria.

The TSPA model for the seismic scenario is very similar to the TSPA model for the nominal scenario, with two major exceptions: (1) failed areas on the drip shield, waste package or cladding are determined by sampling stochastic parameters in abstractions for damage to EBS components, rather than by the Integrated Waste Package Degradation (IWPD) Model for corrosion processes; and (2) a single seismic event occurs at a random time during each realization. The output from each calculated realization is a time history of dose to the reasonably maximally exposed individual.

In calculating structural damage from a seismic event, the horizontal PGV is used as the measure of the amplitude of the ground motion (BSC 2003 [DIRS 161812]). PGV is appropriate for the response of a rock mass to dynamic loading because the change in stress across a weak compression wave is directly proportional to the particle velocity. The horizontal PGV values have been calculated for the 10^{-6} per year and 10^{-7} per year mean annual exceedance frequencies at the emplacement drifts (called Point B in the probabilistic seismic hazard analyses). The horizontal PGV value for the 10^{-6} per year ground motions is 2.44 m/s (DTN: MO0303DPGVB106.002 [DIRS 162712]). The horizontal PGV value for the 10^{-7} per year ground motions is 5.35 m/s (DTN: MO0210PGVPB107.000 [DIRS 162713]).

The scaling analysis is, based on the Point A hazard curve defined by the probabilistic seismic hazard analyses expert elicitation (DTN: MO03061E9PSHA1.000 [DIRS 163721], file h_vel_extended.frac_mean). A scaling factor of 0.7963 results in an error of +7.6 and -1.7 percent with respect to the two known values at Point B. PGV values over the range of annual exceedance frequencies can be determined by interpolation, with the resulting values shown in Table 24 (BSC 2003 [DIRS 161812], Table I-2)

Table 24. Interpolated Values on the Scaled PGV Hazard Curve for Point B

Annual Exceedance Frequency (1/yr)	Interpolated PGV at Point B (cm/s)	Comments
5×10^{-4}	18.1	
10^{-4}	38.8	
5×10^{-5}	55.0	
10^{-5}	106.7	
10^{-6}	262.4	Error of +7.5% relative to the exact value of 244 cm/s
10^{-7}	525.8	Error of –1.7% relative to the exact value of 535 cm/s
1×10^{-8}	1073	

6.3.16.1 Waste Package Damage

The failure criterion for Alloy 22 is defined as a uniform distribution between 80 and 90 percent of the yield strength (BSC 2003 [DIRS 161812], Section 6.3.1). In other words, there is uncertainty in the value of the appropriate residual stress threshold for Alloy 22. Waste package damage values, i.e. percent of total outer surface area exceeding the threshold value at the two extremes (80 and 90 percent) of the stress threshold. Since the failed area is defined by the elements of the finite-element grid whose residual stress exceeds the value of the stress threshold, it follows that the failed area for the 90 percent threshold will always be less than or equal to the failed area for the 80 percent threshold.

The damaged areas for 15 different realizations are summarized in the *Seismic Consequence Abstraction* (BSC 2003 [DIRS 161812], Table 6) for an annual frequency of occurrence of 10^{-6} per year and in (BSC 2003 [DIRS 161812], Table 7) for an annual frequency of occurrence of 10^{-7} per year. The percent failed WP area from all realizations for these two cases varies from as low as 0.05% to as high as 1.84%. The mean damage and standard deviation of the damage is also presented in these tables. For both cases, the mean damage for the 80 percent residual stress threshold is approximately twice as large as the mean damage for the 90 percent stress threshold. Note also that the variability in damage (i.e. the ratio of the maximum damage to the minimum damage for a given ground motion level) from the ground motions is approximately a factor of 10 at a given residual stress threshold. The uncertainty in damage is dominated by the uncertainty in ground motion, rather than the uncertainty in the residual stress threshold.

The results also demonstrate that the cumulative damage area is dominated by the contribution from end-to-end impacts of adjacent waste packages. In particular, the damaged area from waste package to pallet impacts is much smaller than the damage due to the end-to-end impacts of adjacent waste packages, with the exception of realization number 14 in both tables. The damage from end-to-end impacts is the dominant contribution to total damage because the adjacent waste package is conservatively represented as an essentially rigid wall anchored to the invert.

The model abstractions for waste package response to vibratory ground motions and for drip shield response to vibratory ground motions and rockfall are simple numerical fits to the percent failed surface area as a function of PGV. The fits involve selecting the most appropriate distribution to represent the variability of damage as a function of PGV. The appropriate distributions and functional fits have been developed and documented in the *Seismic Consequence Abstraction* (BSC 2003 [DIRS 161812], Attachments II, IV and VI).

The damage abstraction selected for the TSPA-LA calculations is a relationship between the Bayesian upper bound and the corresponding seismic hazard level, as measured by horizontal PGV. The PGV levels corresponding to the 10^{-6} and 10^{-7} per year hazard levels are 2.44 m/s and 5.35 m/s, respectively (BSC 2003 [DIRS 161812], Section 6.4). As described, a linear fit to the calculated Bayesian upper bounds and these PGV values produces the following linear relationship (BSC 2003 [DIRS 161812], Section 6.5.1):

$$D_{ub} = \mathrm{MAX}(0.0,\ 0.383 * PGV - 0.305), \qquad \text{(Eq. 61)}$$

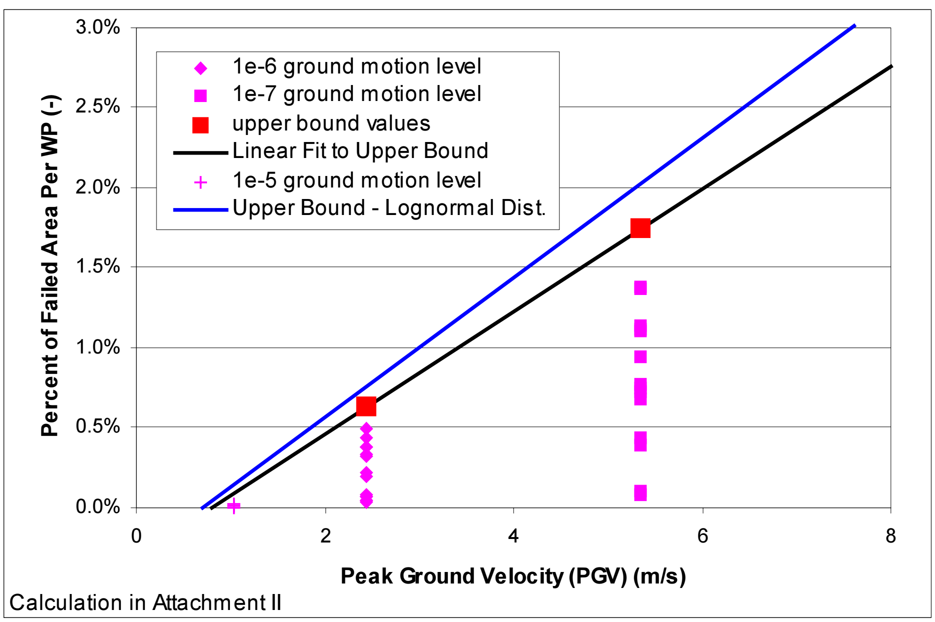
where D_{ub} = Bayesian upper bound of the uniform distribution of the percent of damaged area on the surface of the waste package at a given PGV. The MAX function ensures that the value of D_{ub} cannot be less than 0 percent. These calculations are documented in the *Seismic Consequence Abstraction* (BSC 2003 [DIRS 161812], Attachment II).

An independent technical review of this model abstraction as described by Equation 61 has been performed. The result of this review is presented in the *Seismic Consequence Abstraction* (BSC 2003 [DIRS 161812], Attachment III).

A comparison of a lognormal distribution at PGV of 2.44 m/s and 5.35 m/s with the uniform distribution represented in Equation 61 identifies values of D_{ub} (in the units of percent damaged area) where the uniform distribution is nonconservative with respect to the lognormal distribution, i.e. the uniform damage surface significantly underestimates exceedance probability for damage greater than 0.60 percent. However, this nonconservatism at higher damage values can be easily corrected by changing Equation 61 to slightly increase the linear upper bound for damage, D_{ub}. The nonconservatism can be eliminated if D_{ub} is defined as:

$$D_{ub} = 0.436(\text{PGV}) - 0.305 \quad \text{(Eq. 62)}$$

instead of using Equation 61. D_{ub} has the units of percent damage, so that a PGV of 5.35 m/s results in damage of 2.0 percent. Details of the comparison between the lognormal distribution and the uniform distribution are presented in Figure 19 of this report from the *Seismic Consequence Abstraction* (BSC 2003 [DIRS 161812], Attachment II, Figure II-5) which compares the modified upper bound for the lognormal fit to the original upper bound for the uniform distribution.



Source: BSC 2003 [DIRS 161812], Attachment II, Figure II-5

Figure 19. Comparison of Upper Bounds Based on a Lognormal Distribution (Blue Curve) with the Bayesian Upper Bound

Until additional structural response calculations are available at PGV values below 2.44 m/s and above 5.35 m/s, it is prudent to choose the more conservative fit (Equation 62) for the upper bound of the uniform distribution for waste package damage for TSPA-LA.

The damage to the waste package is applied to all waste packages in the repository, except for those packages that experience a juvenile failure. There is no spatial variability for damage to the waste package.

6.3.16.2 Failed Area Abstraction For The Drip Shield

Vibratory ground motion has the potential to damage the drip shield as a barrier to flow. This damage may occur due to the mechanical response of the drip shield to impacts from the waste package, emplacement pallet or invert. Damage may also occur due to the mechanical response of the drip shield to impacts from rock blocks or rockfall that are induced by the ground motions. In addition to damage caused by impact, it is also possible that adjacent drip shields will be separated during a high amplitude ground motion. Separated drip shields could allow seepage to fall directly on a waste package(s), and therefore have the same effect as damage caused by impact. Note that both mechanisms (damage due to impact and separation) have been observed in the structural response calculations for ground motions at the 10^{-6} per year and 10^{-7} per year levels.

Vibratory ground motions have the potential to eject large rock blocks in the nonlithophysal zone. The mechanical response of the drip shield to impact by a large rock block has the potential to damage the drip shield as a barrier to flow. This damage could also occur because of separation between two adjacent drip shields from vibratory ground motions. Development of an abstraction for damage to the drip shield due to rockfall induced by vibratory ground motion in the nonlithophysal zone involves the steps described in Figure 20.

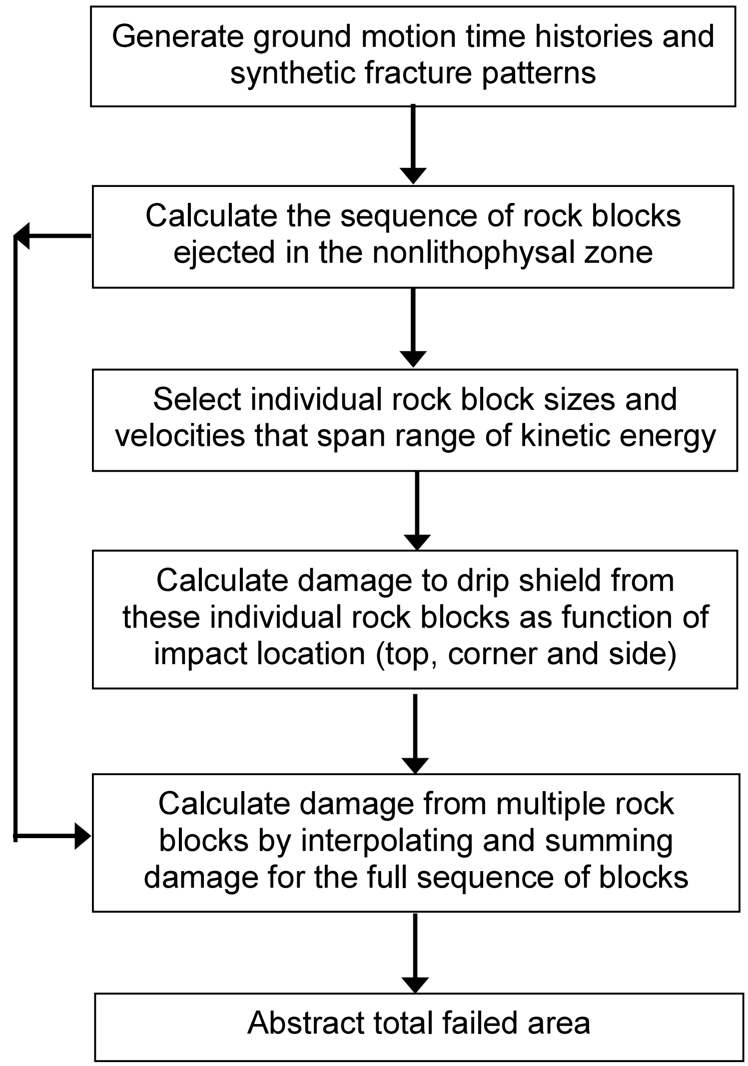


Figure 20. Flow Chart of the Drip Shield Damage Abstraction Methodology

Using the catalog of damage results for individual rock blocks in *Seismic Consequence Abstraction* (BSC 2003 [DIRS 161812], Table 12), the failed areas for multi-block rockfalls at the 10^{-6} per year and 10^{-7} per year ground motion levels are calculated by interpolation and are shown in Table 25 (BSC 2003 [DIRS 161812], Table 13).

Table 25. Statistics for Damaged Area From Multiple Rockfalls on the Drip Shield at 10^{-6} and 10^{-7} Annual Exceedance Frequencies

	Failed Area at the 10^{-6} Level (%)	**Failed Area at the 10^{-7} Level (%)**
Mean	1.698	3.405
Median	0.049	0.941
Standard Deviation	5.165	9.322
Minimum	0	0
Maximum	32.245	63.568

Note that the spread in the failed area reflects: (a) the uncertainty associated with the ground motion time histories corresponding to a given annual exceedance probability, and (b) the geologic uncertainty regarding the exact configuration of the fracture system near the emplacement drifts. This uncertainty is represented in the rockfall calculations through the synthetic fracture pattern.

6.3.16.3 Damage Abstraction for Multiple Drip Shields

The rockfall calculations in the nonlithophysal zone are based on a tunnel length segment of 25 meters (BSC 2003 [DIRS 162711], Section 6.3.1). Since the length of an individual drip shield is 5805 mm (BSC 2003 [DIRS 165304], Table 1), the damage from multiple block impacts will be shared between 25/5.805 = 4.31 drip shields, rather than being applied to a single drip shield. Note that the overlap between adjacent drip shields is ignored in this calculation because it is a relatively small length compared to the overall length of the drip shield. Given the presence of multiple drip shields, it is necessary where appropriate to modify the damage abstraction developed in *Seismic Consequence Abstraction* (BSC 2003 [DIRS 161812], Section 6.6.1) to account for the presence of multiple drip shields. This modification results in the following equations representing the fraction of cases with no damage and the fraction of cases with damage, respectively:

A power law fit to the fraction of cases with no damage is given by:

$$F = \text{MIN}(1.0, 0.601 * (PGV)^{-0.735}) \quad \text{(Eq. 63)}$$

where F is the fraction of rockfall cases without failure. The MIN function ensures that the value of F cannot be greater than 1.0.

This power law fit to the fraction of cases with no damage (Equation 63) is unchanged by the effective number of drip shields exposed to the rock fall. The percentage of the DS failed surface area is given by a log-triangular distribution modified because the damage is distributed among 4 to 5 drip shields (BSC 2003 [DIRS 161812], Section 6.6.1),

$$M = (0.0088/4.31) \times (PGV)^{3.7767} \quad \text{(Eq. 64)}$$

$$M = 0.00204 \times (PGV)^{3.7767} \quad \text{(Eq. 65)}$$

will represent the mode of the log triangular distribution for the damage to each drip shield in the nonlithophysal zones. The fixed upper and lower bounds of the log-triangular distribution, 0.001 and 100 percent, are not being changed because these bounds are limiting values.

6.4 CONSIDERATION OF ALTERNATIVE CONCEPTUAL MODELS

The Technical Work Plan (TWP) for this activity (BSC 2002 [DIRS 161132], Attachment B, Section B6.4) states:

> "The Integrated Waste Package Degradation Model is an abstraction model of models developed in supporting documents. Alternative conceptual models were considered, as appropriate, during the model development activities in the supporting documents. On this basis, alternative conceptual models for the features, events, and processes represented in the Integrated Waste Package Degradation Model will have been appropriately considered before implementation within the Integrated Waste Package Degradation Model. Therefore, no further consideration of alternative conceptual models will be performed within the *Waste Package and Drip Shield Degradation*, ANL-EBS-PA-000001."

Therefore no further consideration of alternative conceptual models will be performed within this report.

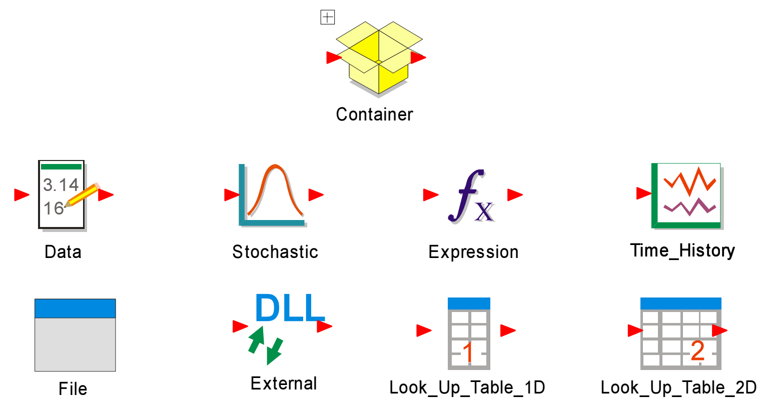
6.5 MODEL FORMULATION FOR THE BASE-CASE MODEL

The IWPD Model makes use of several software packages. These are listed in Section 3. The WAPDEG software is a dynamic-link library (DLL), which is responsible for modeling the variability in WP degradation. The GoldSim software is used to pass input to the WAPDEG software and is responsible for treating the uncertainty in the WAPDEG inputs. The GoldSim software also calls several other DLLs that are used to model uncertainty in various inputs to the WAPDEG software. These include the SCCD DLL, for the treatment of uncertainty in stress and stress intensity factor profiles, and the CWD DLL, for the treatment of uncertainty in the number and size of closure lid weld (manufacturing) defects. Throughout this section, reference will be made to various parts of the GoldSim model file as well as to the various input files, parameters, and parameter distributions used in waste package degradation modeling.

6.5.1 GoldSim Implementation Overview

In this section, a brief overview of a GoldSim model file that calls the WAPDEG software is presented. A more detailed description of the GoldSim software can be found in *GoldSim Graphical Simulation Environment: User's Guide* (GoldSim Technology Group 2002 [DIRS 160643]). GoldSim is a graphical simulation environment, used in this technical product to prepare an input file for the WAPDEG software. A typical GoldSim model simulation run contains multiple realizations. Each realization is equally likely, and represents one particular sampling of the uncertain parameters. A multiple realization simulation is run in distributed processing mode, with a master computer directing tens of slave processors. The details of GoldSim's distributed processing mode can be found in *GoldSim Distributed Processing Module: User's Guide* (GoldSim Technology Group 2002 [DIRS 160578]).

The GoldSim graphical elements used to develop an input data set for the WAPDEG software are illustrated in Figure 21.

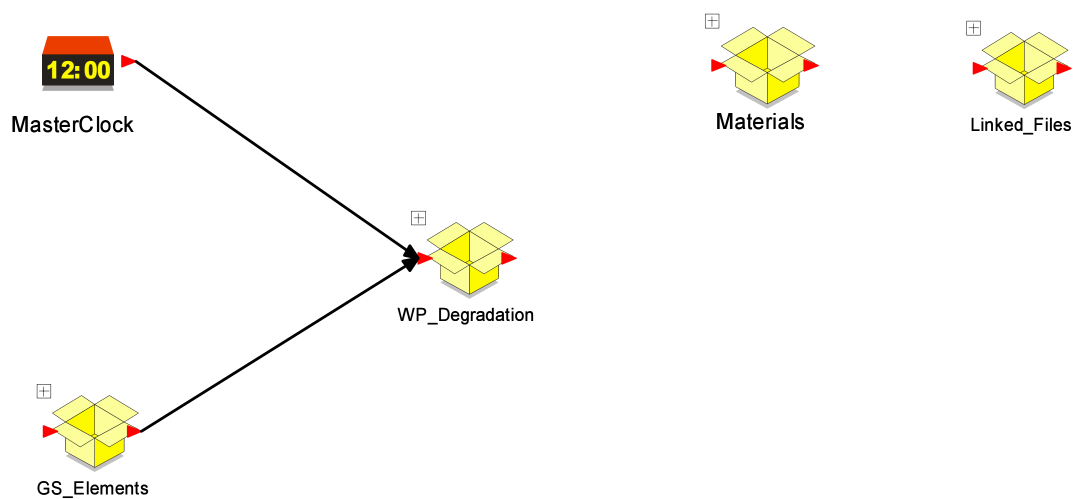


Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 21. Graphical Elements Used in the GoldSim Software.

Container elements are similar to subdirectories on a hard disk in that other graphical elements reside within them. Data elements are fixed values (or vectors of values). Stochastic elements define distributions, which are typically sampled once per realization. Expression elements are used to evaluate expressions (e.g., to multiply a data element by a stochastic value). Time_History elements are used to graph results (e.g., the contents of a Look_Up_Table_1D element). File elements contain the file names that will be passed to each processor used for the simulation runs. The corresponding files must be present in the master directory. External elements are used to call external dynamic link libraries (DLLs), such as the WAPDEG software. Look_Up_Table_1D and Look_Up_Table_2D elements are typically used to store tables of input values or output values associated with external elements.

A schematic of a portion of the GoldSim model file, which calls the WAPDEG software, is shown in Figure 22.



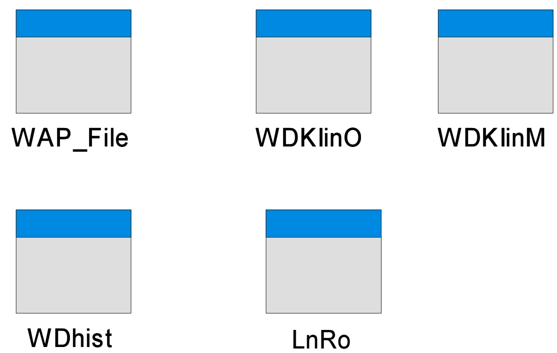
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 22. GoldSim Model File Calling the WAPDEG Software

Figure 22 is a screen capture of the top-level view of the GoldSim model file used in this analysis. The MasterClock is a built-in GoldSim element, which contains GoldSim-specific input parameters. The only GoldSim-specific parameters that impact the model results are the random seed used and the number of realizations.

The Materials container element is a built-in GoldSim element, which is not used in this analysis.

The contents of the Linked_Files container element are shown in Figure 23.

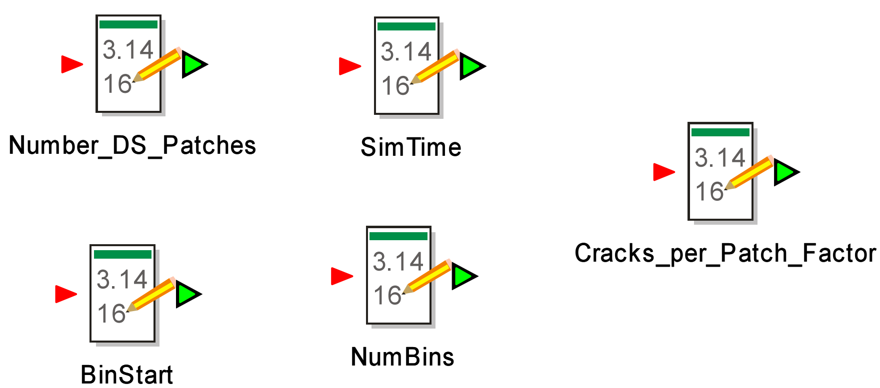


Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 23. Contents of the Linked_Files Container Element.

The file elements within the Linked_Files container element are linked to file names to be passed to slave processors. For instance the WAP_File element is linked to the file "WD4DLL.WAP", a required file for the execution of the WAPDEG software.

The contents of the GS_Elements container element are shown in Figure 24. These elements contain global parameters, that are defined within the GoldSim model, but which are used by the WAPDEG software.



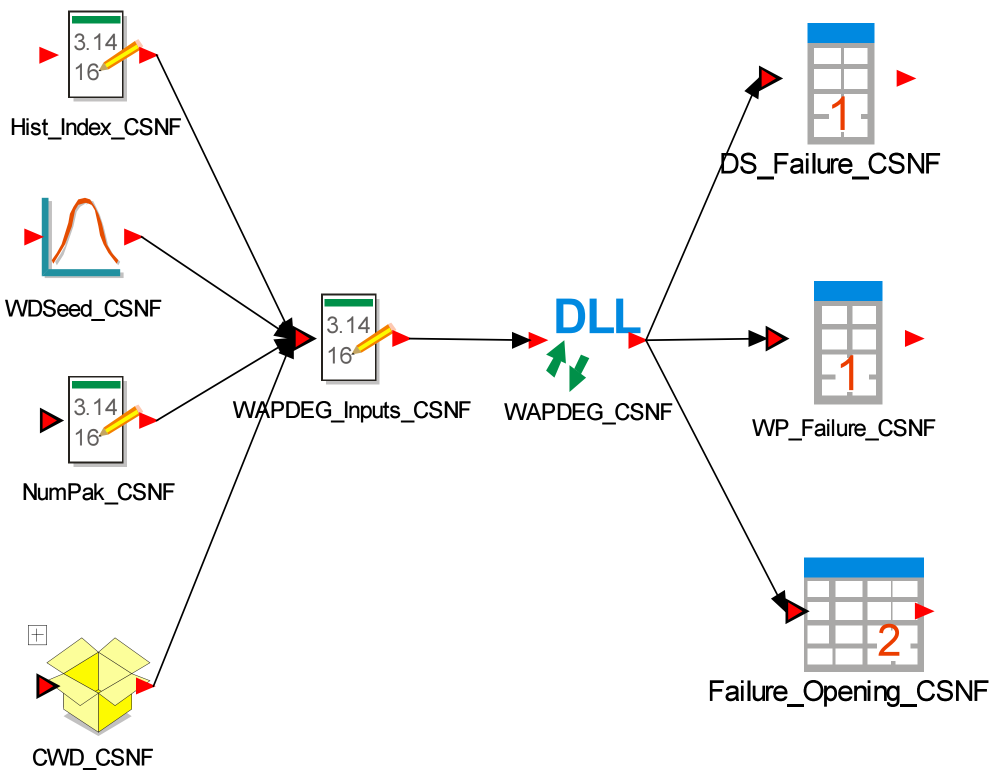
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 24. Contents of the GS_Elements Container Element.

The contents of the WP_Degradation container element will be discussed later in this document, in relation to specific degradation modes.

6.5.2 WAPDEG-GoldSim Interface Overview

GoldSim interacts with the WAPDEG DLL through an external element. The TSPA-LA model file will typically call the WAPDEG DLL several times per GoldSim realization. The exact number of calls will depend on the scenario class being run. A graphical representation of the interface between the GoldSim software and the WAPDEG DLL is shown in Figure 25, for simulation of CSNF WP degradation (the interface and input for CDSP WP degradation are almost identical to those for CSNF WP degradation, differences will be mentioned when appropriate throughout this section).



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 25. Interface Between the GoldSim Software and the WAPDEG DLL for CSNF Waste Packages (these are the contents of the IWPD_CSNF Container Element as depicted in Figure 26).

At each call, the WAPDEG DLL, represented by the external element WAPDEG_CSNF, is passed a vector of 2000 real numbers, via a vector data element, WAPDEG_Inputs_CSNF. The values in the WAPDEG input vector specify degradation models and degradation model parameters.

The contents of the WAPDEG input vector are reproduced in Attachment I (Table I-1) and will be discussed in more detail in the following sections. All values in the WAPDEG input vector are real numbers. Those that do not change, and are not defined by TSPA-LA model components, are explicitly stated. The rest are represented by variable names, defined in the TSPA-LA model itself. Certain parameters in the WAPDEG input vector reproduced in Attachment I (Table I-1) depend on the WP configuration (CSNF or CDSP) being simulated. The values for the CSNF WP configuration are shown first, with the corresponding CDSP WP configuration value given afterwards in brackets.

Since only real numbers are passed between GoldSim and the WAPDEG DLL, and since some of the degradation model parameters are represented by distributions and tables, stored in text files, an additional communication mechanism is needed. GoldSim and WAPDEG share a "file index" file, WD4DLL.WAP. The contents of this file, for a typical TSPA-LA model file, are listed in Table 26. Note that the line numbers and the column headings in Table 26 are not part of the WD4DLL.WAP file, but are included for clarity.

Table 26. Contents of WD4DLL.WAP File.

Line	File Name
1	WDenv_00_07wheader.ou
2	WDenv_00wh.ou
3	EMPTY
4	WDKlinO.fil
5	WDKlinM.fil
6	WDKISCCO.fil
7	WDStressO.fil
8	WDKISCCM.fil
9	WDStressM.fil
10	WDCWDNDO_CSNF.cdf
11	WDCWDSizeO_CSNF.cdf
12	WDCWDNDM_CSNF.cdf
13	WDCWDSizeM_CSNF.cdf
14	WDCWDNDO_CDSP.cdf
15	WDCWDSizeO_CDSP.cdf
16	WDCWDNDM_CDSP.cdf
17	WDCWDSizeM_CDSP.cdf
18	WDlnRGC.cdf

Using the WD4DLL.WAP file, GoldSim and WAPDEG can share file indices (line numbers in the WD4DLL.WAP file) in place of actual file names. The 2000 real numbers and the contents of the files identified in the WD4DLL.WAP file are the only inputs to the WAPDEG DLL.

In the TSPA-LA model, the drip shield and waste package degradation processes are discretized at the spatial bin/fuel type level. The repository is divided into five spatially defined bins. Each bin contains a different number of waste packages and is subject to different environment conditions. There are potentially two different major types of waste package configurations, designated as Commercial Spent Nuclear Fuel (CSNF) and Co-Disposal (CDSP) waste packages.

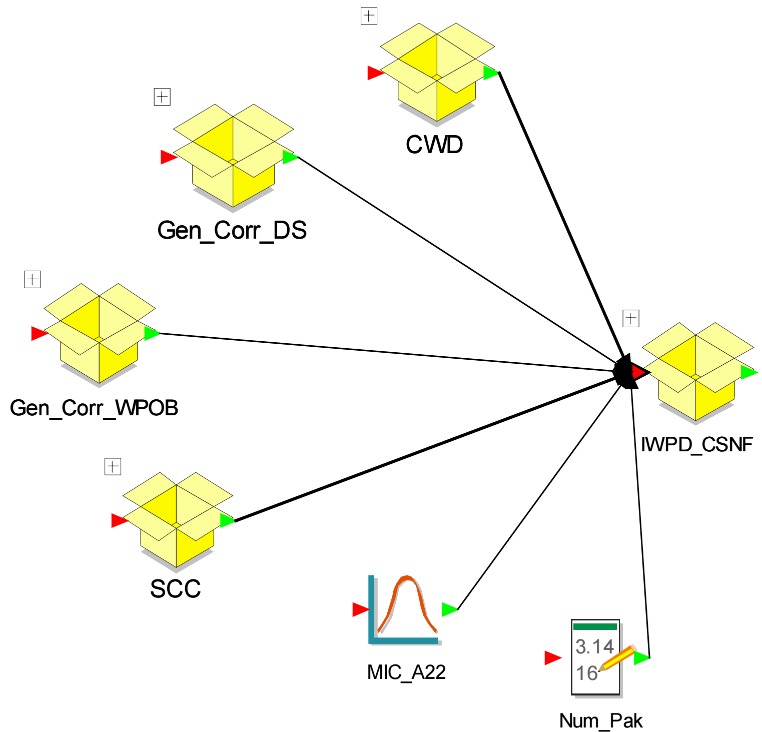
Figure 25 shows four input links to the WAPDEG_Inputs_CSNF vector. These are all a function of the fuel type and/or history and environment variables. The data element, NumPak_CSNF, defines the number of CSNF waste packages in the bin. The data element, Hist_Index_CSNF, contains the file index linking the file containing the WP thermal histories to a line number and file name in the WD4DLL.WAP file. WDSeed_CSNF is a stochastic element characterized by a uniform distribution between 1 and 2^{31}-1 (the maximum positive 32-bit integer). WDSeed_CSNF is used to generate a different integer for each WAPDEG DLL call, to seed the random number generator within the WAPDEG software. The container element, CWD_CSNF, holds some of the parameters required for the calculation of the weld flaw probability for the closure lids. The conceptual model for weld flaws is discussed in Section 6.3.8.2 and the WAPDEG implementation of this conceptual model is described in Section 6.5.8.

Figure 25 also illustrates the output produced by the WAPDEG DLL. There are two one-dimensional table elements and one two-dimensional table element linked to the WAPDEG_CSNF external element. The DS_Failure_CSNF element receives a one-dimensional table of drip shield first failure times. The WP_Failure_CSNF element receives a one-dimensional table of waste package first failure times. The waste package first failure time is defined to be the first penetration by any mechanism (patch, pit, crack) of the waste package inner layer. The format of both of these tables is similar; the first column containing the drip shield or waste package first failure times in years (sorted in increasing order) and the second column containing the cumulative fraction of drip shields or waste packages failed. The Failure_Opening_CSNF element receives a two dimensional table containing 33 columns. The number of rows is determined by the input parameter "NumBins". The column contents are explained in Table 27. Note that waste package failure (for the purposes of averaging) is defined as any penetration (patch, pit, or crack) of the waste package layer 2 (the modeled inner layer in Figure 3). If there are penetrations of layer 1 (the modeled outer layer in Figure 3) of a waste package, but no waste package failures (penetrations of layer 2), the corresponding average number of patch, pit, or crack failures being reported is set to zero.

Table 27. Column Contents of the Failure_Opening_CSNF Element.

Column Number	Contents
1	average number of patch failures (per failed drip shield) on the drip shield top
2	average number of pit failures (per failed drip shield) on the drip shield top
3	average number of crack failures (per failed drip shield) on the drip shield top
4	average number of patch failures (per failed drip shield) on the drip shield side
5	average number of pit failures (per failed drip shield) on the drip shield side
6	average number of crack failures (per failed drip shield) on the drip shield side
7	the cumulative fraction of first patch failures on the drip shield (top and side)
8	the cumulative fraction of first pit failures on the drip shield (top and side)
9	the cumulative fraction of first crack failures on the drip shield (top and side)
10	average number of patch failures (per failed waste package) on the waste package layer 1 top
11	average number of pit failures (per failed waste package) on the waste package layer 1 top
12	average number of crack failures (per failed waste package) on the waste package layer 1 top
13	average number of patch failures (per failed waste package) on the waste package layer 1 side
14	average number of pit failures (per failed waste package) on the waste package layer 1 side
15	average number of crack failures (per failed waste package) on the waste package layer 1 side
16	average number of patch failures (per failed waste package) on the waste package layer 1 bottom
17	average number of pit failures (per failed waste package) on the waste package layer 1 bottom
18	average number of crack failures (per failed waste package) on the waste package layer 1 bottom
19	the cumulative fraction of first patch failures on the waste package layer 1 (top, side, and bottom)
20	the cumulative fraction of first pit failures on the waste package layer 1 (top, side, and bottom)
21	the cumulative fraction of first crack failures on the waste package layer 1 (top, side, and bottom)
22	average number of patch failures (per failed waste package) on the waste package layer 2 top
23	average number of pit failures (per failed waste package) on the waste package layer 2 top
24	average number of crack failures (per failed waste package) on the waste package layer 2 top
25	average number of patch failures (per failed waste package) on the waste package layer 2 side
26	average number of pit failures (per failed waste package) on the waste package layer 2 side
27	average number of crack failures (per failed waste package) on the waste package layer 2 side
28	average number of patch failures (per failed waste package) on the waste package layer 2 bottom
29	average number of pit failures (per failed waste package) on the waste package layer 2 bottom
30	average number of crack failures (per failed waste package) on the waste package layer 2 bottom
31	the cumulative fraction of first patch failures on the waste package layer 2 (top, side, and bottom)
32	the cumulative fraction of first pit failures on the waste package layer 2 (top, side, and bottom)
33	the cumulative fraction of first crack failures on the waste package layer 2 (top, side, and bottom)

There are additional input links to the WAPDEG_Inputs_CSNF vector. Some of these are in the global parameter container, GS_Elements, and were discussed in Section 6.5.1. The implementation of the conceptual models for degradation due to general corrosion of Alloy 22 and Titanium Grade 7, and for stress corrosion cracking (SCC) of Alloy 22 is done in separate container elements. These are shown in Figure 26 (WP_Degradation Container) and discussed in the following sections.



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 26. Other Input Links to IWPD_CSNF (contents of the WP_Degradation Container).

6.5.3 Number of Patches and Number Waste Package-Drip Shields Design Input

The drip shield plate thickness is used directly in the input to the WAPDEG DLL (see line 40 of Table I-1). The WAPDEG software does not require the DS surface area, only the number of DS patches need be specified. Since the variation in the general corrosion rate of the DS is considered to be due only to uncertainty (Section 6.3.3), each DS is modeled by one patch (see line 52 of Table I-1).

In Section 6.3.2 the CSNF and CDSP waste package (WP) surface areas and patch sizes were calculated. The number of WP patches was determined to be 1014 for CSNF WPs and 1106 for CDSP WPs (Section 6.3.2). This data is entered on line 29 of Table I-1.

Note that since the WAPDEG software calculates the number of patches by dividing the surface area entered by the patch area entered, the “number of patches data” for both the DS and the WP is actually entered as a surface area and the patch area is entered with the value "1" (see lines 32 to 36 and lines 54 to 58 of Table I-1).

The drip shield and waste container surface areas are also divided into fractions. The drip shield has a top and side fraction. The top fraction is defined in line 53 of the WAPDEG input vector. The waste package has a top, bottom and side fraction. The top fraction and bottom fraction are entered on lines 30 and 31, respectively, of the WAPDEG input vector. The fraction assigned to side patches is obtained by subtracting the data entered for the other fraction(s) from one. The fraction assigned to side patches of the waste container is identified with the closure lid region, for modeling purposes.

In the TSPA Model, the drip shield and waste package degradation processes are expected to be simulated at the spatial bin/fuel type level. The number of IWPD Model simulations per TSPA Model realization depends on the scenario class being run. The WAPDEG software runs twice for each of the five spatially fixed bins, once for the CSNF waste packages in that bin and once for CDSP waste packages. If the spatially fixed bin contains fewer than 500 DS/WP pairs, all CSNF and CDSP DS/WP pairs in the bin should be simulated. If the bin contains more than 500 DS/WP pairs, then only up to 500 CSNF and 500 CDSP DS/WP pairs should be simulated. The impact of this modeling assumption is analyzed by the sensitivity studies in Section 6.6.4.

6.5.4 Waste Package Design Input

As explained in Section 6.3.2, the dual Alloy 22 lid design for the waste package outer barrier (WPOB) requires that outer barrier be modeled as two layers. The outer modeled layer is 25 mm thick (the thickness of the outer closure lid) and the inner modeled layer is 10 mm thick (the thickness of the middle closure lid). The WAPDEG input vector defines these two layer thicknesses in lines 4 and 17 of the WAPDEG input vector (Table I-1).

In addition, each layer is modeled as being composed of two different regions, the closure lid region and the shell region. The closure lid thicknesses (both outer and middle) are the same for CSNF and CDSP waste packages, but the thickness of the shell region is different (20 mm for the CSNF WP, 25 mm for the CDSP WP). The WAPDEG software assigns a fraction of the total WP surface area to top and bottom surfaces. The side fraction is obtained by subtracting the sum of the top and bottom fractions from one. This area assignment, for the WPOB, is done in lines 30 and 31 of the WAPDEG input vector (Table I-1). The top and bottom area fractions are associated with the shell region and the side fraction is associated with the closure lid region. The fractions are not the same for both WP types. The area fraction assigned to "side" (closure lid) patches is calculated to be 0.032 (0.038 for CDSP WPs) in Section 6.3.2.1.

The two-layer implementation of the WPOB also requires that the general corrosion rate be adjusted. The general corrosion rate applied to the outer layer is set to a large value. The general corrosion rate applied to the inner layer is modified by the ratio of the inner to outer shell layer thicknesses. The effect of this adjustment to general corrosion rate is then removed, for the closure lid regions only. Thus the original general corrosion rate is applied to both closure lids. However, the outer layer shell region degrades immediately and the inner layer shell region degrades at the correct rate for the 20 mm (or 25 mm) WPOB barrier shell.

The implementation of the two-layer WPOB in the WAPDEG software is done in two places. First, the error term in the General Linear Model functional form, used to model general corrosion (BSC 2002 [DIRS 162606], Section 4.2.6.5), is changed. The second change is to modify the multipliers used in the SCC Slip Dissolution event used to model the SCC degradation (BSC 2002 [DIRS 162606], Section 4.2.7.5).

The functional form used for the General Linear Model (BSC 2002 [DIRS 162606], Section 4.2.6.5), in its most general form, is given by

$$D = \exp\left(c_0 + \sum_{j=1}^{N} c_j E_j + \varepsilon\right)\exp\left(-\frac{Q}{T}\right) t^n \qquad \text{(Eq. 66)}$$

where

D = corrosion depth (mm)
N = number of terms
c_0 = constant
c_j = the j^{th} coefficient
E_j = the j^{th} exposure condition
ε = error term
Q = activation energy
T = temperature (K)
n = time exponent

The General Linear Model (GLM) functional form is used by the WAPDEG software to implement the general corrosion conceptual model. The general form defined by Equation 66 includes a constant term, N terms that depend on exposure conditions, as well as an error term, ε. The abstracted general corrosion model presented in Equations 23 through 26 (Section 6.3.4) does not require the full generality of Equation 66. The particular form used in the TSPA-LA model implementation involves a constant term, the activation energy term, and the error term. This implementation is discussed in more detail in Section 6.5.7. The discussion in this section is limited to an explanation of how the error term, ε, is used to implement the two-layer WPOB model. Note that the error term is an implementation feature, not a part of the conceptual model.

The outer layer error term is set to the natural log of 10^{14} in lines 111 to 115 and lines 210 to 214 of the WAPDEG input vector. The error term that applies to the inner layer is set to the natural log of the ratio of 10 to 20 (or the natural log of the ratio of 10 to 25 for CDSP WPs). The inner layer error term is defined in lines 150 to 154 and lines 249 to 253 of the WAPDEG input vector.

Inspection of the functional form in Equation 66 shows that setting the error term, ε, to a large value effectively causes instantaneous degradation of the outer layer. Using the error term for the inner layer to modify the corrosion rate by the ratio of thicknesses causes the inner layer to degrade at the correct rate for the WPOB shell region.

The closure lid region SCC degradation is modeled in the WAPDEG input vector using a SCC Slip Dissolution event (BSC 2002 [DIRS 162606], Section 4.2.7.5). As noted above, the closure lid region of the waste package is identified with the side fraction of the surface area. To maintain the original general corrosion rate in the closure lid region, the effect of the multipliers (imposed by adjusting the error term) is removed in the closure lid region only (i.e. for side patches only).

The input data for the Slip Dissolution event is contained in lines 331 to 408 of Table I-1, for the outer layer. Examination of lines 337 to 339 of Table I-1 shows that only side patches are impacted by this event data. Examination of line 395 to 406 shows that one of the event effects is to accelerate the general corrosion rate by a factor of 1.00E-14, which cancels the large multiplier on the general corrosion rate for the closure lid region (side patches).

The input data for the Slip Dissolution event for the inner layer is contained in lines 409 to 486 of Table I-1, for the inner layer. Examination of lines 415 to 417 shows that only side patches are impacted by this event data. Examination of line 473 to 484 shows that one of the event effects is to accelerate the general corrosion rate by a factor of 20/10 = 2 (or 25/10 = 2.5 for CDSP WPs) This cancels the previously added multiplier on the general corrosion rate.

6.5.5 Waste Package and Drip Shield Exposure Conditions Implementation

The exposure condition inputs to the IWPD Model analysis are derived from an abstraction of temperature and relative humidity behavior that gives parameterized inputs for waste package and drip shield exposure conditions. For a description of the algorithm used to develop the exposure conditions file, refer to Section 6.3.13.

Eight different thermal hydrologic histories were created and combined in one exposure file (WDenv_00_07wheader.ou), to use in the IWPD Model simulations documented in this report. Each thermal hydrologic history is considered to represent the behavior of 1/8 (0.125) of the drip shields and waste packages simulated. The format of the thermal hydrology input file conforms to the WAPDEG Table Format (BSC 2002 [DIRS 162606], Section 4.2.4). The first few lines of the first and second set of exposure histories are shown below

```
! 1st comment line
! 2nd comment line
! 3rd comment line
#  8  5
#  181
#  0.125
!           t           wpT         wpRH        dsT           dsRH
            1            96     0.577473          96      0.577473
         69.9            96     0.577473          96      0.577473
           70           160    0.2017962         160     0.2017962
     74.40632      139.4507    0.2724015    139.4507     0.2724015
        .             .            .            .             .
        .             .            .            .             .
        .             .            .            .             .
#  181
#  0.125
!           t           wpT         wpRH        dsT           dsRH
            1            96    0.6144519          96     0.6144519
         69.9            96    0.6144519          96     0.6144519
          70            160    0.100933          160     0.100933
     74.40632      139.4507    0.1401267    139.4507     0.1401267
        .             .            .            .             .
        .             .            .            .             .
```

. . . . .

The first 3 lines in the example file (beginning with exclamation points) are comment lines. The user can enter as many comment lines as desired. The WAPDEG software ignores these lines. The user can enter comments designed to enhance traceability and uniquely identify the exposure history file. The next line (# 8 5) is a header line which indicates that the exposure history file contains 8 exposure histories each with 5 columns. The next line (# 181) is a header line which indicates that the first exposure history contains 181 rows of exposure data. This is followed by (# 0.125) a header line containing the fraction of waste packages to which the exposure history applies (1/8 in this case). The next line again begins with an exclamation point and is a comment line, typically used for column labels. Only one comment line is allowed in this position. The header lines are followed by exposure data, typically consisting of the time, temperature, and relative humidity on the drip shield and waste container surfaces. The next exposure history is preceded by two header lines indicating that it consists of 181 rows and applies to 1/8 of the drip shield waste package pairs.

The WAPDEG input vector (see line 67 of Table I-1) specifies the file index corresponding to the exposure conditions file to be used. In the TSPA-LA model, the exposure conditions will vary with spatial bin and fuel type.

Water conditions (BSC 2002 [DIRS 162606], Section 3.2.3, 4.2.5.6, 4.2.5.7, and 4.2.5.8) are the mechanism used in the WAPDEG software to apply corrosion processes to the waste container barriers. The IWPD Model defines two water conditions, associated with environments expected in the repository. The first, identified by the numerical label "1", corresponds to the environment under the drip shield and is referred to as the "DSInside" water condition. The second, identified by the numerical label "2", corresponds to the environment above the drip shield and is referred to as the "DSOutside" water condition.

The water condition that applies to the outer (top) surface of the drip shield is defined in the drip sequence data. A drip sequence (BSC 2002 [DIRS 162606], Section 3.2.2 and 4.2.5.6) is made up of one or more phases, where each phase lasts a specified length of time and is characterized by a constant water contact condition. In the TSPA-LA model, only one drip sequence, with one phase, is defined. Lines 68 to 85 of the WAPDEG input vector in Table I-1 define the drip sequence. The water condition number corresponding to this drip sequence is "2" ("DSOutside" water). The drip sequence initially applies to all patches (top and side) on the outer (top) surface of the drip shield. When a drip shield patch penetrates, the drip sequence water condition is transferred to the patches of the underlying WPOB. Since the DS is modeled with only one patch, when the DS fails, all patches of the outer layer of the underlying waste package become subject to the drip sequence water condition ("DSOutside" water).

The water condition that applies to the inner (bottom) surface of the drip shield is defined by the "Drip Shield Initial Water Condition" (BSC 2002 [DIRS 162606], Section 4.2.5.4). For the TSPA-LA model, the water condition in effect for the drip shield inner (bottom) surface is specified in line 65 of the WAPDEG input vector to be condition "1" ("DSInside" water condition).

6.5.6 Drip Shield General Corrosion Abstraction Model Implementation

General corrosion is the only drip shield (DS) degradation process modeled by the WAPDEG software (Section 6.3.4). General corrosion is modeled separately for the DS outer (top) and inner (bottom) surfaces. Two cumulative distribution functions (CDFs) were developed for general corrosion of Titanium Grade 7 (Section 4.1.2), one applicable to the inner surface of the DS (Table 4) and one for the outer surface (Table 5). These CDFs are reproduced in the stochastic elements WDDSOInGC and WDDSOutGC, which are inputs to the WAPDEG DLL (see Figure 27).

Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 27. Contents of the Gen_Corr_DS Container Element

The general corrosion of Titanium Grade 7 is modeled in the WAPDEG software using the Power Law functional form (BSC 2002 [DIRS 162606], Section 4.2.6.6). The Power Law functional form has the general representation

$$D = B\,t^{n} \qquad \text{(Eq. 67)}$$

where

D = corrosion depth (mm)
t = time (yr)
n = time exponent

Values for B are obtained by fitting experimental data. In the current implementation, the time exponent is one.

In the WAPDEG software, every general corrosion functional form is associated with a single water condition and barrier. Therefore, two implementations of the Power Law functional form are required to define the two possible states of Titanium Grade 7 general corrosion.

The Power Law functional form data is defined in the WAPDEG input vector in lines 165 to 185 ("DSInside" water) and lines 264 to 284 ("DSOutside" water). The B term in Equation 67 is input to the WAPDEG software as a sampled value from the stochastic WDDSInGC, for the DS inner surface and as a sampled value from the stochastic WDDSOutGC, for the DS outer surface.

The exponent, n, of the time term, t, in Equation 67 is set to one (see lines 180 to 184 and lines 279 to 283).

Note that the "inside-out" corrosion of the DS proceeds with the water condition defined by the "Drip Shield Initial Water Condition". The water condition defined on line 288 applies only to "inside-out" corrosion of the WPOB layers (BSC 2002 [DIRS 162606], Section 4.2.5.4 and Section 4.2.5.10).

Uncertainty in the general corrosion of titanium is captured by the two stochastics WDDSOutGC and WDDSInGC. These stochastics are sampled once for every TSPA-LA realization and apply to all drip shields.

6.5.7 Waste Package Outer Barrier General Corrosion Abstraction Model Implementation

The conceptual model for general corrosion of the WPOB is presented in Equations 23 through 26 (Section 6.3.4). The rate of general corrosion of the Alloy 22 waste package outer barrier is expected to be a function of exposure temperature, with the temperature dependence following an Arrhenius relationship (see Section 6.3.4, Equation 23).

The conceptual model for general corrosion of Alloy 22 is implemented by the WAPDEG software using the General Linear Model (GLM) functional form (BSC 2002 [DIRS 162606], Section 4.2.6.5). The most general form of the GLM is given by Equation 66 (Section 6.5.4). The specific form used for the TSPA-LA model implementation of the Alloy 22 corrosion rate is

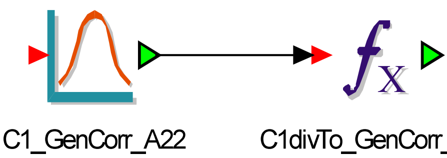
$$D = \exp\left(\ln(R_0) + \frac{C_1}{333.15} + \varepsilon\right)\exp\left(-\frac{C_1}{T}\right)\ t^n \qquad \text{(Eq. 68)}$$

where D is corrosion depth (mm), t is time (yr), and T is exposure temperature (K). This implementation involves a constant term ($\ln(R_o) + C_1/333.15$), the activation energy (C_1), and an error term, ε. The constant term has two components, $\ln(R_o)$ and $C_1/333.15$. $\ln(R_o)$ is sampled from the (natural logarithm of the) general corrosion rate distribution obtained from the 5-year crevice geometry samples. C_1 is sampled from a distribution determined by fitting the short-term polarization resistance data for Alloy 22 to the Arrhenius relation. The derivation of these two parameters is described in more detail in Section 6.3.4. The constant, 333.15 in the denominator of the second term is related to the temperature at which the experimental data was collected (Section 4.1.3.1). The error term, ε, is used to adjust the corrosion rate for the dual lid design. This adjustment is required because the lids and outer shell are of different thicknesses. Note that the error term is an implementation feature, not a part of the conceptual model.

In the WAPDEG software, every general corrosion functional form is associated with a single water condition and barrier. Both “DSInside” and “DSOutside” water conditions can potentially contact the waste package outer barrier. However, the WPOB general corrosion conceptual model (Section 6.3.4) concludes that the same general corrosion rate model should be applied to all surfaces of the waste package outer barrier. Therefore, four almost identical implementations of the GLM functional form are defined, one for each combination of layer and water condition. These four definitions differ only in the error term data.

The GLM functional form data is defined in the WAPDEG input vector in lines 90 to 125 (WPOB outer layer, “DSInside” water), lines 129 to 164 (WPOB inner layer, “DSInside” water), lines 189 to 224 (WPOB outer layer, “DSOutside” water), and lines 228 to 263 (WPOB inner layer, “DSOutside” water). Since the same general corrosion model applies to both layers and water conditions, these data sections contain essentially the same information. Therefore only the first (lines 90 to 125) will be discussed in detail.

The first two terms of the GLM specification are defined in lines 100 to 104 (ln(R_o) and lines 105 to 110 (C_1/ 333.15), respectively. The ln(R_o) term in Equation 68 is input to the WAPDEG software as a CDF. Line 101 of the WAPDEG input vector specifies the file index for this CDF (line 18 in Table 26). The C_1 term, is given by a normal distribution with mean of 3116.47 and a standard deviation of 296.47 truncated at ± 3 standard deviations (see Table 7). This normal distribution is defined in the stochastic element C1_GenCorr_A22 (see lines 116 to 120). The related term, C_1/333.15, is given by the expression element, C1divTo_GenCorr_A22 (see Figure 28). The exponent, n, of the time term, t, in Equation 68 is one (see lines 121 to 125). The function of the error term, ε, is explained in Section 6.5.4.



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 28. Contents of the Gen_Corr_WPOB Container Element

Uncertainty in the general corrosion of Alloy 22 is captured by the stochastic C1_GenCorr_A22. This stochastic is sampled once for every TSPA-LA realization and applies to all WPOB layers.

Variability in the general corrosion of Alloy 22 is represented by the implementation of the ln(R_0) CDF. The barrier variance sharing for the CDF is set to zero (lines 95 to 99). The CDF is therefore sampled once for every patch of each WPOB. Each patch on the WPOB surface will have a different corrosion rate. This captures the variation in the general corrosion rate over the waste package surface.

Variability in the general corrosion of Alloy 22 is also expressed in Equation 68 through the exposure temperature variable, which varies spatially and temporally, according to the thermal hydrologic history files.

6.5.8 Manufacturing Defect Abstraction Model Implementation

Weld flaws in waste package closure lid welds are the only manufacturing defects identified as having the potential to affect waste package performance (Section 6.3.12). The weld flaws in the closure lid welds are likely sites for stress corrosion cracking (SCC), and are therefore modeled as part of the IWPD Model SCC analysis (Section 6.3.8.2).

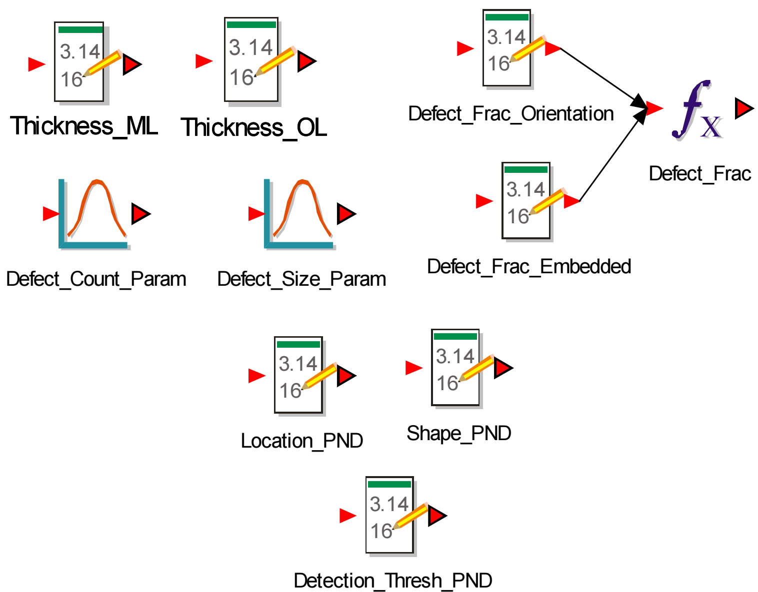
Stress corrosion cracking (SCC) is modeled in the WAPDEG software by the use of a SCC Slip Dissolution event (BSC 2002 [DIRS 162606], Section 3.3.2.1.1 and Section 4.2.7.5). The SCC Slip Dissolution event will be described in more detail in Section 6.5.10. When a SCC Slip Dissolution event includes defect (weld) flaws, the defect flaw density and size distribution are defined by a Manufacturing Defects event (BSC 2002 [DIRS 162606], Section 3.3.2.1 and Section 4.2.7.2).

In the WAPDEG software, a corrosion-affecting event can apply to one barrier and one or more water conditions and can have effects specific to that event, as well as generic effects. The

Manufacturing Defects event has only one specific effect, to introduce manufacturing defects onto patches.

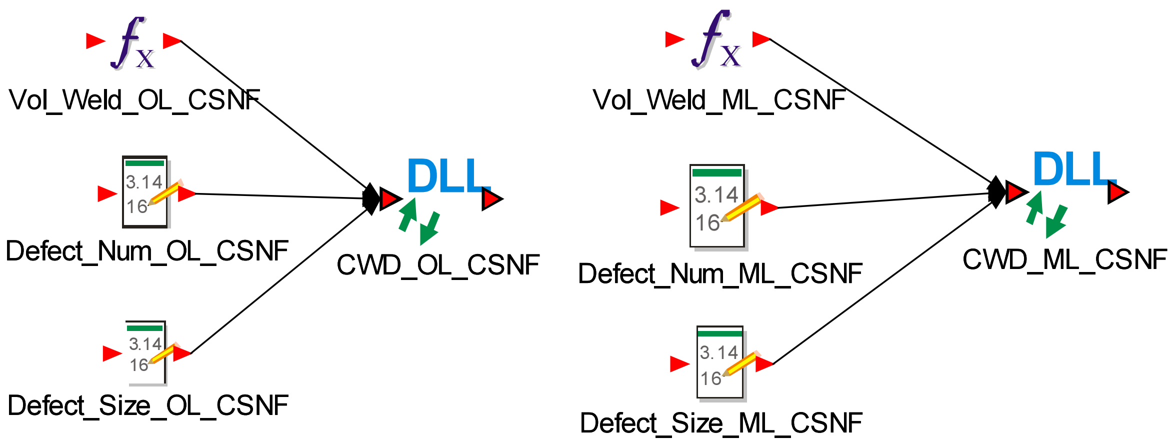
A separate Manufacturing Defects event must be defined for the outer and middle closure lids. The closure lids can potentially be subject to both exposure conditions, therefore both water conditions ("DSInside" and "DSOutside" water) are defined. Two Manufacturing Defect events are defined for the TSPA-LA model in lines 291 to 310 (outer closure lid) and lines 311 to 331 (middle closure lid) of the WAPDEG input vector (Table I-1). The inputs to the Manufacturing Defects event consist of a probability that a barrier has manufacturing defects, a distribution for the number of manufacturing defects per barrier (defect density), and a defect size distribution.

In the TSPA-LA model, the defect probability, and the defect density and size distributions are calculated by the CWD DLL (see Figure 25 and Figure 26).



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 29. Contents of the CWD Container Element (Global CWD DLL Inputs)



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 30. Contents of the CWD_CSNF Container Element

The CWD software computes the cumulative probability of a manufacturing defect based on the probability for the non-detection of weld defects. Inputs to this calculation are the weld thickness, the weld volume, the defect fraction considered, a detection threshold, a characteristic flaw size, a shape factor, a defect count parameter, and a defect size parameter. The details of this calculation are given in Section 6.3.8.2.

The global input parameters to the CWD DLL software are held in the container element CWD (see Figure 29). The weld thickness is given by the data elements Thickness_OL and Thickness_ML (for the outer and middle closure lids). The defect fraction considered is calculated in the expression element, Defect_Frac, as the product of the fraction of defects capable of propagation based on orientation (Defect_Frac_Orientation) and the fraction of embedded manufacturing defect flaws to propagate (Defect_Frac_Embedded). The detection threshold is defined in the data element Detection_Thresh_PND. The characteristic flaw size and shape factor are defined in the data elements Location_PND and Shape_PND, respectively. The defect count parameter is given by a gamma distribution defined in the stochastic element Defect_Count_Param. The defect size parameter is given by a gamma distribution defined in the stochastic element Defect_Size_Param. The values of all of these parameters are taken from Table 9.

The local input parameters to the CWD DLL are held in the container CWD_CSNF (CWD_CDSP). The contents of the CWD_CSNF container element are shown in Figure 30. The input parameter, weld volume (Vol_Weld_OL_CSNF and Vol_Weld_ML_CSNF in Figure 30), is not globally defined, but depends on the waste package type. The values for both WP types and both lids are given in Table 9.

The output of the CWD software consists of two tables, and the probability of the occurrence of at least one defect per waste package. The four data elements, Defect_Num_OL_CSNF, Defect_Size_OL_CSNF, Defect_Num_ML_CSNF, and Defect_Size_ML_CSNF contain the file indices for the CWD software output tables. These output tables contain distributions for the density and size of defect flaws, on the outer and middle closure lids. The CWD outputs are direct inputs to the Manufacturing Defects event in WAPDEG software.

The probability of at least one defect is input at lines 296 and 316 of the WAPDEG input vector (Table I-1), for the outer and middle closure lids, respectively. The file indices corresponding to the number of flaws distribution are input at lines 297 to 301 and lines 317 to 321 of the WAPDEG input vector(Table I-1), for the outer and middle closure lids, respectively. The file indices corresponding to the flaw size distribution are input at lines 302 to 306 and lines 322 to 326 of the WAPDEG input vector (Table I-1), for the outer and middle closure lids, respectively.

Uncertainty is inherent in the calculation of the probability of at least one defect, via the probability for non-detection (PND) function. The calculation of this function uses the parameters Detection_Thresh_PND, Location_PND, and Shape_PND. Uncertainty in the defect flaw density and size is represented by the uncertain parameters (Defect_Count_Param and Defect_Size_Param) that form components of the calculation of the density and size distributions.

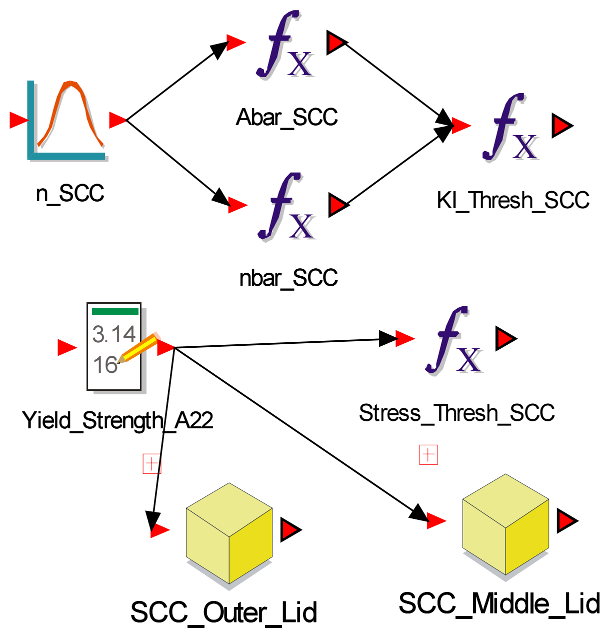
Spatial variability in the defect flaw density and size results from the density and size distributions, which form the input to the Manufacturing Defects event. These distributions are sampled once for each layer of each waste package. They are then randomly distributed to SCC patches on the WPOB layers (BSC 2002 [DIRS 162606], Section 4.2.7.2).

6.5.9 Stress and Stress Intensity Factor Profile Abstraction Model Implementation

The dominant component of stress in the WPOB closure lid weld regions has been determined to be hoop stress, which promotes radially oriented crack growth. The stress and stress intensity factor profiles are modeled in the WAPDEG software as part of a SCC Slip Dissolution event (BSC 2002 [DIRS 162606], Section 3.3.2.1.1 and Section 4.2.7.5). The SCC Slip Dissolution event will be described in more detail in Section 6.5.10. The part of the event data that pertains to the stress and stress intensity factor will be discussed here.

The SCC Slip Dissolution event requires as input, a stress intensity factor, K_I , versus depth table, and a stress versus depth table.

In the TSPA-LA model, these tables are produced by the SCCD DLL (see Figure 26). In particular, the SCCD software calculates the variation in stress and stress intensity versus depth and angle. Inputs to this calculation are four regression coefficients from the model abstraction for stress versus depth, the sine of the fracture angle, the number of angles to be calculated, the expected yield strength, the yield strength scaling factor, and the angular amplitude of the stress variation. Also required is an uncertain deviation from median yield strength range and a table of stress intensity versus depth. The details of this calculation are given in the SMR for the SCCD software (BSC 2000 [DIRS 161757]).



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 31. Contents of the SCC Container Element

The input parameters to the SCCD DLL software are held in the container element SCC (see Figure 31). The global parameter, yield strength, is defined in Table 11 and input via the data element Yield_Strength_A22. The remaining input parameters are barrier-dependent, and are defined for the outer and middle closure lids in the container elements SCC_Outer_Lid and SCC_Middle_Lid. The contents of the container element SCC_Outer_Lid are shown in Figure 32. The contents of the corresponding container for the middle lid are entirely analogous.

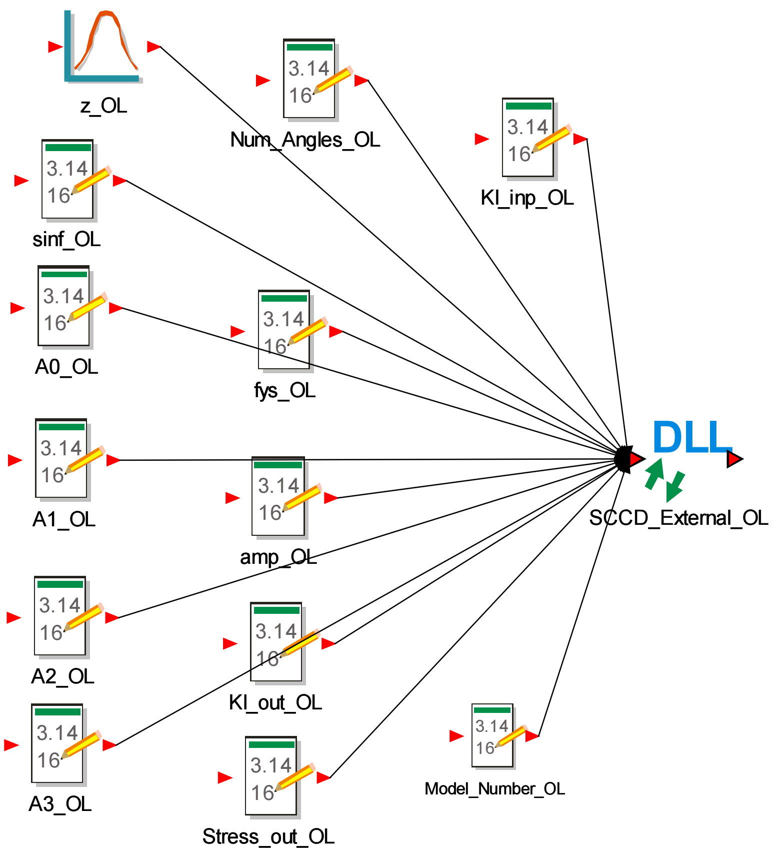
The four regression coefficients are defined in Table 12, for both lids. The outer lid values are stored in data elements A0_OL, A1_OL, A2_OL, and A3_OL. The sine of the fracture angle is defined in the data element sinf_OL. This value is always one, since only radial cracks are considered. The number of angles for which the calculation will be performed is set in the data element Num_Angles_OL. The yield strength scaling factor, fys_OL, is defined in Section 6.3.8.1 to be 15 per cent of the yield strength. The angular amplitude of the stress variation, amp_OL, is defined by Equation 10 (17.236893). The input table of stress intensity factor versus depth is defined in Table 13. The WD4DLL.WAP file index for this table is contained in the data element KI_inp_OL.

Uncertainty in the stress and stress intensity factor profiles is included via an uncertainty scaling factor, z, given by

$$z = \left(\frac{z\_OL * Yield\_Strength\_A22 * fys\_OL}{3} \right) \quad \text{(Eq. 69)}$$

z_OL represents the uncertain variation away from the median value and is sampled from a truncated normal distribution with a mean of zero, a standard deviation of one, and is truncated at three standard deviations. The uncertainty scaling factor, z, then has standard deviation given by 5% of yield strength (since fys_OL = 0.15), as specified in Table 11.

Two implementations of the uncertainty are possible, according to the value in the data element, Model_Number_OL. Details of the two uncertainty implementations are given in the SMR for the SCCD software (BSC 2000 [DIRS 161757]).



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 32. Contents of SCC_Outer_Lid Container Element

Outputs of the SCCD DLL are stress and stress intensity tables, as a function of depth, calculated at a number of angles (equally spaced and in the range 0 to π radians, inclusive). The two data elements, Stress_out_OL and KI_out_OL contain the file indices for the SCCD software output tables. The SCCD outputs are direct inputs to the SCC Slip Dissolution event in WAPDEG software.

The WD4DLL.WAP file indices corresponding to the tables of stress intensity versus depth and stress versus depth tables are input at lines 340 and 341 and lines 418 and 419 of the WAPDEG input vector (Table I-1), for the outer and middle closure lids, respectively.

6.5.10 Slip Dissolution Abstraction Model Implementation

Stress corrosion cracking (SCC) is modeled in the WAPDEG software by the use of a SCC Slip Dissolution event (BSC 2002 [DIRS 162606], Section 3.3.2.1.1 and Section 4.2.7.5). In the WAPDEG software cracking can be initiated at incipient flaws and/or defect flaws. Stress corrosion cracking due to both incipient flaws and defect flaws is modeled by the SCC Slip Dissolution Model Event.

In the WAPDEG software, a corrosion-affecting event can apply to one barrier and one or more water conditions and can have effects specific to that event, as well as generic effects. The SCC Slip Dissolution event has one specific effect, to initiate SCC.

A separate SCC Slip Dissolution event must be defined for each closure lid (outer and middle). The closure lids can potentially be subject to both DSInside and DSOutside exposure conditions, therefore both water conditions are included. The two SCC Slip Dissolution events are defined for the TSPA-LA model in lines 331 to 408 (outer closure lid) and lines 409 to 486 (middle closure lid) of the WAPDEG input vector (Table I-1). Incipient flaw cracks are automatically included in the event, but defect flaw cracks must be specifically included (lines 336 and 414 of the WAPDEG input vector). Note that the event is restricted to apply only to side patches (closure lid region), by the data entered at lines 337 to 339 and lines 415 to 417.

Using this event, cracks, once initiated, grow at a rate given by:

$$V = \overline{A}\left(K_I\right)^{\overline{n}} \tag{Eq. 70}$$

where

- V = crack velocity
- $\overline{A}$ = Pre-exponential factor
- K_I = Stress intensity factor
- $\overline{n}$ = Repassivation rate (or slope)

The crack growth parameters ($\overline{A}$ and $\overline{n}$) are defined by Equations 16 and 17 (Section 4.1.7) and by the repassivation slope in Table 14. They are input to the WAPDEG input vector at lines 352 to 361 and at lines 430 to 439. The parameters Abar_SCC and nbar_SCC correspond to the TSPA-LA expression elements of the same name, in the SCC container element (see Figure 31). Abar_SCC and nbar_SCC are a function of the repassivation slope, n_SCC. The repassivation slope is sampled from the stochastic element, n_SCC, defined by a truncated normal distribution (at ± 2 sds), with a mean of 1.304 and a standard deviation of 0.16 (see Table 14).

The number of incipient flaws per patch (incipient flaw density) is defined in the barrier definition data of the WAPDEG input vector. This definition is found in lines 11 to 15, for the outer closure lid and lines 24 to 28 for the middle closure lid. The incipient flaw densities are defined to be 6 cracks per patch and 15 cracks per patch, respectively (Section 6.3.8). The data for the incipient flaw densities is developed in Section 6.3.8. The number of weld flaws per patch (defect flaw density) is defined by the Manufacturing Defects event for each closure lid (see Section 6.5.8). The SCC Slip Dissolution event requires data for incipient crack size. The incipient crack size is defined in Table 14 and is input at lines 362 to 366 and at lines 440 to lines 444 of the WAPDEG input vector.

The SCC Slip Dissolution event also requires both a stress threshold and/or a stress intensity factor threshold, for crack growth initiation. These thresholds are separately defined for incipient and defect flaw cracks. The values of stress threshold and stress intensity factor threshold are defined in Table 14. They are contained in the TSPA-LA model expression elements Stress_Thresh_SCC and KI_Thresh_SCC. The thresholds for the incipient flaws are defined in lines 373 to 382 and in lines 451 to 460 of the WAPDEG input vector. The thresholds for the defect flaws are entered in lines 383 to 392 and lines 461 to 470 of the WAPDEG input vector. Note that both the incipient and defect flaws use the same stress intensity factor threshold. However, the defect (weld) flaws do not require a stress threshold to nucleate (see Section 4.1.7) and therefore a relatively large negative number (-600) is input as the stress threshold.

Uncertainty in the crack growth and in the stress intensity factor threshold is represented by the uncertainty in the repassivation slope. The repassivation slope is sampled by the stochastic element n_SCC, once every TSPA-LA realization. The stress and stress intensity factor tables, produced by the SCCD DLL, include uncertainty due to the use of a scaling factor that describes the deviation from the median stress/stress intensity profile. This scaling factor is sampled by the stochastic element z_OL, once every TSPA-LA realization. Uncertainty in the probability of occurrence and the density and size distributions for defect flaws is included via the stochastic elements (Defect_Count_Param and Defect_Size_Param) that form part of the CWD calculation (Section 6.5.8). Note that there is no uncertainty associated with the density and size distribution of the incipient flaws. These are explicitly defined (lines 12, 25, 363 and 441).

Spatial variability is included in the crack growth model via the stress versus depth and stress intensity factor versus depth tables. A new set of tables is calculated for every TSPA-LA realization. The tables are sampled for every patch that is subject to SCC. Spatial variability in the density and size of the defect flaws is also included, as described in Section 6.5.8.

6.5.11 Waste Package Outer Barrier Microbially Influenced Corrosion (MIC) Abstraction Model Implementation

The effect of MIC on the general corrosion of the WPOB is described in Section 6.3.9.2. Equation 56 defines a MIC factor, f_{MIC}, that is a multiplier to the general corrosion rate. The MIC factor is applied to the WPOB general corrosion rate when the relative humidity at the WPOB surface is above 90%.

MIC is modeled in the WAPDEG software by the use of a MIC event (BSC 2002 [DIRS 162606], Section 4.2.7.10). The WAPDEG input vector for the TSPA-LA model defines two MIC events, one for the outer layer (lines 487 to 520 of Table I-1) and one for the inner layer (lines 521 to 554 of Table I-1).

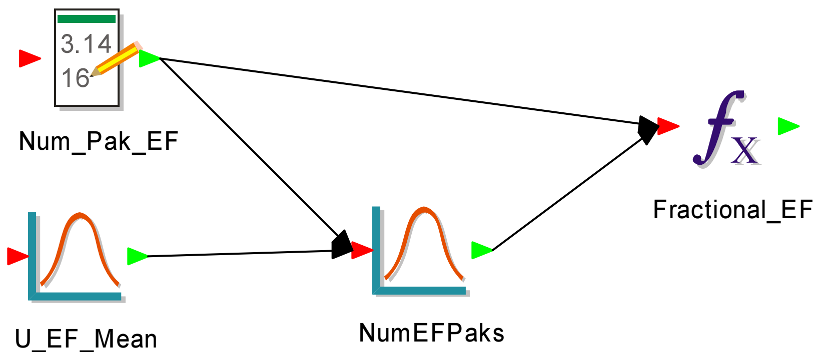
In both cases MIC is applied to the whole surface area (see lines 492 and 526 of Table I-1). The threshold RH for initiation of MIC is a fixed value of 0.9 (Table 15) and is entered (as a fraction) in lines 499 to 503 and lines 533 to 537 of Table I-1.

The MIC factor is input to the WAPDEG software as a sampled value from the stochastic MIC_A22 (see Figure 26). This stochastic is defined to be uniformly distributed between 1 and 2 (Table 15). It is entered in lines 514 to 518 of the WAPDEG input vector, for the outer layer, and in lines 548 to 552, for the inner layer. The same value is used for both layers.

Uncertainty in the MIC factor is represented by the stochastic element MIC_A22. There is no variability in the MIC factor (the MIC factor is applied to the whole WPOB surface area).

6.5.12 Implementation of Early Failure of Waste Packages

The Early Failure implementation consists of specifying the number of WPs to be considered as potentially subject to early failure and the distribution for the failure rate per WP. The distribution for the failure rate was discussed in Sections 4.1.9 and 6.3.12.2 of this report. A sample GoldSim implementation is shown in Figure 33.



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 33. Example GoldSim Implementation to Determine the Fraction of Early Failed Waste Packages.

The values used in the GoldSim elements in Figure 33 are summarized in Table 28.

Table 28. Waste Package Early Failure Parameters and Their Sources

Parameter Name	Parameter Source	Parameter Value	Units
Num_Pak_EF Number of packages considered	This is a TSPA model parameter to be specified by TSPA Model at runtime	e.g., 11184 (representative value, see discussion under Parameter Source)	N/A
U_EF_Mean Evaluation probability per WP (Uncertain Poisson intensity)	BSC 2003 [DIRS 164475], Section 7, Table 20	Log normal distribution with a geometric mean of 7.2×10^{-6} and a geometric sd of 15^(1/1.645) truncated at 7.44213E-3	per WP
NumEFPaks Number of Early Failed WP in the realization	BSC 2003 [DIRS 164475], Section 7, Table 20	Poisson Distribution with intensity Num_Pak_EF*U_EF_Mean	# WP/realization
Fractional_EF Fraction of Early Failed WP in the realization	This report	NumEFPaks/Num_Pak_EF	fraction of WP/realization

The value of Num_Pak_EF should be chosen appropriately for the purpose of the study. For example, if one wanted to know how many (or what fraction of) WPs will undergo early failure in a given realization, one should set Num_Pak_EF equal to the total number of WPs (i.e. 11184) (Section 4.1.1). Alternatively, if one wanted to know how many CDSP WPs will undergo early failure in a given realiztion, one should set Num_Pak_EF equal to the total number of CDSP WPs (i.e. 3412) (Section 4.1.1). In the case of the TSPA-LA Early Failure Analysis, three types of WPs are expected to be considered; CDSP WPs, CSNF WPs with zirconium-based cladding on the waste form, and CSNF WPs with stainless steel-based cladding on the waste form. The separation of CSNF WP configurations is made for the purposes of incorporating differences in waste form degradation.

A marginal distribution for the number of early failed WPs which incorporates the uncertainty variation is analysed here. This may be evaluated by integrating the Poisson pdf with the rate of early failure pdf (given by the log normal distribution) over their given ranges. This integration results in the marginal distribution for number of early failed WPs given the total number of WPs ($N = 11184$). Certain approximations must be made to evaluate this integral, since an analytical solution to the integral does not exit. The integral is approximated numerically over its domain from zero to the truncated upper bound. The log normal pdf is also adjusted to its truncated upper bound representation so that the pdf properly integrates to one over its effective range. This upper bound is picked so that it is as large as any of the rate values from the Monte Carlo study to which the log normal was fitted. The marginal distribution integral is represented below, where $f(x)$ and $F(x)$ are the pdf and CDF of the lognormal distribution, N is the population of packages considered, and n is the count of early failed WPs.

$$p(n) = \int_0^{\lambda_m} (\lambda N)^n \cdot \frac{\exp(-\lambda N)}{n!} \cdot \frac{f(\lambda)}{F(\lambda_m)} \cdot d\lambda \qquad \text{(Eq. 71)}$$

The discrete pdf, $p(n)$, evaluated for values of $n = 0, 1, 2, \ldots$, gives the probability of n packages being failed early. The integral upper bound, represented by λ_m, is 7.44213E-3 for numerically evaluating the marginal distribution.

Evaluating this marginal pdf for various values of n provides the following results. Only 17 percent of the realizations have early failures, 83 percent of realizations have no early failed waste packages (Table 29). Realizations with only one early failure account for 11.4 percent of realizations and 3 percent of realizations have two early failed waste packages. This leaves 2.6 percent of the remaining realizations having three or more failed waste packages.

Table 29. Early Failure Waste Package Unconditional Probability Values

n (Number of WPs)	p(n)
0	0.830177156
1	0.114170546
2	0.029481907
≥3	0.026170391

Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

A second pdf may be derived from the pdf (Equation 71) given that at least one WP has undergone early failure by renormalizing the probabilities associated with having at least one early failed WP. This second pdf is called a conditional distribution (i.e. conditional on the fact that at least one failure has occurred). For purposes of constructing a pdf table, we must pick a maximum value of $n = n_m$ such that having a value of n larger may be neglected. The value chosen here (n_m = 111) is the count associated with the standard deviation times three upper value for, $\lambda_m N$, the expected number of early failures for the maximum rate. The probability of all count values larger than n_m is small, 1.7E-9. The conditional pdf, $pc(n)$, is given below by normalizing the individual probabilities of failure (*p(n)*) by the sum of the probabilities (*p(n)*) for $n = 1, 2, \ldots, n_m$ (Equation 72). Values for this pdf are in Table 47.

$$pc(n) = \frac{p(n)}{\sum_{i=1}^{n_m} p(i)}, \qquad (n = 1,2,\ldots,n_m) \qquad \text{(Eq. 72)}$$

The distributions above may be sampled directly for unconditional or conditional counts of early failed WPs, respectively. If it is then required to partition this count between differing package types this may be done by expressing the count as a sample from a multinomial distribution. The parameters for the multinomial distribution would be *n* and the probabilities of each waste package type, where these probabilities are given by the ratio of the number of packages in the repository for that type (N_i, such that $N = \Sigma N_i$) to the total of number of all package types (i.e. *N*). To generate a multinomial distribution, a simple way is to work with the marginals since they are binomials. The generation is done sequentially. Each succeeding conditional marginal is a binomial. As an example, an implementation for three (waste form) WP types would be performed as in Table 30.

Table 30. Multinomial Sampling Algorithm (Three WP Types)

1. Sample a value for n.
2. Sample n_1 as a Binomial(n, p = N_1/N).
3. Sample n_2 as a Binomial(n – n_1, p = N_2/(N-N_1)).
4. Sample n_3 as a Binomial(n – n_1 – n_2, p = N_3/(N-N_1-N_2) = 1). That is n_3 = n – n_1-n_2.

While the analysis above provides counts of early failed WPs, the effect and time of an early failure are presented in the discussion that follows.

Since an improperly heat treated WP might be susceptible to aging and phase instability, it is not possible to identify a single and specific mechanism of degradation. For these reasons, the following recommendations are made in the *Analysis of Mechanisms for Early Waste Package/Drip Shield Failure* (BSC 2003 [DIRS 164475], Section 6.4.8) for evaluating WP early failure

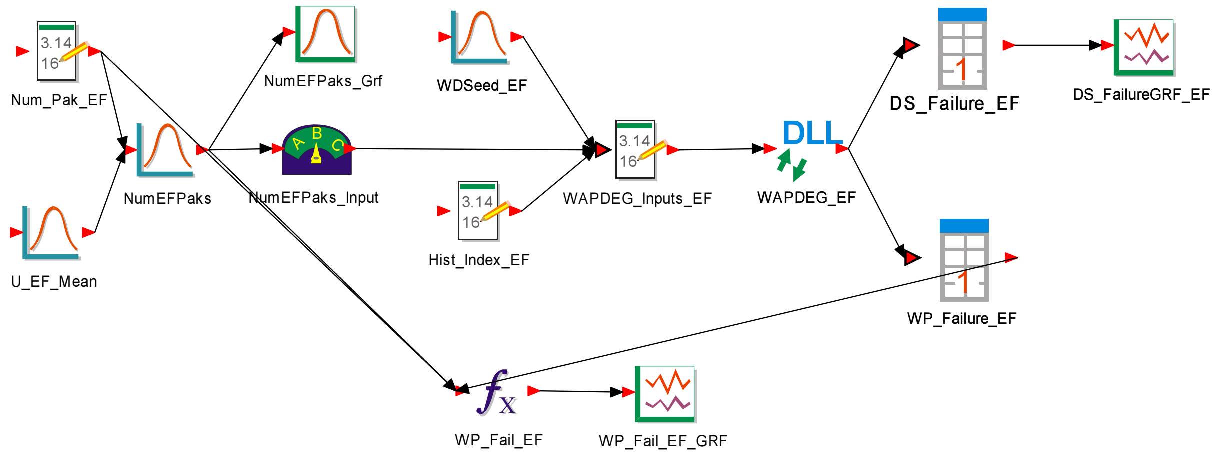
- A failure of the WP outer barrier shell and outer and middle closure lids should be assumed as well as the failure of the stainless steel structural inner shell and its lid.

- The affected WPs should be assumed to fail immediately upon initiation of degradation processes.

- The entire WP surface area should be considered affected by WP early failure.

- The materials of the entire affected area should be assumed lost upon failure of the WPs because the affected area could be subjected to stress corrosion cracking and enhanced localized and general corrosion.

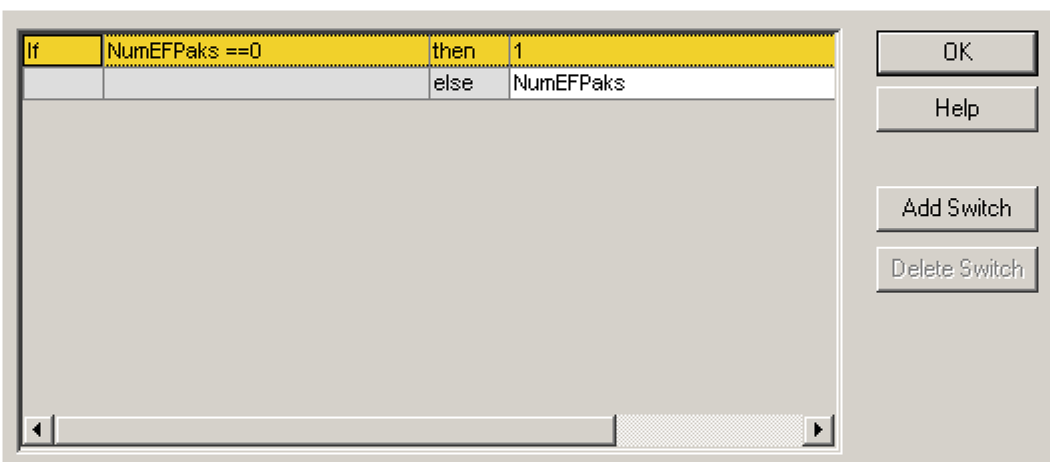
An example GoldSim implementation which determines the number and failure time of early failed waste packages is shown in Figure 34.



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 34. Example GoldSim Implementation to Determine the Number and Failure Time of Early Failed Waste Packages.

It is expected that not all of this implementation will be used; it is provided to guide the implementation of the Early Failure Analysis in TSPA. The parameters Num_Pak_EF, U_EF_Mean, and NumEFPaks are familiar from the previous figure. The element labeled NumEFPaks_GRF is merely a graphical element used to show the user a plot of the number of early failed WPs per realization. It has no effect on the results of the calculation and can be removed. The element labeled NumEFPaks_Input is a switch element whose contents are shown in Figure 35.



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 35. Contents of NumEFPaks_Input Element.

The effect of this element is clear; if the number of sampled WPs subject to early failure is zero then the number of WPs modeled by the WAPDEG software is set to one, if the number of sampled WPs subject to early failure is one or more then the number of WPs modeled by the WAPDEG software is unchanged. This is done so that the WAPDEG software is not called with zero WPs (which would result in an error).

The element WDSeed_EF provides the WAPDEG software with a seed value (through the WAPDEG_Inputs_EF element). Similarly, the Hist_Index_EF provides the WAPDEG software with the file index for the thermal hydrologic history file index (the line number in the WD4DLL.WAP file) to be used (through the WAPDEG_Inputs_EF element). The contents of the WAPDEG_Inputs_EF element are shown in Table 31

Table 31. Contents of the WAPDEG_Inputs_EF Element

Row	Value	Input Description	Comments/Units
1	Realization	Realization Number	
2	1	Number of Barriers	
3	1	Barrier Type	A22 OB
4	25	Barrier Thickness	mm
5	0.75	Barrier Mechanical Failure Fraction	fraction
6	1000	Barrier Pit Density Distribution Index	Fixed
7	0	Parameter1	/mm^2
8	0	Parameter 2	
9	0	Parameter 3	
10	0	Parameter 4	
11	1000	Barrier Crack Density Distribution Index	Fixed
12	0	Parameter1	/mm^2
13	0	Parameter 2	
14	0	Parameter 3	
15	0	Parameter 4	
16	1	Waste Container Surface Area	mm^2
17	1	Waste Container Top Fraction	fraction
18	0	Waste Container Bottom Fraction	fraction
19	1000	Waste Container Patch Size Distribution Index	Fixed
20	1	Parameter1	mm^2
21	0	Parameter 2	
22	0	Parameter 3	
23	0	Parameter 4	
24	-1	Apply Size Boolean	TRUE
25	-1	Drip Shield Present Boolean	TRUE
26	3	Drip Shield Type	Ti7 DS
27	15	Drip Shield Thickness	mm
28	0.75	Drip Shield Mechanical Failure Fraction	fraction
29	1000	Drip Shield Pit Density Distribution Index	Fixed
30	0	Parameter1	/mm^2
31	0	Parameter 2	
32	0	Parameter 3	
33	0	Parameter 4	
34	1000	Drip Shield Crack Density Distribution Index	Fixed
35	0	Parameter1	/mm^2
36	0	Parameter 2	
37	0	Parameter 3	
38	0	Parameter 4	
39	Number_DS_Patches	Drip Shield Surface Area	mm^2
40	1	Drip Shield Top Fraction	fraction
41	1000	Drip Shield Patch Size Distribution Index	Fixed
42	1	Parameter1	mm^2
43	0	Parameter 2	
44	0	Parameter 3	
45	0	Parameter 4	
46	-1	Drip Shield Apply Size Boolean	TRUE
47	1000	Drip Shield Fractional Area Affected Distribution Index	Fixed
48	1	Parameter1	fraction

Row	Value	Input Description	Comments/Units
49	0	Parameter 2	
50	0	Parameter 3	
51	0	Parameter 4	
52	1	Initial Water Condition under DS	DSInside
53	NumEFPaks_Input	Total Number of Waste Packages	
54	Hist_Index_EF	Index Number of T/H File to Read	
55	1	Number of Drip Sequences	
56	1	Number of Phases - Drip Sequence #1	
57	1000	Fraction of Top Patches Subject to Sequence Distribution Number	Fixed
58	1	Parameter1	fraction
59	0	Parameter 2	
60	0	Parameter 3	
61	0	Parameter 4	
62	1000	Fraction of Side Patches Subject to Sequence Distribution Number	Fixed
63	1	Parameter1	fraction
64	0	Parameter 2	
65	0	Parameter 3	
66	0	Parameter 4	
67	1000	Fraction of Bottom Patches Subject to Sequence Distribution Number	Fixed
68	1	Parameter1	fraction
69	0	Parameter 2	
70	0	Parameter 3	
71	0	Parameter 4	
72	2	Water Condition for Last Phase	DSOutside
73	4	Number of Corrosion Models	
74	1	Water Condition Index Number	DSInside
75	1	Corrosion Mechanism Index (1, 2, or 3)	General
76	1	Layer Composition Index	A22 OB
77	6	Functional Form Index	Power Law
78	2	Number of Levels for Variance Sharing	
79	1000	Barrier Variance Sharing Distribution Index	Fixed
80	1	Parameter1	fraction
81	0	Parameter 2	
82	0	Parameter 3	
83	0	Parameter 4	
84	1000	B term distribution	Fixed
85	1.00E+14	Parameter1	
86	0	Parameter 2	
87	0	Parameter 3	
88	0	Parameter 4	
89	1000	n term distribution	Fixed
90	1	Parameter1	
91	0	Parameter 2	
92	0	Parameter 3	
93	0	Parameter 4	
94	0	Sample Type	
95	1	Water Condition Index	DSInside
96	1	Corrosion Mechanism Index (1, 2, or 3)	General
97	3	Layer Composition Index	Ti7 DS
98	6	Functional Form Index - D = B*t^n	Power Law

Row	Value	Input Description	Comments/Units
99	2	Number of Levels for Variance Sharing	
100	1000	Barrier Variance Sharing Distribution Index	Fixed
101	1	Parameter1	fraction
102	0	Parameter 2	
103	0	Parameter 3	
104	0	Parameter 4	
105	1000	B Distribution Index	Fixed
106	WDDSInGC	Parameter1	mm/yr
107	0	Parameter 2	
108	0	Parameter 3	
109	0	Parameter 4	
110	1000	n Distribution Index	Fixed
111	1	Parameter1	
112	0	Parameter 2	
113	0	Parameter 3	
114	0	Parameter 4	
115	0	Sample Type	
116	2	Water Condition Index	DSOutside
117	1	Corrosion Mechanism Index (1, 2, or 3)	General
118	1	Layer Composition Index	A22 OB
119	6	Functional Form Index	Power Law
120	2	Number of Levels for Variance Sharing	
121	1000	Barrier Variance Sharing Distribution Index	Fixed
122	1	Parameter1	fraction
123	0	Parameter 2	
124	0	Parameter 3	
125	0	Parameter 4	
126	1000	B term distribution	Fixed
127	1.00E+14	Parameter1	
128	0	Parameter 2	
129	0	Parameter 3	
130	0	Parameter 4	
131	1000	n term distribution	Fixed
132	1	Parameter1	
133	0	Parameter 2	
134	0	Parameter 3	
135	0	Parameter 4	
136	0	Sample Type	
137	2	Water Condition Index	DSOutside
138	1	Corrosion Mechanism Index (1, 2, or 3)	General
139	3	Layer Composition Index	Ti7 DS
140	6	Functional Form Index - D = B*t^n	Power Law
141	2	Number of Levels for Variance Sharing	
142	1000	Barrier Variance Sharing Distribution Index	Fixed
143	1	Parameter1	
144	0	Parameter 2	
145	0	Parameter 3	
146	0	Parameter 4	
147	1000	B Distribution Index	Fixed
148	WDDSOutGC	Parameter1	mm/yr
149	0	Parameter 2	
150	0	Parameter 3	
151	0	Parameter 4	
152	1000	n Distribution Index	Fixed
153	1	Parameter1	

Row	Value	Input Description	Comments/Units
154	0	Parameter 2	
155	0	Parameter 3	
156	0	Parameter 4	
157	0	Sample Type	
158	0	Number of General Thresholds	
159	0	Number of Pit Temperature Thresholds	
160	-1	Inside Out Corrosion Logical	TRUE
161	2	Water Condition for Inside Out Corrosion	DSOutside
162	0	Interface Corrosion Logical	FALSE
163	0	Number of Events	
164	WDSeed_EF	Seed for the random number generator	
165	NumBins	Number of bins for reporting penetrations with time	
166	BinStart	Bin Start Time	
167	0	Number of summary times for reporting penetrations	
168	0	Do Subset of Total Package Logical	FALSE
169	1	Number of First Package	
170	1	Number of Last Package	
171	SimTime	Simulation Time	
172	11	Number of Output files	
173	0	Generate OUT file logical	
174	0	Generate AUX file logical	
175	0	Generate PIT file logical	
176	0	Generate CRK file logical	
177	0	Generate PAT file logical	
178	0	Generate THK file logical	
179	0	Generate EVN file logical	
180	0	Generate DET file logical	
181	0	Generate INA file logical	
182	0	Generate OUA file logical	
183	0	Generate PDZ file logical	

Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

This WAPDEG input vector is much simplified compared to the nominal WAPDEG input vector. The WAPDEG_Inputs_EF vector contains input for modeling NumEFPaks_Input number of DS/WP pairs. The DS performance is unaffected by early failure processes (Section 6.3.12.1), thus it is modeled with the same general corrosion rates used in the nominal IWPD Model (see lines 106 and 147 in Table 31). A very high (10^{14} mm/yr general corrosion rate is chosen for the single-barrier WP (line 126 of Table 31) resulting in immediate failure of the entire WP barrier upon initiation of degradation. The DS_Failure_EF and WP_Failure_EF elements contain the output of the WAPDEG software. The WP_Fail_EF element contains WP_Failure_EF*(NumEFPaks/Num_Pak_EF) which is zero when NumEFPaks is zero and gives the fraction of early failed WPs failed versus time. The WP_Fail_EF_GRF element is a graph element which has no effect on the simulation results.

6.6 BASE-CASE MODEL RESULTS

6.6.1 Overview

The previous sections of this report have documented the inputs to the Integrated Waste Package Degradation (IWPD) Model nominal-case analysis. In this Section, the results of a representative IWPD Model analysis for waste package and drip shield degradation are presented. The information in this section is provided only as a demonstration of an example set of model outputs. The waste package and drip shield degradation analyses to be presented in this Section are for 300 realizations of the IWPD Model to account for the uncertainty analysis of the uncertain simulation parameters. Each IWPD Model realization corresponds to a complete IWPD Model run to represent the variability in the degradation processes for a given number of waste package and drip shield pairs.

Sensitivities using other choices of number of waste package and drip shield pairs are discussed in the next section.

The input parameters and their values were discussed in Section 6.5. Further specification of model inputs and recommendations for implementation can be found in Section 8.1. The IWPD Model analysis results (i.e. fraction of drip shields and waste packages failed versus time and the number of crack and patch penetrations per failed drip shield/waste package versus time) are reported as a group of "degradation profile curves" that represent the potential range of the output parameters. The analysis results are presented for the upper and lower bounds, mean, and 95^{th}, 75^{th}, 25^{th} and 5^{th} percentiles as a function of time for the following output parameters:

- Waste package first breach (or failure)
- Drip shield first breach (or failure)
- Waste package first crack penetration
- Waste package first patch penetration
- Waste package number of crack penetrations per failed waste package
- Waste package number of patch penetrations per failed waste package
- Drip shield number of patch penetrations per failed drip shield

Note that localized corrosion is not explicitly discussed in this section. Also note that stress corrosion cracking (SCC) of the drip shield is not modeled (see Section 6.3.7), thus no crack penetration failures for the drip shield are calculated. Therefore, for the drip shield, the first patch penetration versus time profile is equivalent to the first breach versus time profile.

The upper and lower bounds, mean, and 95^{th}, 75^{th}, 25^{th} and 5^{th} percentile curves do not correspond to single realizations. They are summary statistics related to consideration of all 300 realizations. In the bullets below, the origin of the upper and lower bound, mean, and 95^{th}, 75^{th}, 25^{th} and 5^{th} percentile curves for first breach of the waste package are discussed. Similar wording (not included for the sake of brevity) could be applied for discussion of origins of the drip shield first breach curves, waste package first crack penetration curves, etc.

- At each point in time the upper bound curve shows the realization with the greatest fraction of waste packages failed calculated in any one of the 300 realizations. This may not be the same realization at each point in time. The upper bound curve becomes non-zero at the time of failure of first waste package in all of the 300 realizations.

- At each point in time the 95^{th} percentile curve shows the realization with the 285^{th} greatest fraction of waste packages failed, i.e. 3*95 = 285 realizations out of 300 have smaller fraction of waste packages failed calculated in any one of the 300 realizations. This may not be the same realization at each point in time. The 95th percentile curve becomes non-zero at the time when at least 3*5 = 15 realizations have at least one waste package failure.

- At each point in time the 75th percentile curve shows the realization calculated in any one of the 300 realizations with the 225th greatest fraction of waste packages failed, i.e. 3*75 = 225 realizations out of 300 have smaller fraction of waste packages failed. This may not be the same realization at each point in time. The 75th percentile curve becomes non-zero at the time when at least 3*25 = 75 realizations have at least one waste package failure.

- At each point in time the 25th percentile curve shows the realization calculated in any one of the 300 realizations with the 75th greatest fraction of waste packages failed, i.e. 3*25 = 75 realizations out of 300 have smaller fraction of waste packages failed. This may not be the same realization at each point in time. The 25th percentile curve becomes non-zero at the time when at least 3*75 = 225 realizations have at least one waste package failure.

- At each point in time the 5th percentile curve shows the realization calculated in any one of the 300 realizations with the 15th greatest fraction of waste packages failed, i.e. 3*5 = 15 realizations out of 300 have smaller fraction of waste packages failed. This may not be the same realization at each point in time. The 5th percentile curve becomes non-zero at the time when at least 3*95 = 285 realizations have at least one waste package failure.

- At each point in time the mean curve shows the mean of all the fractions of waste packages failed in all of the 300 realizations. The mean curve becomes non-zero at the time of failure of first waste package in all of the 300 realizations.

6.6.2 Commercial Spent Nuclear Fuel Integrated Waste Package Degradation Model Base-Case Results

The Commercial Spent Nuclear Fuel (CSNF) Waste Packages (WPs) are simulated using 1014 patches (Section 6.3.2). The CSNF WPOB shell thickness is 20 mm (Section 4.1.1).

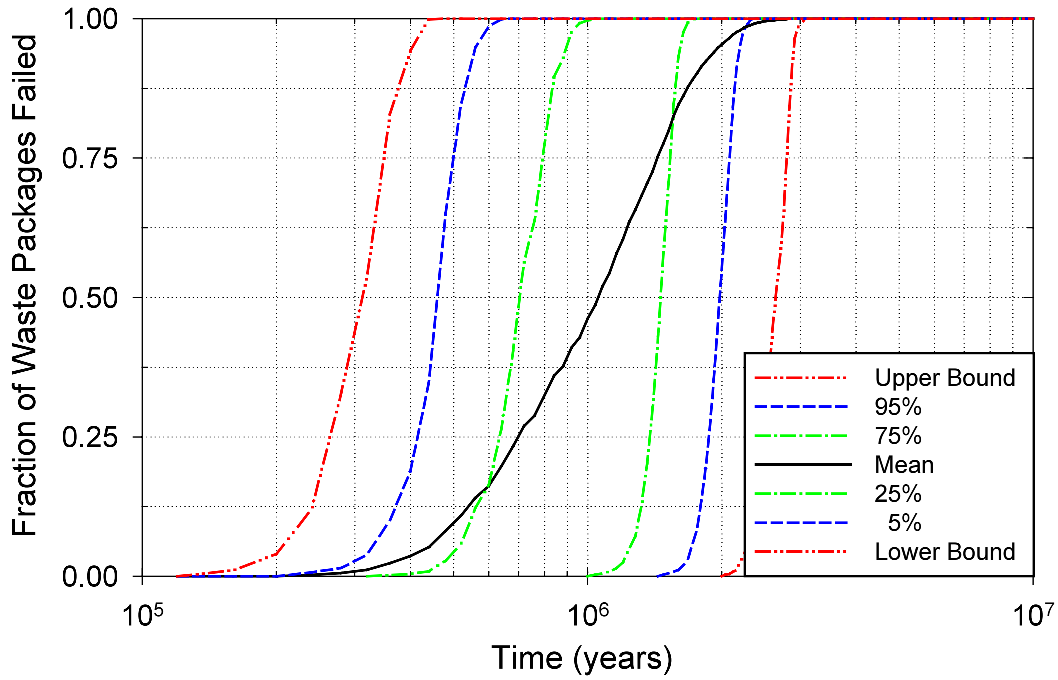
Figure 36 shows the upper and lower bounds, mean, and 95th, 75th, 25th and 5th percentile confidence intervals of the first breach profile for CSNF waste packages versus time. The upper bound profile, which is the upper extreme of the probable range of the first breach time, indicates that the earliest possible first breach time for a waste package is about 120,000 years. Note that the estimated earliest possible first breach time has a very low probability. It can be shown by comparing with the upper bound profile in Figure 38 (showing the first crack breach profiles of waste packages with time) that the first breach is by SCC crack penetration (see the discussion of the results in Figure 38 and Figure 39 later in this Section). The median estimate (50% of waste packages failed) of the first breach time of the upper bound profile is about 310,000 years. The median estimate of the first breach time of the mean profile is about 1.06 million years. The time to fail 10 percent of waste packages for the upper bound and mean profiles is about 230,000 and 320,000 years, respectively.

Figure 37 shows the first breach profiles of CSNF drip shields with time. Because SCC and localized corrosion of the drip shields are not modeled in this Section, the first breach profiles shown in the figure are all by general corrosion only. Both the upper and under sides of the drip shield are exposed to the exposure conditions in the emplacement drift and are subject to general corrosion. Thus, in the analysis, the general corrosion rate for the drip shields is sampled twice independently, once for the upper side and the once for the under side. There is no variability in DS failure times. This is shown in the failure profiles in that the fraction of failed drip shields rises quickly from zero to one. For the upper bound drip shield failure profile, the drip shields fail at about 47,500 years. For the 95th percentile profile, the drip shields fail at about 92,500 years. The median estimate of the first breach time of the mean profile is about 310,000 years. Since the drip shields are modeled with one patch, the entire surface of a failed drip shield fails at one time.

Figure 38 and Figure 39 show respectively the first crack penetration and patch penetration profiles of the CSNF waste packages with time. The first crack breach times of the upper bound and 95th percentile profiles are about 120,000 and 240,000 years, respectively (Figure 38), and the first patch breach times of the upper and 95th percentile profiles are about 480,000 and 560,000 years, respectively (Figure 39). Comparison of the first crack and patch breach profiles with the first breach profiles in Figure 36 indicates that the initial breach (or failure) of the waste packages is generally by SCC crack penetration in the Alloy 22 waste package outer barrier middle closure lid welds. For the 75th percentile profiles in the figures, the first crack and patch penetration times are about 360,000 and 840,000 years, respectively.

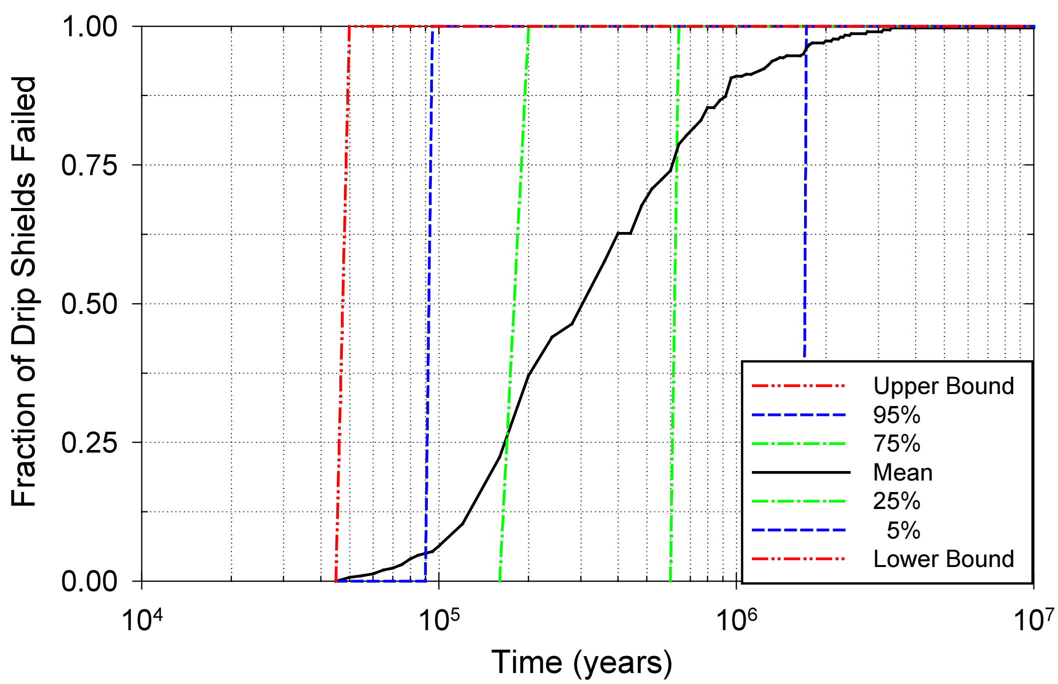
Figure 40 shows the profile for the average number of crack penetrations per failed CSNF waste package. As discussed for Figure 38, the upper bound and 95th percentile profiles show the first crack penetration at about 120,000 and 240,000 years, respectively. The mean profile never develops more than about 382 cracks. SCC cracks in passive alloys such as Alloy 22 tend to be very tight (i.e. small crack opening displacement) by nature (BSC 2003 [DIRS 161234], Section 6.3.7). The opposing sides of through-wall SCC cracks will continue to corrode at very low passive corrosion rates until the gap region of the tight crack opening is "plugged" by the corrosion product particles and precipitates such as carbonate present in the water. Any water transport through this oxide/salt filled crack area will be mainly by diffusion-type transport processes (BSC 2003 [DIRS 161234], Section 6.3.7). Thus, both the effective water flow rate into the waste packages and the radionuclide release rate from the waste packages through the SCC cracks would be expected to be extremely low and should not contribute significantly to the overall radionuclide release rate from the potential repository.

Figure 41 presents the profile for the average number of patch openings per failed waste package. For the upper bound profile, which again represents an extremely low probability case, the average first patch breach occurs at about 480,000 years (see also Figure 39), and about 10 patches on average (about 1 percent of the waste package surface area) are breached by 825,000 years. For the mean profile, there will be only about 2.5 patch openings (on average) in each of the failed waste packages by 1 million years.



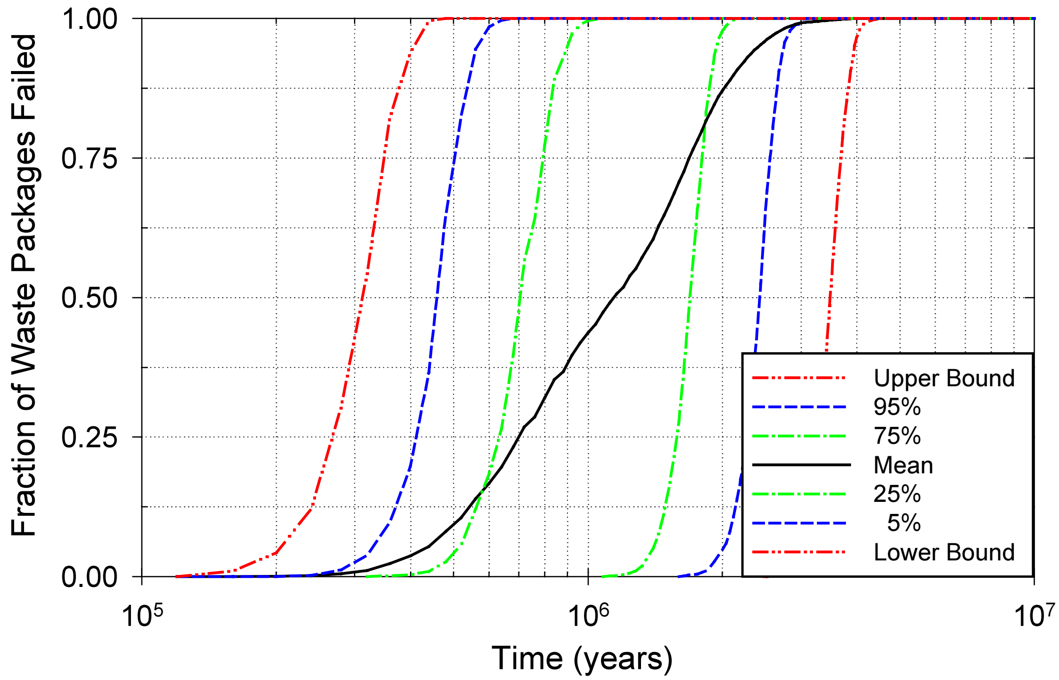
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 36. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Breach Profile of CSNF Waste Packages With Time for the IWPD Model



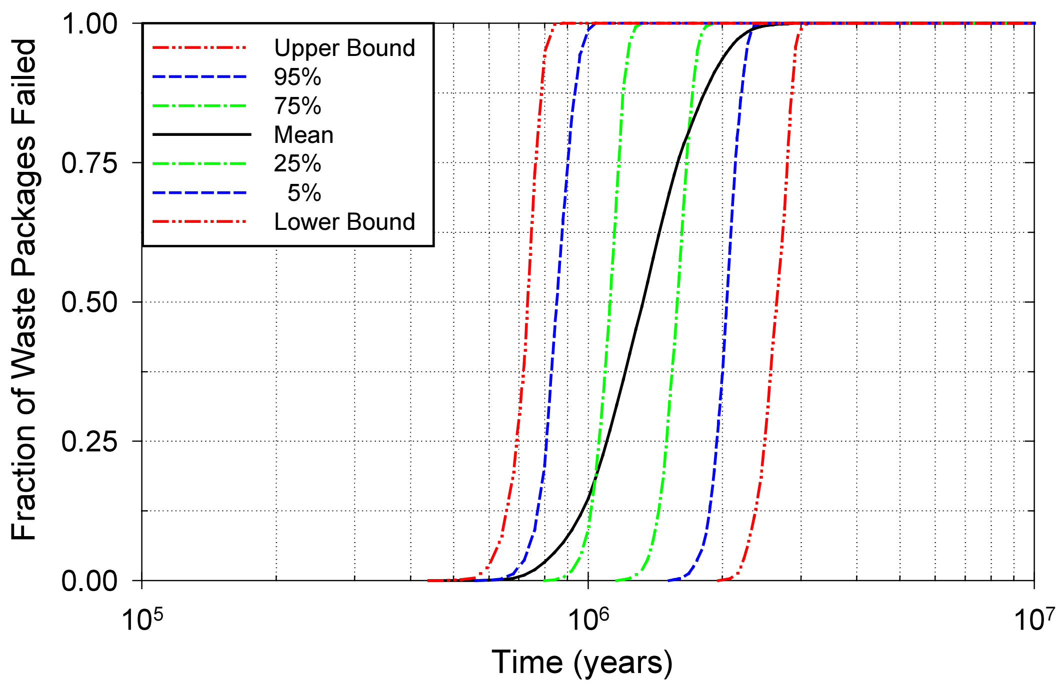
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 37. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Breach Profile of CSNF Drip Shields With Time for the IWPD Model



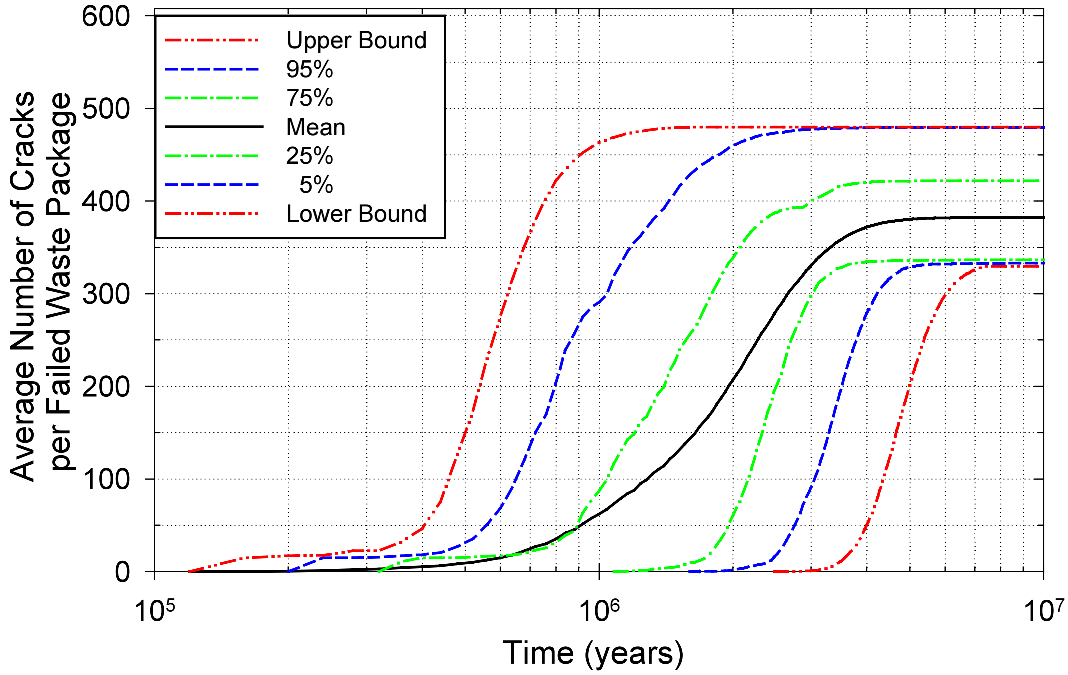
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 38. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Crack Breach Profile of CSNF Waste Packages With Time for the IWPD Model



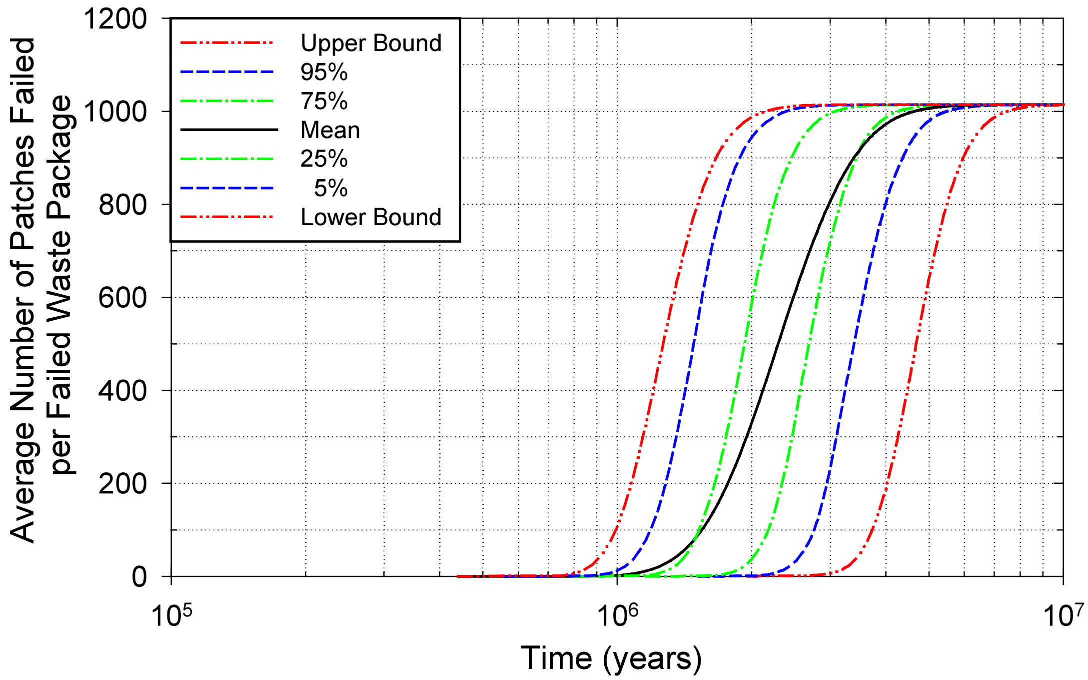
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 39. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Patch Breach Profile of CSNF Waste Packages With Time for the IWPD Model



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 40. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Average Number of Crack Penetrations per Failed CSNF Waste Package Profile With Time for the IWPD Model



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 41. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Average Number of Patch Penetrations per Failed CSNF Waste Package Profile With Time for the IWPD Model

6.6.3 Co-Disposal Waste Package Integrated Waste Package Degradation Model Base-Case Results

The Co-Disposal (CDSP) Waste Packages (WPs) are simulated using 1106 patches (Section 6.3.2). The CDSP WPOB shell thickness is 25 mm (Section 4.1.1).

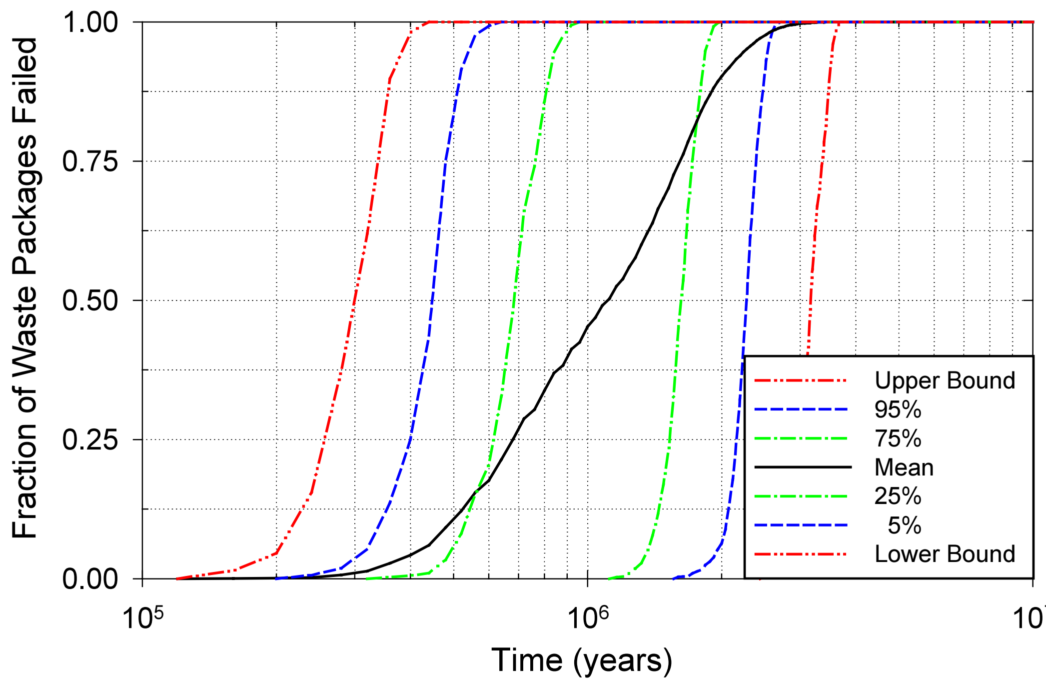
Figure 42 shows the upper and lower bounds, mean, and 95th, 75th, 25th and 5th percentile confidence intervals of the first breach profile for CDSP waste packages versus time. The upper bound profile, which is the upper extreme of the probable range of the first breach time, indicates that the earliest possible first breach time for a waste package is about 120,000 years. Note that the estimated earliest possible first breach time has a very low probability. It can be shown by comparing with the upper bound profile in Figure 44 (showing the first crack breach profiles of waste packages with time) that the first breach is by SCC crack penetration (see the discussion of the results in Figure 44 and Figure 45 later in this Section). The median estimate (50% of waste packages failed) of the first breach time of the upper bound profile is about 310,000 years. The median estimate of the first breach time of the mean profile is about 1.12 million years. The time to fail 10 percent of waste packages for the upper bound and mean profiles is about 220,000 and 485,000 years, respectively.

Figure 43 shows the first breach profiles of CDSP drip shields with time. Because SCC and localized corrosion of the drip shields are not modeled in this Section, the first breach profiles shown in the figure are all by general corrosion only. Both the upper and under sides of the drip shield are exposed to the exposure conditions in the emplacement drift and are subject to general corrosion. Thus, in the analysis, the general corrosion rate for the drip shields is sampled twice independently, once for the upper side and the once for the under side. There is no variability in DS failure times. This is shown in the failure profiles in that the fraction of failed drip shields rises quickly from zero to one. For the upper bound drip shield failure profile, the drip shields all fail at about 47,500 years. For the 95th percentile profile, the drip shields all fail at about 92,500 years. The median estimate of the first breach time of the mean profile is about 310,000 years. Since the drip shields are modeled with one patch, the entire surface of a failed drip shield fails at one time. Note that the CSNF and CDSP DS failure curves are identical since there is no difference between the DSs for the 2 WP types.

Figure 44 and Figure 45 show respectively the first crack penetration and patch penetration profiles of the CDSP waste packages with time. The first crack breach times of the upper bound and 95th percentile profiles are about 120,000 and 200,000 years respectively (Figure 44), and the first patch breach times of the upper and 95th percentile profiles are about 560,000 and 720,000 years, respectively (Figure 45). Comparison of the first crack and patch breach profiles with the first breach profiles in Figure 42 indicates that the initial breach (or failure) of the waste packages is generally by SCC crack penetration in the Alloy 22 waste package outer barrier middle closure lid welds. For the 75th percentile profiles in the figures, the first crack and patch penetration times are about 360,000 and 920,000 years, respectively.

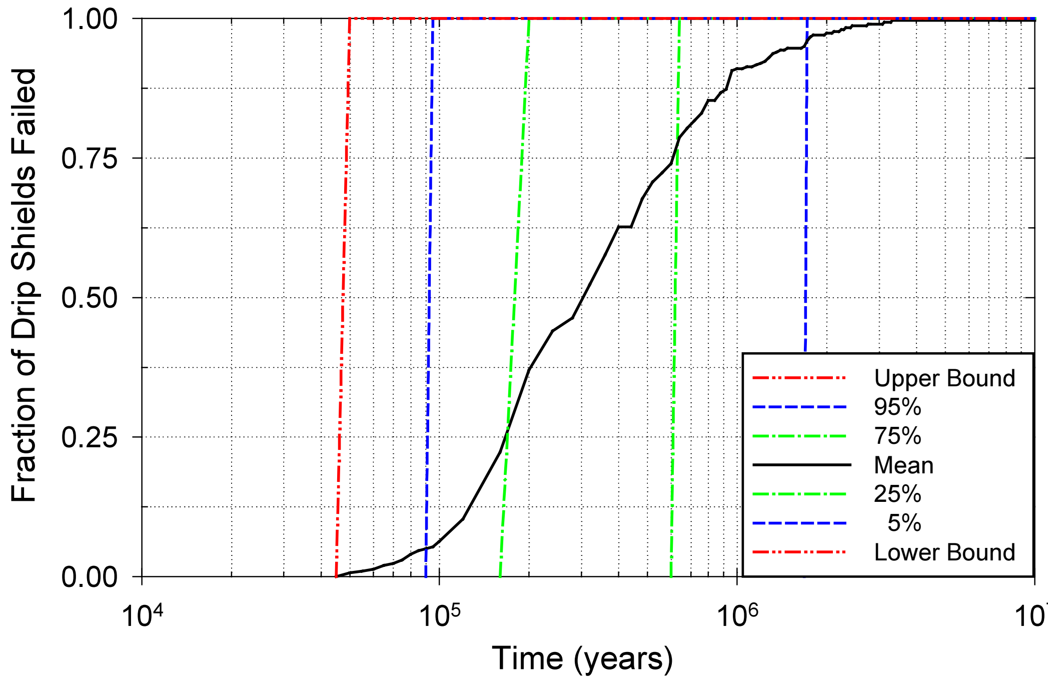
Figure 46 shows the profile for the average number of crack penetrations per failed CDSP waste package. As discussed for Figure 44, the upper bound and 95th percentile profiles show the first crack penetration at about 120,000 and 200,000 years, respectively. The mean profile never develops more than about 522 cracks. SCC cracks in passive alloys such as Alloy 22 tend to be very tight (i.e. small crack opening displacement) by nature (BSC 2003 [DIRS 161234], Section 6.3.7). The opposing sides of through-wall SCC cracks will continue to corrode at very low passive corrosion rates until the gap region of the tight crack opening is "plugged" by the corrosion product particles and precipitates such as carbonate present in the water. Any water transport through this oxide/salt filled crack area will be mainly by diffusion-type transport processes (BSC 2003 [DIRS 161234], Section 6.3.7). Thus, both the effective water flow rate into the waste packages and the radionuclide release rate from the waste packages through the SCC cracks would be expected to be extremely low and should not contribute significantly to the overall radionuclide release rate from the potential repository.

Figure 47 presents the profile for the average number of patch openings per failed waste package. For the upper bound profile, which again represents an extremely low probability case, the first patch breach occurs at about 560,000 years (see also Figure 45), and about 13 patches (on average) (about 1 percent of the waste package surface area) are breached by 1 million years. For the mean profile, there will be only about 0.28 of a patch opening (on average) in each of the failed waste packages by 1 million years.



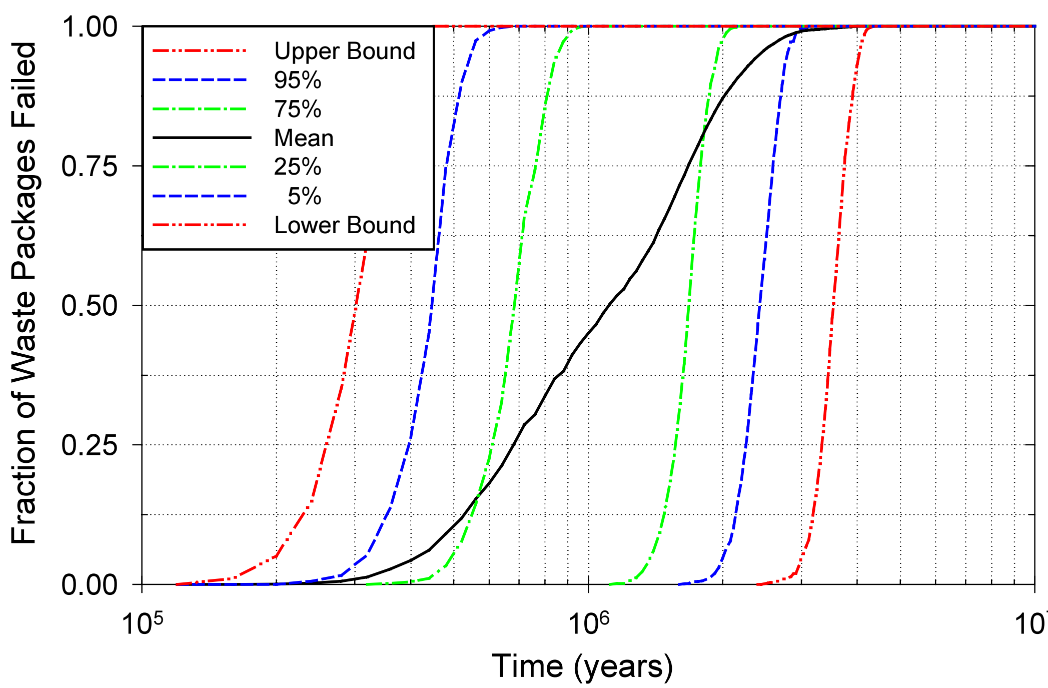
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 42. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Breach Profile of CDSP Waste Packages With Time for the IWPD Model



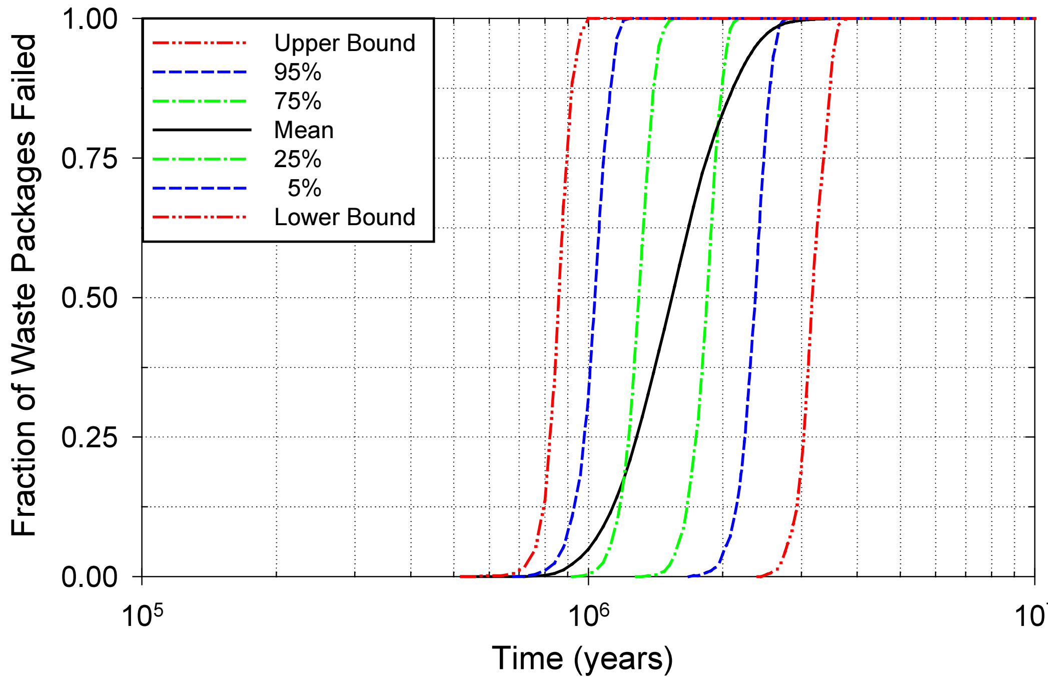
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 43. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Breach Profile of CDSP Drip Shields With Time for the IWPD Model



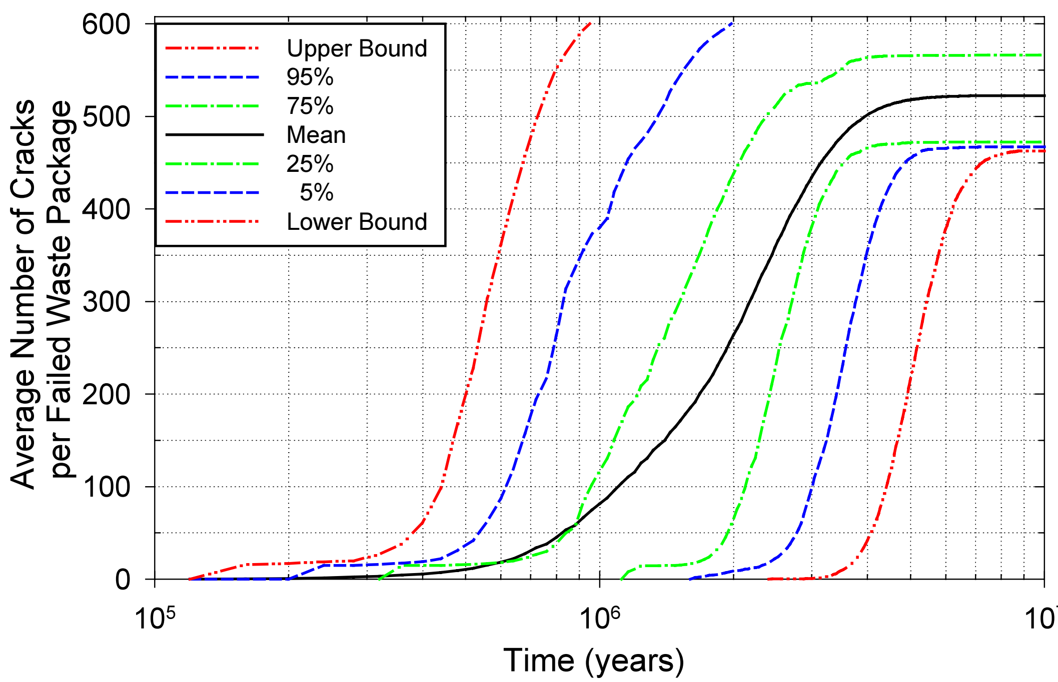
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 44. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Crack Breach Profile of CDSP Waste Packages With Time for the IWPD Model



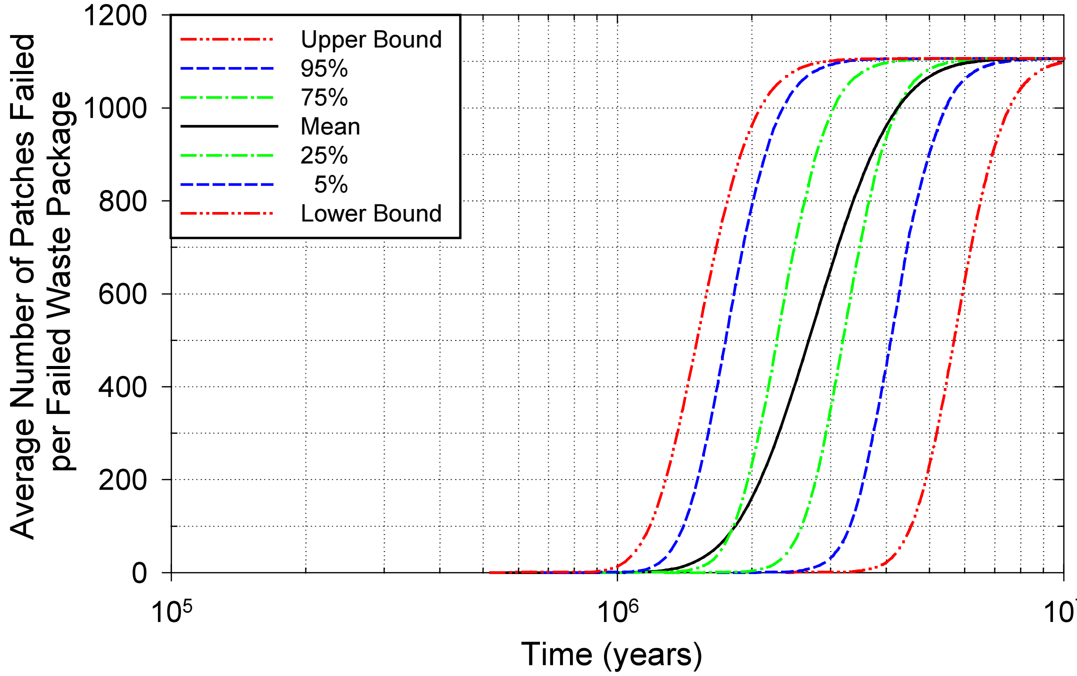
Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 45. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Patch Breach Profile of CDSP Waste Packages With Time for the IWPD Model



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 46. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Average Number of Crack Penetrations per Failed CDSP Waste Package Profile With Time for the IWPD Model



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 47. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Average Number of Patch Penetrations per Failed CDSP Waste Package Profile With Time for the IWPD Model

6.6.4 Number of Drip Shield and Waste Package Pairs Sensitivity Study

Among the activities listed in the governing Technical Work Plan (BSC 2002 [DIRS 161132], Attachment B, Section B6.4) to be performed to generate confidence in the model during model development are:

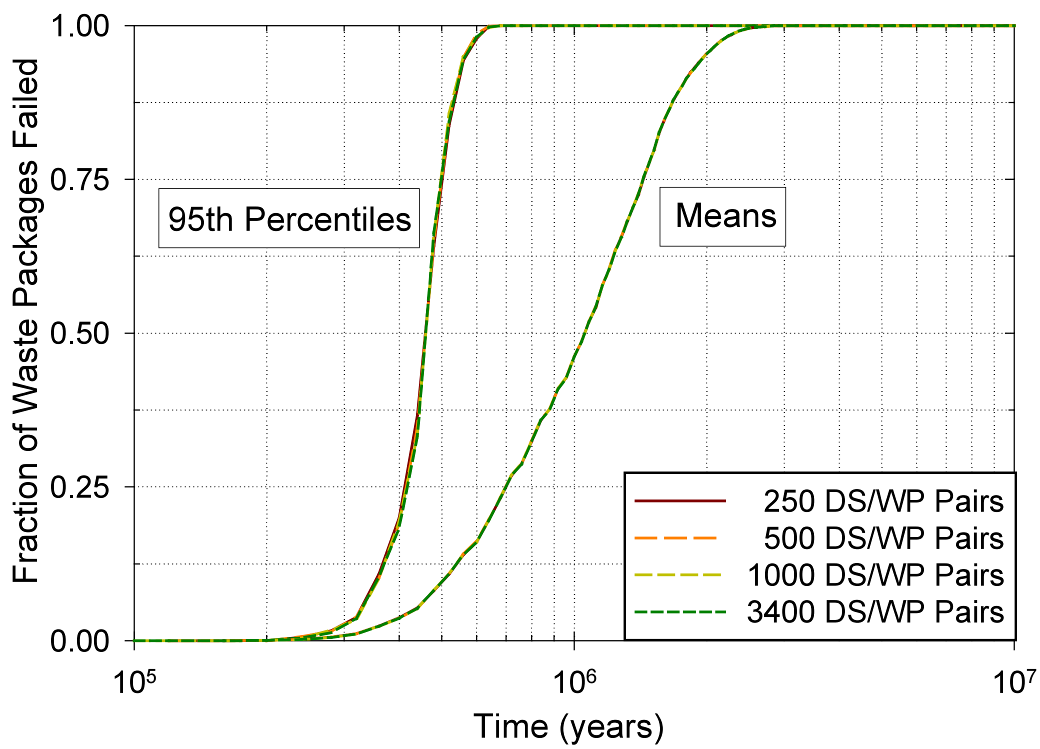
- Simulations with various numbers of waste package and drip shield pairs for the purpose of determining the appropriate number of waste package and drip shield pairs to use in nominal simulations.

- Simulations with various numbers of waste package and drip shield "patches" for the purpose of determining the appropriate number of patches to use in nominal simulations.

The simulations referred to in the second bullet (simulations with various numbers of waste package and drip shield patches) are not necessary since the analyses in this report have developed a technical basis for the particular choice of the number of patches used in nominal Integrated Waste Package Degradation (IWPD) Model simulations (Section 6.3.4).

The simulations referred to in the first bullet (simulations with various numbers of waste package and drip shield pairs) are relevant and are discussed in this Section.

The IWPD Model was executed with 250, 500, 1000, and 3400 DS/WP pairs for the purpose of determining the appropriate number of waste package and drip shield pairs to use in nominal simulations. The mean and 95th percentile WP first failure curves are shown in Figure 48 for all cases. Figure 48 clearly shows that the IWPD Model results are not very sensitive to the number of DS/WP pairs simulated over the range investigated. However, it should be noted that the TSPA Model will use thermal hydrologic history files which differ from those used in these analyses. On this basis, it is recommended that the TSPA Model use the lesser of the number of DS/WP pairs to be simulated and 500 DS/WP pairs. This choice is obviously appropriate when less than 500 DS/WP pairs are to be simulated and balances the need for accuracy with the need for reasonable execution time when more than 500 DS/WP pairs are to be simulated. It is expected that, in the TSPA Model, the drip shield and waste package degradation processes will be simulated at the spatial bin/fuel type level. The number of IWPD Model simulations per TSPA Model realization depends on the scenario class being run. The IWPD Model is evaluated twice for each of the five spatially fixed bins, once for the CSNF waste packages in that bin and once for CDSP waste packages. If the spatially fixed bin contains fewer than 500 DS/WP pairs, all CSNF and CDSP DS/WP pairs in the bin should be simulated. If the bin contains more than 500 DS/WP pairs, then only 500 CSNF and 500 CDSP DS/WP pairs need to be simulated.



Output DTN: MO0310MWDWAPAN.002 [DIRS 165800]

Figure 48. The 95th Percentile Confidence Intervals and Means Using 250, 500, 1000, and 3400 Drip Shield/Waste Package Pairs of the First Breach of CSNF Waste Package Profile With Time for the IWPD Model

6.7 DESCRIPTION OF BARRIER CAPABILITIES

10 CFR 63 [DIRS 156605] defines a barrier as "any material, structure, or feature that, for a period to be determined by NRC, prevents or substantially reduces the rate of movement of water or radionuclides from the Yucca Mountain repository to the accessible environment, or prevents

the release or substantially reduces the release rate of radionuclides from the waste." 10 CFR 63.102(h) and 10 CFR 63.113(a) require that the repository system must include multiple barriers, both natural and engineered. The capability of a barrier is defined by its ability to achieve one or more of the functions described above: i.e. the extent to which it can prevent or delay the movement of water or radionuclides, or prevent or reduce the release rate from the waste. In this document, two barriers are considered; the drip shield and the waste package. These barriers contribute to waste isolation by keeping water away from the waste forms for their lifetime.

6.7.1 Summary of Barrier Capabilities

The reader should note that the results of the analyses documented in Section 6.6 are for illustrative purposes only. The drip shield and waste package degradation profiles presented in this Section 6.6 result from the use of representative thermal hydrologic history files (Section 6.3.13) produced for the purpose of allowing the IWPD Model to be exercised in this report. The actual drip shield and waste package degradation profiles which will be used in the TSPA-LA Model will make use of the actual thermal hydrologic history files appropriate for the repository. Nonetheless the drip shield and waste package degradation profiles presented in this Section 6.6 do provide evidence that the IWPD Model implementation functions properly.

Furthermore, the effects of igneous and seismic events and localized corrosion on drip shield and waste package performance were not evaluated in this report.

6.7.1.1 Summary of Drip Shield Barrier Capabilities

Drip shields will be installed over the waste packages prior to repository closure. The drip shields divert any moisture that might seep from the drift walls, including condensed water vapor, around the waste packages to the drift floor for thousands of years. The drip shields will be made of titanium alloy, which provides corrosion resistance and structural strength. The drip shields limit any damage arising to waste packages in the event of expected rockfalls, as the emplacement drifts degrade over time. Because of the low corrosion rate of titanium alloy, the initial breaches of the drip shields are not expected to occur until approximately 35,000 years (Section 6.3.3), and the median estimate of the mean time to initial breaching of drip shields is approximately 310,000 years. Therefore, even in the event of a breach of a waste package before its corresponding drip shield, advective transport of radionuclides cannot occur until after 35,000 years and is likely to be delayed even longer.

6.7.1.2 Summary of Waste Package Barrier Capabilities

Waste packages prevent any contact between water and waste as long as they are intact, and limit water flow and potential radionuclide migration even after the waste packages are breached. The waste packages have a dual-metal design containing two concentric cylinders. The inner vessel cylinder is a 50 mm thick layer of 316 stainless steel. The outer barrier cylinder is a 20 mm or 25 mm thick layer of Alloy 22, a corrosion resistant nickel-based alloy. Alloy 22 protects the 316 stainless steel inner vessel cylinder from corrosion, while the 316 stainless steel inner vessel provides structural support for the thinner Alloy 22 outer barrier cylinder. The corrosion rates of Alloy 22 are so low that it is not expected that any waste packages would be breached by general corrosion or stress corrosion cracking during the first 10,000 years: models indicate that the time to initial breaching of the waste packages is on the order of one hundred thousand years (Section 6.6). Analyses of the potential for premature failures of waste packages by processes other than corrosion (e.g., improper heat treatment or damage by rockfall) indicate a very low probability that packages would be breached before 10,000 years. Even after that time, the slow failure rate of waste packages, and the low rate of water movement through them, would limit releases of radionuclides for many tens of thousands of years.

7. VALIDATION

The Integrated Waste Package Degradation (IWPD) Model is an abstraction model composed of models developed in documents, which serve as input to this report. These documents include:

- *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2003 [DIRS 161235]) contains the
  - General and Localized Corrosion Model for Waste Package
- *General Corrosion and Localized Corrosion of Drip Shield* (BSC 2003 [DIRS 161236]) contains the
  - General and Localized Corrosion Model for Drip Shield
- *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material* (BSC 2003 [DIRS 161234]) contains the
  - Stress Corrosion Cracking Models for Waste Package and Drip Shield

Within these documents, discussions of, and rationale for, selection of the appropriate number of data sets to be used for model development as well as the appropriate number of data points contained within each data set are provided. These documents also provide guidance as to the acceptable limit of variation of the experimental values from those obtained from the model predicted values.

This model was validated using the approach described in the AP-SIII.10Q, *Models*, procedure. This procedure calls for the determination of the level of confidence required for the model and identifies criteria that can be utilized to show that the level of confidence has been achieved.

7.1 DETERMINATION OF LEVEL OF CONFIDENCE REQUIRED

The current Technical Work Plan for this report (BSC 2002 [DIRS 161132], Attachment B, Section B6.2) states that the IWPD Model warrants a "high level of confidence." This statement was based on the previous version of the IWPD Model, which incorporated all of the component models for the waste package and the drip shield relevant to TSPA. The localized corrosion model for the waste package outer barrier, which could potentially cause failure of the waste packages at times significantly less than any other degradation mode, was included in the previous version of the IWPD Model but is not included in the current version of the IWPD Model. In addition, in the previous version of the IWPD Model, failure times for the drip shields and waste packages could be predicted independent of the TSPA Model.

The *Scientific Processes Guidelines Manual* (BSC 2002 [DIRS 160313], Appendix B) suggests that models requiring "high level of confidence" should be validated using a Level III validation approach. It is believed that this determination would be appropriate for the previous version of the IWPD Model. However, the current version of the IWPD Model as planned for delivery to TSPA does not include some of the key features previously included. These features are: detailed thermal-hydrologic information needed for initiating corrosion processes and a localized corrosion model as a function of physical and environmental conditions.

The IWPD Model now consists primarily of the general corrosion and stress corrosion cracking models. When these models are exercised using representative thermal hydrologic histories, waste package and drip shield lifetimes are predicted to be in excess of 100,000 years which is significantly longer than the regulatory period. While these results should be used only for illustrative purposes (as the thermal hydrologic histories used are not obtained from upstream models), they suggest that the IWPD Model as currently developed and delivered to TSPA, requires only a Level I validation approach.

On the basis of the above arguments, the validation criteria used for model validation are consistent with those required for Level I validation and are different from those cited in the Technical Work Plan applicable to this activity.

7.2 IDENTIFICATION AND DOCUMENTATION OF CRITERIA TO BE USED TO DETERMINE THAT THE REQUIRED LEVEL OF CONFIDENCE HAS BEEN OBTAINED

AP-SIII.10Q identifies several criteria that can be utilized to show that the level of confidence has been achieved. Criterion 5.3.3.c.6 is appropriate for this model. This criterion states:

> "Corroboration of abstraction or system model results to the results of the mathematical model(s) from which the abstraction or system model was derived, including cooroboration with results of auxiliary analyses used to provide additional confidence in system model results."

The Technical Work Plan for this report (BSC 2002 [DIRS 161132], Attachment B, Section B6.5) states that the postdevelopment validation activities for the Integrated Waste Package Degradation (IWPD) Model will consist primarily of corroboration of abstraction model results to the results of the validated abstraction model(s) from which the abstraction was derived. Each model will be implemented as specified in the model reports (listed above) which serve as inputs to this report. This is assured by preparation of the model documentation in accordance with the AP-SIII.10Q, *Models*, procedure. This approach is consistent with Section 5.3.3.c.6 of the AP-SIII.10Q, *Models*, procedure.

In addition, the Technical Work Plan (TWP) (BSC 2002 [DIRS 161132], Attachment B, Section B6.3) for this report identified the following criteria to be used to determine that the required level of confidence has been obtained for the IWPD Model. These criteria are primarily related to confidence building during model development although they do provide additional confidence in the IWPD Model results consistent with AP-SIII.10Q, Section 5.3.3.c.6.

> Criterion One: Has each model implemented within the Integrated Waste Package Degradation Model, achieved its required level of confidence?

Criterion Two. Is the model used to evaluate performance unlikely to underestimate the actual degradation and failure of engineered barriers?

Criterion Three: Are the parameters used in the Integrated Waste Package Degradation Model obtained from appropriately controlled sources?

Criterion Four: Is the WAPDEG software within which the Integrated Waste Package Degradation Model is implemented qualified?

7.3 DOCUMENTATION OF ACTIVITIES TO BE PERFORMED TO GENERATE CONFIDENCE IN THE MODEL DURING MODEL DEVELOPMENT

Postdevelopment validation activities for the Integrated Waste Package Degradation (IWPD) Model consist primarily of corroboration of abstraction model results to the results of the validated abstraction model(s) from which the abstraction was derived. Each model was implemented as specified in the model reports (listed above) which serve as inputs to this report. As noted above, the IWPD Model is limited to the general corrosion and stress corrosion cracking of the waste package outer barrier and the drip shield. The abstracted models for each degradation mode in the IWPD Model are exactly those generated in the degradation mode process models. The IWPD Model basically provides the pathway through the degradation modes for TSPA by applying the selected environmental conditions for a collection of waste packages and drip shields. Since the WAPDEG code is validated (qualified), one can be confident that each model was implemented properly. Since the IWPD Model inputs are consistent with those defined in the supporting documents, one can be confident that the models were implemented as specified and with appropriate inputs. Further assurance can be gained from the fact that the model documentation was prepared in accordance with the AP-SIII.10Q, *Models*, procedure.

Among the activities listed in the governing Technical Work Plan (BSC 2002 [DIRS 161132], Attachment B, Section B6.4) to be performed to generate confidence in the model during model development are:

- Simulations with various numbers of waste package and drip shield pairs for the purpose of determining the appropriate number of waste package and drip shield pairs to use in nominal simulations.

- Simulations with various numbers of waste package and drip shield “patches” for the purpose of determining the appropriate number of patches to use in nominal simulations.

The simulations referred to in the second bullet (simulations with various numbers of waste package and drip shield patches) are not necessary since the analyses in this report have developed a technical basis for the particular choice of the number of patches used in nominal Integrated Waste Package Degradation (IWPD) Model simulations (Section 6.3.4). The simulations referred to in the first bullet (simulations with various numbers of waste package and drip shield pairs) are relevant and are discussed in Section 6.6.4.

The TWP Criteria One and Three are satisfied by the fact that each document which provides input to the IWPD Model has been documented, checked, and approved in accordance with the AP-SIII.10Q, *Models*, procedure. Similarly, the post-development validation activities for the Integrated Waste Package Degradation Model listed in the TWP (BSC 2002 [DIRS 161132], Attachment B, Section B6.5) which consist of corroboration of abstraction model results to the results of the validated abstraction model(s) from which the abstraction was derived. Each model was implemented within the WAPDEG code as specified in the documents (listed previously), which serve as inputs to this report. Since the WAPDEG code is validated (qualified), full model validation results from verification that the WAPDEG inputs are consistent with those defined in these supporting documents. This is assured by preparation of the model documentation in accordance with AP-SIII.10Q and by the checking process outlined in AP-SIII.10Q. Therefore the answer to the questions posed by Criteria One and Three are "YES."

TWP Criterion Two is satisfied by the use of conservative modeling assumptions such as

- No performance credit is taken for the stainless steel inner vessel after breach of the waste package outer barrier (Section 6.3).

- The waste package surface area used in this report ignores the area of the lid regions (Section 6.3.2). This results in a conservative measure of the fraction of WP surface area subjected to stress corrosion cracking.

- The general corrosion rate re-scaling for patch size (Section 6.3.4) effectively results in the highest of four sampled general corrosion rates being used for each modeled patch.

- The distribution of general corrosion rates for Alloy 22 obtained from specimens exposed at both 60 and 90°C is applied at 60°C (Section 6.3.4).

- The stress and stress intensity profiles are not readjusted for the effects of progressive wall thinning due to general corrosion

Therefore the answer to the question posed by Criterion Two is "YES."

TWP Criterion Four is satisfied by consultation of the Baseline of Qualified Software maintained by the Project's Software Configuration management Department and consultation of the Document Input Reference System for documents relevant to the qualification of WAPDEG V. 4.07 (e.g., BSC 2002 [DIRS 161240] and BSC 2002 [DIRS 162606]), CWD V. 2.0 (e.g., BSC 2003 [DIRS 162809]), SCCD V. 2.01 (e.g., BSC 2000 [DIRS 161757]), and GoldSim V. 7.50.100 (e.g., BSC 2003 [DIRS 161572]). Therefore the answer to the question posed by Criterion Four is "YES."

On this basis, the validation criteria from AP-SIII.10Q related to corroboration and the validation criteria listed in the TWP governing this report (BSC 2002 [DIRS 161132], Attachment B, Section B6) have been satisfied and the IWPD Model is valid for use in TSPA-LA.

7.4 TECHNICAL ERROR REPORTS ADDRESSED

Technical Error Report TER-02-0015 is addressed in this report. The description of the technical error identified two issues:

1. Subsequent to preparation of the previous version of this report, an independent model validation review indicated that the model validation was not consistent with the *Models* procedure (now AP-SIII.10Q).

2. The previous version of this report was classified as Bin 3 per the *Model Validation Status Review* (BSC 2001 [DIRS 156257], Section 6.10.8). This classification was a result of the assertion that a model (having to do with SCC of weld regions) was missing that should have been incorporated (BSC 2001 [DIRS 156257], Section 6.10.8).

TER-02-0015 Issue 1 is satisfied by the issuance of this report and its preparation in accordance with the AP-SIII.10Q, *Models* procedure.

TER-02-0015 Issue 2 is satisfied by the fact that the *WAPDEG Analysis of Waste Package and Drip Shield Degradation* report uses the outputs from model reports (see Section 6.1) which have also been prepared and validated in accordance with the AP-SIII.10Q, *Models* procedure. That is the model reports which provide input to this report have been determined to be complete and appropriate for their intended use.

8. CONCLUSIONS

8.1 MODEL OUTPUTS

The results of all outputs documented in this report are tracked by DTN: MO0310MWDWAPAN.002 [DIRS 165800]. All distributions sampled within GoldSim are uncertainty distributions and all distributions sampled within the WAPDEG DLL are variability distributions.

8.1.1 Developed Outputs

The outputs discussed in this section are inputs to the TSPA Integrated Waste Package Degradation (IWPD) Model implementation.

8.1.1.1 Nominal Integrated Waste Package Degradation Model Outputs

Since the Integrated Waste Package Degradation (IWPD) Model is implemented directly in the TSPA Model, the inputs to the IWPD Model are outputs to the TSPA Model documentation. For example, the files identified in the Linked_Files container element (Figure 23), are inputs to the IWPD Model and must accompany the TSPA Model if the IWPD Model is to be run properly within the TSPA Model. Therefore the files identified in the Linked_Files container element (Figure 23) would also be documented in the TSPA Model documentation since they serve as inputs to the IWPD Model component of the larger TSPA Model. The primary outputs of this report are the WAPDEG input vector (Table I-1) and the external input files which must accompany the IWPD Model GoldSim implementation (Attachment II).

In addition, the contents of the IWPD Model GoldSim implementation are outputs of this report.

The elements in the Linked_Files container element (Figure 23) and their values are listed in Table 32.

Table 32. Contents of Linked_Files Container

Element Name	Description	Value
WAP_File	List of filenames	WD4DLL.WAP (see Attachment II)
WDKlinO	Stress intensity vs depth for outer lid	WDKlinO.fil (see Attachment II)
WDKlinM	Stress intensity vs depth for middle lid	WDKlinM.fil (see Attachment II)
WDhist	List of T/RH files	WDenv_00_07wheader.ou (it is expected that TSPA will generate their own list of T/RH files)
LnRo	CDF for the natural logarithm of the general corrosion rate for Alloy 22	WDlnRGC.cdf (see Attachment II)

The elements in the GS_Elements container element (Figure 24) and their values are listed in Table 33.

Table 33. Contents of GS_Elements Container

Element Name	Description	Value
Number_DS_Patches	Number of patches per drip shield	1
SimTime	Length of Simulation (years)	1.0E7
BinStart	Start time for bins (years)	1000
NumBins	Number of log-spaced time bins in WAPDEG tables	300
Cracks_per_Patch_Factor	Number of cracks per patch for middle lid	15

The GoldSim elements which do not vary with WP configuration (i.e. CSNF or CDSP) are treated in separate container elements as illustrated in Figure 26. The elements in Figure 26 and their values are listed in Table 34.

Table 34. Contents of WP_Degradation Container (see Figure 26)

Element Name	Description	Value
MIC_A22	MIC general corrosion enhancement factor	Uniform between 1 and 2
Gen_Corr_DS (Container)	General corrosion of the DS	See Table 35
Gen_Corr_WPOB (Container)	General corrosion of the WPOB	See Table 36
CWD (Container)	Closure Weld Defect treatment	See Table 37
SCC (Container)	SCC Inputs	See Table 38
IWPD_CSNF (Container)	Inputs for CSNF WP modeling	See Table 41
IWPD_CDSP (Container) (not shown in Figure 26)	Inputs for CDSP WP modeling	See Table 42

The elements in the Gen_Corr_DS container element (Figure 27) and their values are listed in Table 41.

Table 35. Contents of the Gen_Corr_DS Container Element

Element Name	Description	Value
WDDSOutGC	Outside surface general corrosion rate	CDF in Table 5 of

Element Name	Description	Value
	for DS	this report
WDDSInGC	Inside surface general corrosion rate for DS	CDF in Table 4 of this report

The elements in the Gen_Corr_WPOB container element (Figure 28) and their values are listed in Table 36.

Table 36. Contents of the Gen_Corr_WPOB Container Element

Element Name	Description	Value
C1_GenCorr_A22	Slope term for T-dependent Alloy 22 general corrosion	See Table 7
C1divTo_GenCorr_A22	Constant term (per realization) for Alloy 22 general corrosion rate	C1_GenCorr_A22/333.15

The elements in the CWD container element (Figure 29) and their values are listed in Table 37.

Table 37. Contents of the CWD Container Element

Element Name	Description	Value
Thickness_ML	Middle lid thickness (mm) (CWD input)	10
Thickness_OL	Outer lid thickness (mm) (CWD input)	25
Defect_Count_Param	Flaw density parameter (flaws per mm^3 of weld) (CWD input)	Gamma distribution with a mean of 7.5/18610540.3277924 and a standard deviation of sqrt(7.5)/18610540.3277924
Defect_Size_Param	Flaw size parameter (1/mm) (CWD input)	Gamma distribution with a mean of 7/31.75 and a standard deviation of sqrt(7)/31.75
Location_PND	Characteristic flaw size for UT PND (mm) (CWD input)	2.5
Shape_PND	Shape factor for probability of non-detection (CWD input)	3
Detection_Thresh_PND	Lower limit for UT probability of non-detection (CWD input)	0.005
Defect_Frac_Orientation	Fraction of defects capable of propagation based on orientation	0.008
Defect_Frac_Embedded	Fraction of embedded manufacturing defect flaws to propagate	0.25
Defect_Frac	Fraction of defects capable of propagation (CWD input)	Defect_Frac_Embedded*Defect_Frac_Orientation

The elements in the SCC container element (Figure 31) and their values are listed in Table 38.

Table 38. Contents of the SCC Container Element

Element Name	Description	Value
n_SCC	SCC growth rate exponent (repassivation rate)	Truncated normal (at ±2 sd) with a mean of 1.304 and sd of 0.16.
Abar_SCC	SCC growth rate pre-exponent	(7.8E-2) * ((n_SCC)^3.6) * ((4.1E-14)^(n_SCC)) *60*60*24*365.25
nbar_SCC	4*n	4*n_SCC
KI_Thresh_SCC	Stress Intensity Factor Threshold	(7.23E-06/Abar_SCC)^(1/nbar_SCC)
Yield_Strength_A22	Yield Strength of Alloy 22 (MPa)	285
Stress_Thresh_SCC	Stress threshold for SCC nucleation	0.9*Yield_Strength_A22

Element Name	Description	Value
	(MPa)	
SCC_Outer_Lid (Container)	SCC Inputs for Outer Lid	See Table 39
SCC_Middle_Lid (Container)	SCC Inputs for Middle Lid	See Table 40

The elements in the SCC_Outer_Lid container element (Figure 32) and their values are listed in Table 39.

Table 39. Contents of the SCC_Outer_Lid Container Element

Element Name	Description	Value
z_OL	Uncertain deviation from median yield strength range for outer lid (SCCD input)	Truncated normal (at ±3 sd) with a mean of 0 and sd of 1
Num_Angles_OL	Number of angles at which stress intensity factor will be evaluated for outer lid (SCCD input)	5
KI_inp_OL	Line number in WD4DLL.WAP file of the stress intensity factor (KI) versus depth profiles for the outer lid (WDKIinO.fil) (SCCD input)	4
sinf_OL	Sine of the angle of projection that the crack path makes with the outer lid normal (SCCD input)	1
A0_OL	Outer lid stress coefficient (SCCD input)	-292.607
A1_OL	Outer lid stress coefficient (SCCD input)	178.277
A2_OL	Outer lid stress coefficient (SCCD input)	-14.135
A3_OL	Outer lid stress coefficient (SCCD input)	0.320
fys_OL	Outer lid yield strength scaling factor (SSCD input)	0.15
amp_OL	Amplitude of the stress variation with angle, for the outer lid (SCCD input)	17.236893
KI_out_OL	Line number in WD4DLL.WAP file of the filename outer lid KI vs depth profile (SCCD output, WAPDEG input)	6
Stress_out_OL	Line number in WD4DLL.WAP file of the filename for outer lid stress vs depth profile (SCCD output, WAPDEG input)	7
Model_Number_OL	SCC uncertainty model number for outer lid (SCCD input)	1

The elements in the SCC_Middle_Lid container element and their values are listed in Table 40.

Table 40. Contents of the SCC_Middle_Lid Container Element

Element Name	Description	Value
z_ML	Uncertain deviation from median yield strength range for middle lid (SCCD input)	Truncated normal (at ±3 sd) with a mean of 0 and sd of 1
Num_Angles_ML	Number of angles at which stress intensity factor will be evaluated for middle lid (SCCD input)	5
KI_inp_ML	Line number in WD4DLL.WAP file of the stress intensity factor (KI) versus depth profiles for the middle lid (WDKIinO.fil) (SCCD input)	5

Element Name	Description	Value
sinf_ML	Sine of the angle of projection that the crack path makes with the middle lid normal (SCCD input)	1
A0_ML	Middle lid stress coefficient (SCCD input)	219.908
A1_ML	Middle lid stress coefficient (SCCD input)	56.494
A2_ML	Middle lid stress coefficient (SCCD input)	-20.848
A3_ML	Middle lid stress coefficient (SCCD input)	1.083
fys_ML	Middle lid yield strength scaling factor (SSCD input)	0.15
amp_ML	Amplitude of the stress variation with angle, for the middle lid (SCCD input)	17.236893
KI_out_ML	Line number in WD4DLL.WAP file of the filename outer lid KI vs depth profile (SCCD output, WAPDEG input)	8
Stress_out_ML	Line number in WD4DLL.WAP file of the filename for middle lid stress vs depth profile (SCCD output, WAPDEG input)	9
Model_Number_ML	SCC uncertainty model number for middle lid (SCCD input)	1

The elements in the IWPD_CSNF container element (Figure 25) and their values are listed in Table 41.

Table 41. Contents of IWPD_CSNF Container

Element Name	Description	Value
Hist_Index_CSNF	Line number in WD4DLL.WAP file of the filename for the thermal hydrologic and chemistry time history file	1
WDSeed_CSNF	WAPDEG Seed CSNF	Uniform between 1 and $2^{31}-1$
NumPak_CSNF	Number of CSNF waste packages	Expected to be set by TSPA Model
CWD_CSNF (Container)	Closure weld defects treatment for CSNF WPs	See Table 43
WAPDEG_Inputs_CSNF	Input vector to WAPDEG.DLL CSNF	See Attachment I, Table I-1

The elements in the IWPD_CDSP container element and their values are listed in Table 42.

Table 42. Contents of IWPD_CDSP Container Element

Element Name	Description	Value
Hist_Index_CDSP	Line number in WD4DLL.WAP file of the filename for the thermal hydrologic and chemistry time history file	1
WDSeed_CDSP	WAPDEG Seed CDSP	Uniform between 1 and $2^{31}-1$
NumPak_CDSP	Number of CDSP waste packages	Expected to be set by TSPA Model
CWD_CDSP (Container)	Closure weld defects treatment for CDSP	See Table 44
WAPDEG_Inputs_CDSP	Input vector to WAPDEG.DLL CDSP	See Attachment I, Table I-1

The elements in the CWD_CSNF container element (Figure 30) and their values are listed in Table 43.

Table 43. Contents of CWD_CSNF Container Element

Element Name	Description	Value
Vol_Weld_OL_CSNF	Volume of outer lid weld for CSNF WP (CWD input) (mm^3)	1350189
Defect_Num_OL_CSNF	Line number in WD4DLL.WAP file of the filename for CDF of the number of outer lid manufacturing defect flaws for CSNF WPs (CWD output)	10
Defect_Size_OL_CSNF	Line number in WD4DLL.WAP file of the filename for CDF of the length of outer lid manufacturing defect flaws for CSNF WPs (CWD output)	11
Vol_Weld_ML_CSNF	Volume of middle lid weld for CSNF WPs (CWD input) (mm^3)	490478
Defect_Num_ML_CSNF	Line number in WD4DLL.WAP file of the filename for CDF of the number of middle lid manufacturing defect flaws for CSNF WPs (CWD output)	12
Defect_Size_ML_CSNF	Line number in WD4DLL.WAP file of the filename for CDF of the length of middle lid manufacturing defect flaws for CSNF WPs (CWD output)	13

The elements in the CWD_CDSP container element and their values are listed in Table 44.

Table 44. Contents of CWD_CDSP Container Element

Element Name	Description	Value
Vol_Weld_OL_CDSP	Volume of outer lid weld for CDSP WP (CWD input) (mm^3)	1753091
Defect_Num_OL_CDSP	Line number in WD4DLL.WAP file of the filename for CDF of the number of outer lid manufacturing defect flaws for CDSP WP (CWD output)	14
Defect_Size_OL_CDSP	Line number in WD4DLL.WAP file of the filename for CDF of the length of outer lid manufacturing defect flaws for CDSP WP (CWD output)	15
Vol_Weld_ML_CDSP	Volume of middle lid weld for CDSP WP (CWD input) (mm^3)	639901
Defect_Num_ML_CDSP	Line number in WD4DLL.WAP file of the filename for CDF of the number of middle lid manufacturing defect flaws for CDSP WP (CWD output)	16
Defect_Size_ML_CDSP	Line number in WD4DLL.WAP file of the filename for CDF of the length of middle lid manufacturing defect flaws for CDSP WP (CWD output)	17

It is recommended that the WAPDEG DLL be called twice (i.e. once for CSNF and once for CDSP WPs) for each region of the potential repository (i.e. each unique set of thermal hydrologic history files) to be simulated. The input to the WAPDEG DLL consists of the elements in the IWPD_CSNF (Figure 25) (or IWPD_CDSP) container element and the external files created by calls to the CWD DLL (for outer lid of CSNF WPs: WDCWDNDO_CSNF.cdf and WDCWDSizeO_CSNF.cdf; for middle lid of CSNF WPs: WDCWDNDM_CSNF.cdf and WDCWDSizeM_CSNF.cdf; for outer lid of CDSP WPs: WDCWDNDO_CDSP.cdf and WDCWDSizeO_CDSP.cdf; for middle lid of CDSP WPs: WDCWDNDM_CDSP.cdf and WDCWDSizeM_CDSP.cdf) and SCCD DLL (for outer lid: WDKISCCO.fil and WDStressO.fil; for middle lid: WDKISCCM.fil and WDStressM.fil).

8.1.1.2 Waste Package Localized Corrosion Model Outputs

The crevice repassivation potential (E_{rcrev}) is expressed as follows.

$$E_{rcrev} = E^{o}_{rcrev} + \Delta E^{NO_3^-}_{rcrev} \qquad \text{(Eq. 73)}$$

where E^{o}_{rcrev} is the crevice repassivation potential.

The crevice repassivation potential in the absence of nitrate ions is

$$E^{o}_{rcrev} = a_o + a_1 T + a_2 pH + a_3 \log([Cl^-]) + a_4 T \times \log([Cl^-]) \qquad \text{(Eq. 74)}$$

where E^{o}_{rcrev} is in mV vs. the Silver-Silver Chloride (SSC) reference electrode, a_o, a_1, a_2, a_3, and a_4 are constants, T is the temperature (°C), and $[Cl^-]$ is the chloride ion concentration. The median estimated regression coefficients are: a_o = 214.089, a_1 = -3.696, a_2 = 25.284, a_3 = -252.181, and a_4 = 1.414. The covariance matrix resulting from the least squares fitting was determined to be

$$CV = \begin{bmatrix} 2197.7 & -15.159 & -83.254 & -1805.2 & 15.897 \\ -15.159 & 0.22667 & -1.2402 & 18.767 & -0.19963 \\ -83.254 & -1.2402 & 31.826 & -32.372 & 0.74246 \\ -1805.2 & 18.767 & -32.372 & 2906.5 & -28.677 \\ 15.897 & -0.19963 & 0.74246 & -28.677 & 0.29946 \end{bmatrix} \qquad \text{(Eq. 75)}$$

The lower triangular Cholesky factorization, T, of the covariance matrix (such that $T{\cdot}T^T = CV$) is given below.

$$T = \begin{bmatrix} 46.8796331 & 0 & 0 & 0 & 0 \\ -0.32336004 & 0.34943996 & 0 & 0 & 0 \\ -1.7759098 & -5.19247503 & 1.3078025 & 0 & 0 \\ -38.50712731 & 18.07272935 & -5.28748716 & 32.69740173 & 0 \\ 0.33910248 & -0.25749147 & 0.00585517 & -0.33441816 & 0.07935909 \end{bmatrix} \qquad \text{(Eq. 76)}$$

The entire variance of the model is due to uncertainty. It is recommended that the uncertainty of the parameter coefficients of the above model be limited to ±2 sd.

$\Delta E^{NO_3^-}_{rcrev}$ is given by

$$\Delta E^{NO_3^-}_{rcrev} = b_o + b_1 [NO_3^-] + b_2 \frac{[NO_3^-]}{[Cl^-]} \qquad \text{(Eq. 77)}$$

where $\Delta E^{NO_3^-}_{rcrev}$ is in mV vs. SSC, b_o, b_1 and b_2 are constants and other parameters are defined as before. The parameter coefficients resulting from the fitting procedure were determined to be: b_0 = -50.959, b_1 = 115.867, and b_2 = 1045. The linear relationship between $\Delta E^{NO_3^-}_{rcrev}$ and the concentration ratio is applicable for concentration ratios between 0.1 and 1.0. Only the mean value of the $\Delta E_{rcrev}^{NO_3^-}$ is used to determine the crevice repassivation potential (E_{rcrev}).

Variability in the crevice repassivation potential among waste packages is included through the temporally and spatially varying waste package temperature and chemistry exposure conditions.

The long-term corrosion potential model (E_{corr}) for the WPOB is expressed as follows

$$E_{corr} = c_o + c_1 T + c_2 pH + c_3 [Cl^-] + c_4 \log\left(\frac{[NO_3^-]}{[Cl^-]}\right) \quad \text{(Eq. 78)}$$

where E_{corr} is the long-term corrosion potential in mV vs. SSC, c_o, c_1, c_2, c_3, and c_4 are coefficients of the model parameters, and other parameters are defined as before. The median estimated regression coefficients are: $c_0 =$ 365.511, $c_1 =$ 1.853, $c_2 =$ -48.091, $c_3 =$ -29.641, and $c_4 =$ -4.263. The covariance matrix resulting from the least squares fitting was determined to be

$$CV = \begin{bmatrix} 1082.5 & -10.818 & -31.492 & 0.77527 & -37.167 \\ -10.818 & 0.13976 & -0.029431 & -0.1269 & 0.37478 \\ -31.492 & -0.029431 & 6.3919 & 0.42229 & 0.59728 \\ 0.77527 & -0.1269 & 0.42229 & 3.7299 & 6.1905 \\ -37.167 & 0.37478 & 0.59728 & 6.1905 & 18.711 \end{bmatrix} \quad \text{(Eq. 79)}$$

The lower triangular Cholesky factorization, T, of the covariance matrix (such that $T \cdot T^T = CV$) is given below.

$$T = \begin{bmatrix} 32.90136775 & 0 & 0 & 0 & 0 \\ -0.32880092 & 0.17790434 & 0 & 0 & 0 \\ -0.95716386 & -1.9344517 & 1.31667534 & 0 & 0 \\ 0.02356346 & -0.66975495 & -0.646146 & 1.6921195 & 0 \\ -1.12964909 & 0.01883226 & -0.33990853 & 3.55181823 & 2.16877563 \end{bmatrix} \quad \text{(Eq. 80)}$$

The model *should not be used for short-term transient conditions* (BSC 2003 [DIRS 161235], Section 6.4.4). The entire variance of the model is due to uncertainty. It is recommended that the uncertainty of the parameter coefficients of the corrosion potential model be limited to ±2 sd.

Variability in the corrosion potential among waste packages is included through the temporally and spatially varying waste package temperature and chemistry exposure conditions.

The following limitations are identified for the application of the localized corrosion model for Alloy 22 (BSC 2003 [DIRS 161235], Section 1.2):

- Temperature from 20°C up to boiling temperature of $CaCl_2$-containing brines.
- Solution pH from 2 to 12.

- Chloride concentration from a very low non-zero value to 25 molal (*m*, moles/kg water). A value of 0.001 *m* is recommended for the chloride concentration for solutions with no chloride.
- Nitrate concentration from a very low non-zero value to 6 molal (*m*, moles/kg water). A value of 0.001 *m* is recommended for the nitrate concentration for solutions with no nitrate.
- The nitrate to chloride concentration ratio from zero to 1.0 for the crevice repassivation potential model. For solutions with the ratio greater than 1.0, the ratio is limited to 1.0. This ratio range is not applied to the corrosion potential model.

Note that no localized corrosion of the WPOB is expected for any water chemistries with the nitrate concentration greater than the upper bound (6 *m*). Because only nitrate ions are accounted for in the localized corrosion model for the inhibitive effect, the model results for solutions with significant amounts of other potentially inhibitive ions such as carbonate and sulfate (in addition to nitrate ions) are highly conservative. The model results for the beneficial effects of the inhibitive ions combined with the alkaline pH conditions of the typical carbonate waters in the repository are consistent with the experimental observations on the immunity of Alloy 22 to localized corrosion in those waters (BSC 2003 [DIRS 161235], Section 1.2).

8.1.1.3 Waste Package Early Failure Analysis Outputs

A conceptual model for the waste package early failure analysis may involve the full uncertainty and variability specification as outlined in Section 4.1.9 and developed in Section 6.3.12. Alternatively, use of the marginal probability distribution, developed in Section 6.5.12, allows results to be used in a conditional or stratified approach which would allow for computational efficiencies.

Table 45. Waste Package Early Failure Parameters and Their Sources

Parameter Name	Parameter Source	Parameter Value	Units
Num_Pak_EF Number of packages considered	This is a TSPA model parameter to be specified by TSPA Model at runtime	e.g., 11184 (representative value, see discussion under Parameter Source)	N/A
U_EF_Mean Evaluation probability per WP (Uncertain Poisson intensity)	BSC 2003 [DIRS 164475], Section 7, Table 20	Log normal distribution with a geometric mean of 7.2×10^{-6} and a geometric sd of 15^(1/1.645) truncated at 7.44213E-3	per WP
NumEFPaks Number of Early Failed WP in the realization	BSC 2003 [DIRS 164475], Section 7, Table 20	Poisson distribution with intensity Num_Pak_EF*U_EF_Mean	# WP/realization
Fractional_EF Fraction of Early Failed WP in the realization	This report	NumEFPaks/Num_Pak_EF	fraction of WP/realization

Table 46. Early Failure Waste Package Unconditional Probability Values

n (Number of WPs)	p(n)
0	0.830177156
1	0.114170546
2	0.029481907
≥3	0.026170391

Table 47. Early Failure Waste Package Conditional pdf

Conditional Probability	Number of WPs
6.72292043249447E-01	1
1.73603896475176E-01	2
6.62102251738378E-02	3
3.16781457051218E-02	4
1.74664265480460E-02	5
1.05986309693713E-02	6
6.88874646926455E-03	7
4.71473222137090E-03	8
3.35923480253975E-03	9
2.47181818957650E-03	10
1.86749677986347E-03	11
1.44237040765972E-03	12
1.13503969252866E-03	13
9.07649803289940E-04	14
7.36008651370934E-04	15
6.04171817640069E-04	16
5.01345905459817E-04	17
4.20051218756154E-04	18
3.54995977674767E-04	19
3.02366678546451E-04	20
2.59369367847244E-04	21
2.23926363184013E-04	22
1.94471645187147E-04	23
1.69810267359572E-04	24
1.49020132777530E-04	25
1.31382319712795E-04	26
1.16330965064662E-04	27
1.03416750621992E-04	28
9.22799833021864E-05	29
8.26305297934502E-05	30
7.42327072291007E-05	31
6.68937973539920E-05	32
6.04552375285604E-05	33
5.47858084815550E-05	34
4.97763250833152E-05	35
4.53354681692636E-05	36
4.13864895817636E-05	37
3.78645905269958E-05	38
3.47148228178331E-05	39
3.18903989250389E-05	40
2.93513236906451E-05	41
2.70632806669899E-05	42
2.49967211722396E-05	43
2.31261156125399E-05	44
2.14293353591146E-05	45
1.98871401733203E-05	46
1.84827513472259E-05	47
1.72014947430197E-05	48
1.60305010475418E-05	49
1.49584530155581E-05	50
1.39753714138465E-05	51
1.30724329177318E-05	52
1.22418144452487E-05	53
1.14765594142005E-05	54
1.07704622310122E-05	55

Conditional Probability	Number of WPs
1.01179680120012E-05	56
9.51408513147726E-06	57
8.95430871137521E-06	58
8.43455362935730E-06	59
7.95109603336955E-06	60
7.50052270944795E-06	61
7.07968794836482E-06	62
6.68567778292314E-06	63
6.31578160673403E-06	64
5.96747122389443E-06	65
5.63838730892199E-06	66
5.32633307799113E-06	67
5.02927469761981E-06	68
4.74534760973451E-06	69
4.47286756875376E-06	70
4.21034481259677E-06	71
3.95649947572606E-06	72
3.71027614758051E-06	73
3.47085542520984E-06	74
3.23766043150573E-06	75
3.01035657795550E-06	76
2.78884332947732E-06	77
2.57323734345134E-06	78
2.36384705234588E-06	79
2.16113947409198E-06	80
1.96570069703811E-06	81
1.77819203158221E-06	82
1.59930419528470E-06	83
1.42971206779268E-06	84
1.27003250396409E-06	85
1.12078743904329E-06	86
9.82374090487728E-07	87
8.55043505290756E-07	88
7.38888077500076E-07	89
6.33838028935228E-07	90
5.39666263494115E-07	91
4.56000518554527E-07	92
3.82341378459289E-07	93
3.18084501625250E-07	94
2.62545345353809E-07	95
2.14984738019739E-07	96
1.74633823455080E-07	97
1.40717156867760E-07	98
1.12473032823898E-07	99
8.91704420953614E-08	100
7.01223580113182E-08	101
5.46953228642639E-08	102
4.23155263966068E-08	103
3.24717339289036E-08	104
2.47155300757037E-08	105
1.86593991019425E-08	106
1.39731722870978E-08	107
1.03793457798317E-08	108
7.64771967930777E-09	109
5.58974043798139E-09	110
4.05285294051235E-09	111

8.2 SUMMARY

A conceptual model for the nominal case analysis of degradation of drip shield and waste package in the Yucca Mountain repository was developed, incorporating the data and analyses of the individual degradation processes documented in the companion process-level model reports (BSC 2003 [DIRS 161234]; BSC 2003 [DIRS 161235]; BSC 2003 [DIRS 161236]). The conceptual model and the abstractions of the process-level models and their parameters were incorporated into the Integrated Waste Package Degradation (IWPD) Model. The IWPD Model analysis was conducted to develop a detailed description of waste package and drip shield degradation and to develop the degradation abstractions as input to the total system performance assessment (TSPA) analysis.

It should be noted that the results of the analyses documented in Section 6.6 are for illustrative purposes only. The drip shield and waste package degradation profiles presented in this Section 6.6 result from the use of representative thermal hydrologic history files (Section 6.3.13) produced for the purpose of allowing the IWPD Model to be exercised in this report. The actual drip shield and waste package degradation profiles which will be used in the TSPA-LA Model will make use of the actual thermal hydrologic history files appropriate for the repository. Also the results of the localized corrosion (pitting and crevice corrosion) are not presented in this report because evaluation of this degradation mode would require (in addition to of the actual thermal hydrologic history files appropriate for the repository) in-drift geochemical inputs which will only be available to TSPA. Therefore, the localized corrosion model is implemented directly in TSPA. However, the localized corrosion initiation and propagation models for the waste package outer barrier are discussed in Sections 4.1.4 and 6.3.6 and the rationale for exclusion of localized corrosion of the drip shield material is discussed in Section 6.3.5. Nonetheless the drip shield and waste package degradation profiles presented in this Section 6.6 provide evidence that the IWPD Model implementation functions properly.

The waste package and drip shield degradation analyses documented in this report have shown that based on the current general corrosion and stress corrosion cracking model abstractions and modeling assumptions, neither the drip shields nor the waste packages fail within the regulatory time period (10,000 years). The effects of igneous and seismic events and localized corrosion on drip shield and waste package performance were not evaluated in this report. The candidate materials for the drip shield (Titanium Grade 7) and the waste package outer barrier (Alloy 22) are highly corrosion resistant and, under the repository exposure conditions, are not expected to be subject to the degradation processes that, if initiated, could lead to failure within the regulatory time period. Those degradation modes are localized corrosion and stress corrosion cracking (SCC). Both the drip shield and waste package degrade by general corrosion at very low passive dissolution rates. The current experimental data and detailed process-level analyses, upon which the model abstractions incorporated in the IWPD Model are based, are consistent with this conclusion. With the exception of early failure processes (Section 6.3.12), only the closure-lid welds of the waste package, for which complete stress mitigation may not be possible, may be subject to rapidly penetrating corrosion modes under the expected repository conditions (BSC 2003 [DIRS 161234]). Because of potential residual stresses, the closure-lid welds would be subject to SCC.

A dual closure-lid design for the waste package outer barrier has been used, and stress mitigation techniques have been proposed for the outer closure lid weld region. The numerical modeling-based analyses have shown that the hoop stress (driving radial cracks) is the dominant stress in the closure-lid welds that could cause SCC failure of waste package. The analyses also have shown that the above stress mitigation techniques can achieve a substantial stress relief for the closure-lid welds (BSC 2003 [DIRS 161234]). Mitigation of the hoop stress in the Alloy 22 waste package outer barrier outer closure-lid welds has resulted in a stress state such that the corresponding stress intensity factor for the radial crack is negative to a depth of 3 mm from the surface(Figure 15). In the waste package degradation analysis, for a smooth surface without the presence of manufacturing defects, no SCC cracks initiate in the closure-lid welds until the surface layer with a residual stress state less than the stress threshold (0.9*285 MPa = 256.5 MPa) is removed by general corrosion (Figure 13 and Figure 14).

8.3 YUCCA MOUNTAIN REVIEW PLAN CRITERIA

The Waste Package Technical Work Plan (TWP) (BSC 2002 [DIRS 161132], Attachment C, Table C5) has identified acceptance criteria (AC) based on the requirements mentioned in the *Project Requirements Document* (PRD) (Canori and Leitner 2003 [DIRS 161770]) and the *Yucca Mountain Review Plan* (NRC 2003 [DIRS 163274]) (Section 4.2). In this Section, the Sections within this report are identified which address these criteria.

1. System Description and Demonstration of Multiple Barriers (NRC 2003 [DIRS 163274], Section 2.2.1.1.3; Canori and Leitner 2003 [DIRS 161770], PRD-002/T-014, PRD-002/T-016)

   - AC1: Identification of Barriers is Adequate
     - The DS and WP barriers are adequately identified in Section 1.1 and are discussed in more detail in Sections 4.1.1, 6.1, and 6.3.

   - AC2: Description of Barrier Capability to Isolate Waste is Acceptable.
     - The DS and WP description of barrier capability to isolate waste are identified in Section 1.1 and are discussed in Sections 6.1, 6.3, and 6.6. The DS and WP description of barrier capability to isolate waste are summarized in Section 6.7.

   - AC3: Technical Basis for Barrier Capability is Adequately Presented
     - The technical basis for DS and WP barrier capability are discussed throughout this report: proper selection of inputs in Section 4; extensive discussion of conceptual models used in Section 6.3; proper implementation in Section 6.5; and analysis of results in Section 6.6.

2. Degradation of Engineered Barriers (NRC 2003 [DIRS 163274], Section 2.2.1.3.1.3; Canori and Leitner 2003 [DIRS 161770], PRD-002/T-015)

   - AC1: System Description and Model Integration are Adequate
     - The DS and WP system description are adequately identified in Section 1.1 and are discussed in more detail in Sections 4.1.1, 6.1, and 6.3. Model integration issues are addressed in Sections 6.3 and 6.5.

- AC2: Data are Sufficient for Model Justification
  - The data used in the IWPD Model are listed in Section 4.1.1. These data were sufficient to build the Integrated Waste Package Degradation (IWPD) Model described in Sections 6.3 and 6.5. The data and parameters result from activities conducted under a quality assurance program. On this basis the data used are sufficient for justification of the IWPD Model.

- AC3: Data Uncertainty is Characterized and Propagated Through the Model Abstraction
  - The data used in the IWPD Model, including their characterized uncertainty treatments, are listed in Section 4.1.1. The characterized uncertainty treatments are inputs to this report meaning that the characterized uncertainty treatments are implemented within the IWPD Model as specified in the process models feeding this report. The characterized uncertainty treatments are implemented within the IWPD Model (Sections 6.3 and 6.5). On this basis data uncertainty is appropriately characterized and propagated through the model abstraction (IWPD Model).

- AC4: Model Uncertainty is Characterized and Propagated Through the Model Abstraction
  - The models implemented within the IWPD Model, including their characterized uncertainty treatments, are listed in Section 4.1.1. The characterized uncertainty treatments are inputs to this report meaning that the characterized uncertainty treatments are implemented within the IWPD Model as specified in the process models feeding this report. The characterized uncertainty treatments are implemented within the IWPD Model (Sections 6.3 and 6.5). On this basis model uncertainty is appropriately characterized and propagated through the model abstraction (IWPD Model).

- AC5: Model Abstraction Output is Supported by Objective Comparisons
  - The models implemented within the IWPD Model, including their characterized uncertainty treatments, are listed in Section 4.1.1. The characterized uncertainty treatments are inputs to this report meaning that the characterized uncertainty treatments are implemented within the IWPD Model as specified in the process models feeding this report. One notable exception is the use of a patch size which is about four times the size of the crevice geometry samples used to generate the distribution of rates used to model general corrosion of the WPOB (Section 6.3.4). In this instance, a comparison was made between the input general corrosion rate distribution and that resulting from the abstraction methodology (Figure 4). The model abstractions are discussed in Sections 6.3 and 6.5. Model results are presented in Section 6.6. On this basis model abstraction output is supported by objective comparisons (where necessary) in this report.

3. Quantity and Chemistry of Water Contacting Waste Packages and Waste Forms (NRC 2003 [DIRS 163274], Section 2.2.1.3.3.3; Canori and Leitner 2003 [DIRS 161770], PRD-002/T-015)

   The consequences of the Quantity and Chemistry of Water Contacting Waste Packages and Waste Forms are addressed in this report. The consequences include general corrosion, stress corrosion cracking, and localized corrosion.

   - AC1: System Description and Model Integration are Adequate
     - The DS and WP system description are adequately identified in Section 1.1 and are discussed in more detail in Sections 4.1.1, 6.1, and 6.3. Model integration issues are addressed in Sections 6.3 and 6.5.

   - AC2: Data are Sufficient for Model Justification
     - The data used in the IWPD Model are listed in Section 4.1.1. These data were sufficient to build the Integrated Waste Package Degradation (IWPD) Model described in Sections 6.3 and 6.5. The data and parameters result from activities conducted under a quality assurance program. On this basis the data used are sufficient for justification of the IWPD Model.

   - AC3: Data Uncertainty is Characterized and Propagated Through the Model Abstraction
     - The data used in the IWPD Model, including their characterized uncertainty treatments, are listed in Section 4.1.1. The characterized uncertainty treatments are inputs to this report meaning that the characterized uncertainty treatments are implemented within the IWPD Model as specified in the process models feeding this report. The characterized uncertainty treatments are implemented within the IWPD Model (Sections 6.3 and 6.5). On this basis data uncertainty is appropriately characterized and propagated through the model abstraction (IWPD Model).

   - AC4: Model Uncertainty is Characterized and Propagated Through the Model Abstraction
     - The models implemented within the IWPD Model, including their characterized uncertainty treatments, are listed in Section 4.1.1. The characterized uncertainty treatments are inputs to this report meaning that the characterized uncertainty treatments are implemented within the IWPD Model as specified in the process models feeding this report. The characterized uncertainty treatments are implemented within the IWPD Model (Sections 6.3 and 6.5). On this basis model uncertainty is appropriately characterized and propagated through the model abstraction (IWPD Model).

   - AC5: Model Abstraction Output is Supported by Objective Comparisons
     - The models implemented within the IWPD Model, including their characterized uncertainty treatments, are listed in Section 4.1.1. The characterized uncertainty treatments are inputs to this report meaning that the characterized uncertainty

treatments are implemented within the IWPD Model as specified in the process models feeding this report. One notable exception is the use of a patch size which is about four times the size of the crevice geometry samples used to generate the distribution of rates used to model general corrosion of the WPOB (Section 6.3.4). In this instance, a comparison was made between the input general corrosion rate distribution and that resulting from the abstraction methodology (Figure 4). The model abstractions are discussed in Sections 6.3 and 6.5. Model results are presented in Section 6.6. On this basis, model abstraction output is supported by objective comparisons (where necessary) in this report.

9. INPUTS AND REFERENCES

This document may be affected by technical product input information that requires confirmation. Any changes to the document that may occur, as a result of completing the confirmation activities, will be reflected in subsequent revisions. The status of the input information quality may be confirmed by review of the Document Input Reference System database.

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ATTACHMENT I
CONTENTS OF WAPDEG INPUT VECTOR

The contents of the WAPDEG input vector are reproduced below (Table I-1). All values in the WAPDEG input vector are real numbers. Those that do not change, and are not defined by TSPA-LA model components, are explicitly stated. The rest are represented by variable names, defined in the TSPA-LA model itself. Certain of the parameters in the WAPDEG input vector reproduced in Table I-1 depend on the WP configuration (CSNF or CDSP) being simulated. In this case, the value for the CSNF WP is shown first, with the corresponding CDSP WP value given afterwards in brackets.

The DLL links at the end of the vector (i.e. elements 700 and 701) are used to control the calling sequence of the DLLs. Inclusion in the WAPDEG input vector assures that those DLLs are called before WAPDEG is called.

For details of construction of the WAPDEG input vector consult (BSC 2002 [DIRS 162606]).

Table I-1. Contents of WAPDEG Input Vector

Row	Value	Parameter Description	Comments
1	Realization	**Realization Number**	
2	2	**Number of Barriers**	
3	1	**Barrier Type**	**A22 OB**
4	25	Barrier Thickness	mm
5	0.75	Barrier Mechanical Failure Fraction	fraction
6	1000	Barrier Pit Density Distribution Index	Fixed
7	0	Parameter 1	/mm^2
8	0	Parameter 2	
9	0	Parameter 3	
10	0	Parameter 4	
11	1000	Barrier Crack Density Distribution Index	Fixed
12	6	Parameter 1	/mm^2
13	0	Parameter 2	
14	0	Parameter 3	
15	0	Parameter 4	
16	2	**Barrier Type**	**A22 IB**
17	10	Barrier Thickness	mm
18	0.75	Barrier Mechanical Failure Fraction	fraction
19	1000	Barrier Pit Density Distribution Index	
20	0	Parameter 1	/mm^2
21	0	Parameter 2	
22	0	Parameter 3	
23	0	Parameter 4	
24	1000	Barrier Crack Density Distribution Index	Fixed
25	15	Parameter 1	/mm^2
26	0	Parameter 2	
27	0	Parameter 3	
28	0	Parameter 4	
29	1014 (1106)	Waste Container Surface Area	mm^2
30	0.484 (0.481)	Waste Container Top Fraction	fraction
31	0.484 (0.481)	Waste Container Bottom Fraction	fraction
32	1000	Waste Container Patch Area Distribution Index	Fixed
33	1	Parameter 1	mm^2
34	0	Parameter 2	
35	0	Parameter 3	
36	0	Parameter 4	

Row	Value	Parameter Description	Comments
37	-1	Apply Size Boolean	TRUE
38	-1	**Drip Shield Present Boolean**	TRUE
39	3	Drip Shield Type	**Ti7 DS**
40	15	Drip Shield Thickness	mm
41	0.75	Drip Shield Mechanical Failure Fraction	fraction
42	1000	Drip Shield Pit Density Distribution Index	Fixed
43	0	Parameter 1	/mm^2
44	0	Parameter 2	
45	0	Parameter 3	
46	0	Parameter 4	
47	1000	Drip Shield Crack Density Distribution Index	Fixed
48	0	Parameter 1	/mm^2
49	0	Parameter 2	
50	0	Parameter 3	
51	0	Parameter 4	
52	Number_DS_Patches	Drip Shield Surface Area	mm^2
53	1	Drip Shield Top Fraction	fraction
54	1000	Drip Shield Patch Size Distribution Index	Fixed
55	1	Parameter 1	mm^2
56	0	Parameter 2	
57	0	Parameter 3	
58	0	Parameter 4	
59	-1	Drip Shield Apply Size Boolean	TRUE
60	1000	Drip Shield Fractional Area Affected Distribution Index	Fixed
61	1	Parameter 1	fraction
62	0	Parameter 2	
63	0	Parameter 3	
64	0	Parameter 4	
65	1	Initial Water Condition under DS	**DSInside**
66	NumPak_CSNF (NumPak_CDSP)	Total Number of Waste Packages	
67	Hist_Index_CSNF (Hist_Index_CDSP)	Index Number of T/H File to Read	
68	1	**Number of Drip Sequences**	
69	1	**Number of Phases - Drip Sequence #1**	
70	1000	Fraction of Top Patches Subject to Sequence Distribution Number	Fixed
71	1	Parameter 1	fraction
72	0	Parameter 2	
73	0	Parameter 3	
74	0	Parameter 4	
75	1000	Fraction of Side Patches Subject to Sequence Distribution Number	Fixed
76	1	Parameter 1	fraction
77	0	Parameter 2	
78	0	Parameter 3	
79	0	Parameter 4	
80	1000	Fraction of Bottom Patches Subject to Sequence Distribution Number	Fixed
81	1	Parameter 1	fraction
82	0	Parameter 2	
83	0	Parameter 3	
84	0	Parameter 4	
85	2	Water Condition for Last Phase	**DSOutside**
86	6	**Number of Corrosion Models**	
87	1	**Water Condition Index Number**	**DSInside**
88	1	Corrosion Mechanism Index (1, 2, or 3)	**General**

Row	Value	Parameter Description	Comments
89	1	Layer Composition Index	**A22 OB**
90	5	Functional Form Index	General Linear
91	2	Number of terms in model	
92	0	Column number for term 1	
93	0	Column number for term 2	
94	2	Number of Levels for Variance Sharing	
95	1000	Barrier Variance Sharing Distribution Index	Fixed
96	0	Parameter1	fraction
97	0	Parameter 2	
98	0	Parameter 3	
99	0	Parameter 4	
100	2500	Term 1 distribution - ln(R)	File CDF
101	18	Parameter 1	WDlnRGC.cdf
102	0	Parameter 2	
103	0	Parameter 3	
104	0	Parameter 4	
105	1000	Term 2 distribution - C1/To	Fixed
106	C1divTo_GenCorr_A22	Parameter 1	
107	0	Parameter 2	
108	0	Parameter 3	
109	0	Parameter 4	
110	0	Sample Type	
111	1000	Error Term Distribution Index	Fixed
112	3.2236191301917E+01	Parameter 1	ln(10^14)
113	0	Parameter 2	
114	0	Parameter 3	
115	0	Parameter 4	
116	1000	Q Term Distribution Index - C1	Fixed
117	C1_GenCorr_A22	Parameter 1	
118	0	Parameter 2	
119	0	Parameter 3	
120	0	Parameter 4	
121	1000	n Distribution Index	Fixed
122	1	Parameter 1	
123	0	Parameter 2	
124	0	Parameter 3	
125	0	Parameter 4	
126	1	**Water Condition Index Number**	**DSInside**
127	1	Corrosion Mechanism Index Number (1, 2, or 3)	**General**
128	2	Layer Composition Index	**A22 IB**
129	5	Functional Form Index	General Linear
130	2	Number of terms in model	
131	0	Column number for term 1	
132	0	Column number for term 2	
133	2	Number of Levels for Variance Sharing	
134	1000	Barrier Variance Sharing Distribution Index	Fixed
135	0	Parameter1	fraction
136	0	Parameter 2	
137	0	Parameter 3	
138	0	Parameter 4	
139	2500	Term 1 distribution - ln(R)	File CDF
140	18	Parameter 1	WDlnRGC.cdf
141	0	Parameter 2	
142	0	Parameter 3	
143	0	Parameter 4	
144	1000	Term 2 distribution - C1/To	Fixed
145	C1divTo_GenCorr_A22	Parameter 1	
146	0	Parameter 2	

Row	Value	Parameter Description	Comments
147	0	Parameter 3	
148	0	Parameter 4	
149	0	Sample Type	
150	1000	Error Term Distribution Index	Fixed
151	-6.93147180559945E-01 (-9.16290731874155E-01)	Parameter 1	ln(10/20) (ln(10/25))
152	0	Parameter 2	
153	0	Parameter 3	
154	0	Parameter 4	
155	1000	Q Term Distribution Index	Fixed
156	C1_GenCorr_A22	Parameter 1	
157	0	Parameter 2	
158	0	Parameter 3	
159	0	Parameter 4	
160	1000	n Distribution Index	Fixed
161	1	Parameter 1	
162	0	Parameter 2	
163	0	Parameter 3	
164	0	Parameter 4	
165	1	**Water Condition Index**	**DSInside**
166	1	Corrosion Mechanism Index (1, 2, or 3)	**General**
167	3	Layer Composition Index	**Ti7 DS**
168	6	Functional Form Index - D = B*t^n	Power Law
169	2	Number of Levels for Variance Sharing	
170	1000	Barrier Variance Sharing Distribution Index	Fixed
171	1	Parameter 1	fraction
172	0	Parameter 2	
173	0	Parameter 3	
174	0	Parameter 4	
175	1000	B Distribution Index	Fixed
176	WDDSInGC	Parameter 1	mm/yr
177	0	Parameter 2	
178	0	Parameter 3	
179	0	Parameter 4	
180	1000	n Distribution Index	Fixed
181	1	Parameter 1	
182	0	Parameter 2	
183	0	Parameter 3	
184	0	Parameter 4	
185	0	Sample Type	
186	2	**Water Condition Index**	**DSOutside**
187	1	Corrosion Mechanism Index (1, 2, or 3)	**General**
188	1	Layer Composition Index	**A22 OB**
189	5	Functional Form Index	General Linear
190	2	Number of terms in model	
191	0	Column number for term 1	
192	0	Column number for term 2	
193	2	Number of Levels for Variance Sharing	
194	1000	Barrier Variance Sharing Distribution Index	Fixed
195	0	Parameter1	fraction
196	0	Parameter 2	
197	0	Parameter 3	
198	0	Parameter 4	
199	2500	Term 1 distribution - ln(R)	File CDF
200	18	Parameter 1	WDlnRGC.cdf
201	0	Parameter 2	
202	0	Parameter 3	
203	0	Parameter 4	

Row	Value	Parameter Description	Comments
204	1000	Term 2 distribution - C1/To	Fixed
205	C1divTo_GenCorr_A22	Parameter 1	
206	0	Parameter 2	
207	0	Parameter 3	
208	0	Parameter 4	
209	0	Sample Type	
210	1000	Error Term Distribution Index	Fixed
211	3.2236191301917E+01	Parameter 1	ln(10^14)
212	0	Parameter 2	
213	0	Parameter 3	
214	0	Parameter 4	
215	1000	Q Term Distribution Index	Fixed
216	C1_GenCorr_A22	Parameter 1	K
217	0	Parameter 2	
218	0	Parameter 3	
219	0	Parameter 4	
220	1000	n Distribution Index	Fixed
221	1	Parameter 1	
222	0	Parameter 2	
223	0	Parameter 3	
224	0	Parameter 4	
225	2	**Water Condition Index Number**	**DSOutside**
226	1	Corrosion Mechanism Index Number (1, 2, or 3)	**General**
227	2	Layer Composition Index	**A22 IB**
228	5	Functional Form Index	General Linear
229	2	Number of terms in model	
230	0	Column number for term 1	
231	0	Column number for term 2	
232	2	Number of Levels for Variance Sharing	
233	1000	Barrier Variance Sharing Distribution Index	Fixed
234	0	Parameter1	
235	0	Parameter 2	
236	0	Parameter 3	
237	0	Parameter 4	
238	2500	Term 1 distribution - ln(R)	File CDF
239	18	Parameter 1	WDlnRGC.cdf
240	0	Parameter 2	
241	0	Parameter 3	
242	0	Parameter 4	
243	1000	Term 2 distribution - C1/To	Fixed
244	C1divTo_GenCorr_A22	Parameter 1	
245	0	Parameter 2	
246	0	Parameter 3	
247	0	Parameter 4	
248	0	Sample Type	
249	1000	Error Term Distribution Index	Fixed
250	-6.9314718055995E-01 (-9.1629073187416E-01)	Parameter 1	ln(10/20) (ln(10/25))
251	0	Parameter 2	
252	0	Parameter 3	
253	0	Parameter 4	
254	1000	Q Term Distribution Index	Fixed
255	C1_GenCorr_A22	Parameter 1	
256	0	Parameter 2	
257	0	Parameter 3	
258	0	Parameter 4	
259	1000	n Distribution Index	Fixed
260	1	Parameter 1	

Row	Value	Parameter Description	Comments
261	0	Parameter 2	
262	0	Parameter 3	
263	0	Parameter 4	
264	2	**Water Condition Index**	**DSOutside**
265	1	Corrosion Mechanism Index (1, 2, or 3)	**General**
266	3	Layer Composition Index	**Ti7 DS**
267	6	Functional Form Index - D = B*t^n	Power Law
268	2	Number of Levels for Variance Sharing	
269	1000	Barrier Variance Sharing Distribution Index	Fixed
270	1	Parameter 1	
271	0	Parameter 2	
272	0	Parameter 3	
273	0	Parameter 4	
274	1000	B Distribution Index	Fixed
275	WDDSOutGC	Parameter 1	mm/yr
276	0	Parameter 2	
277	0	Parameter 3	
278	0	Parameter 4	
279	1000	n Distribution Index	Fixed
280	1	Parameter 1	
281	0	Parameter 2	
282	0	Parameter 3	
283	0	Parameter 4	
284	0	Sample Type	
285	0	**Number of General Thresholds**	
286	0	**Number of Pit Temperature Thresholds**	
287	-1	Inside Out Corrosion Logical	TRUE
288	2	Water Condition for Inside Out Corrosion	**DSOutside**
289	0	Interface Corrosion Logical	FALSE
290	6	**Number of Events**	
291	2	**Manufacturing Defects Event Index**	
292	1	Barrier Type	**A22 OB**
293	2	Number of Water Conditions	
294	1	Condition Number	**DSInside**
295	2	Condition Number	**DSOutside**
296	CWD_OL_CSNF.FlawProb (CWD_OL_CDSP.FlawProb)	Probability that a Waste Package Has Defects	
297	2600	Number of Flaws Distribution Index	
298	10 (14)	Parameter 1	WDCWDNDO_CSNF.cdf (WDCWDNDO_CDSP.cdf)
299	0	Parameter 2	
300	0	Parameter 3	
301	0	Parameter 4	
302	2500	Flaw Size Distribution Index	File CDF
303	11 (15)	Parameter 1	WDCWDSizeO_CSNF.cdf (WDCWDSizeO_CDSP.cdf)
304	0	Parameter 2	
305	0	Parameter 3	
306	0	Parameter 4	
307	0	Immediate Failure Flag (-1 or 0 for true or false)	FALSE
308	0	Number of Localized Corrosion Modes Initiated (0, 1, or 2)	
309	0	Number of Corrosion Modes Accelerated (0, 1, 2, or 3)	
310	0	Number of Thresholds Reduced (0, 1, or 2)	
311	2	**Manufacturing Defects Event Index**	
312	2	Barrier Type	**A22 IB**
313	2	Number of Water Conditions	

Row	Value	Parameter Description	Comments
314	1	Condition Number	**DSInside**
315	2	Condition Number	**DSOutside**
316	CWD_ML_CSNF.FlawProb (CWD_ML_CDSP.FlawProb)	Probability that a Waste Package Has Defects	
317	2600	Number of Flaws Distribution Index	Discrete PDF
318	12 (16)	Parameter 1	WDCWDNDM_CSNF.cdf (WDCWDNDM_CDSP.cdf)
319	0	Parameter 2	
320	0	Parameter 3	
321	0	Parameter 4	
322	2500	Flaw Size Distribution Index	File CDF
323	13 (17)	Parameter 1	WDCWDSizeM_CSNF.cdf (WDCWDSizeM_CDSP.cdf)
324	0	Parameter 2	
325	0	Parameter 3	
326	0	Parameter 4	
327	0	Immediate Failure Flag (-1 or 0 for true or false)	FALSE
328	0	Number of Localized Corrosion Modes Initiated (0, 1, or 2)	
329	0	Number of Corrosion Modes Accelerated (0, 1, 2, or 3)	
330	0	Number of Thresholds Reduced (0, 1, or 2)	
331	5	**SCC (Slip Dissolution) Event Index**	
332	1	Barrier Type	**A22 OB**
333	2	Number of Water Conditions	
334	1	Condition Number	**DSInside**
335	2	Condition Number	**DSOutside**
336	-1	Include MFD and rockfall cracks?	TRUE
337	0	Fraction of top surface area subject to SCC	fraction
338	1	Fraction of side surface area subject to SCC	fraction
339	0	Fraction of bottom surface area subject to SCC	fraction
340	6	File Index for Lookup Table [KI (col1) vs depth (col2)]	WDKISCCO.fil
341	7	File Index for Lookup Table [stress (col1) vs depth (col2)]	WDStressO.fil
342	1000	Barrier Variance Share Distribution Index (A, n)	Fixed
343	1	Parameter 1	fraction
344	0	Parameter 2	
345	0	Parameter 3	
346	0	Parameter 4	
347	1000	Patch Variance Share Distribution Index (A, n)	Fixed
348	0	Parameter 1	fraction
349	0	Parameter 2	
350	0	Parameter 3	
351	0	Parameter 4	
352	1000	A Distribution Index (velocity = A (KI)**n)	Fixed
353	Abar_SCC	Parameter 1	
354	0	Parameter 2	
355	0	Parameter 3	
356	0	Parameter 4	
357	1000	n Distribution Index	Fixed
358	nbar_SCC	Parameter 1	
359	0	Parameter 2	
360	0	Parameter 3	
361	0	Parameter 4	
362	1000	Incipient Crack Size Distribution Index	Fixed
363	0.05	Parameter 1	mm
364	0	Parameter 2	
365	0	Parameter 3	

Row	Value	Parameter Description	Comments
366	0	Parameter 4	
367	0	Sample Type	
368	1000	Barrier Variance Share Distribution Index (for thresholds)	Fixed
369	1	Parameter 1	fraction
370	0	Parameter 2	
371	0	Parameter 3	
372	0	Parameter 4	
373	1000	Stress Threshold Distribution Index (Incipient)	Fixed
374	Stress_Thresh_SCC	Parameter 1	MPa
375	0	Parameter 2	
376	0	Parameter 3	
377	0	Parameter 4	
378	1000	KI Threshold Distribution Index (Incipient)	Fixed
379	KI_Thresh_SCC	Parameter 1	MPa*sqrt(m)
380	0	Parameter 2	
381	0	Parameter 3	
382	0	Parameter 4	
383	1000	Stress Threshold Distribution Index (MFD)	Fixed
384	-600	Parameter 1	MPa
385	0	Parameter 2	
386	0	Parameter 3	
387	0	Parameter 4	
388	1000	KI Threshold Distribution Index (MFD)	Fixed
389	KI_Thresh_SCC	Parameter 1	MPa*sqrt(m)
390	0	Parameter 2	
391	0	Parameter 3	
392	0	Parameter 4	
393	0	Immediate Failure Flag (-1 or 0 for true or false)	FALSE
394	0	Number of Localized Corrosion Modes Initiated (0, 1, or 2)	
395	1	Number of Corrosion Modes Accelerated (0, 1, 2, or 3)	
396	1	General Corrosion Accelerated	
397	1000	Barrier Variance Share Distribution Index	Fixed
398	1	Parameter 1	fraction
399	0	Parameter 2	
400	0	Parameter 3	
401	0	Parameter 4	
402	1000	Acceleration Factor	Fixed
403	1.00E-14	Parameter 1	
404	0	Parameter 2	
405	0	Parameter 3	
406	0	Parameter 4	
407	0	Sample Type	
408	0	Number of Thresholds Reduced (0, 1, or 2)	
409	5	**SCC (Slip Dissolution) Event Index**	
410	2	Barrier Type	**A22 IB**
411	2	Number of Water Conditions	
412	1	Condition Number	**DSInside**
413	2	Condition Number	**DSOutside**
414	1	Include MFD and rockfall cracks?	TRUE
415	0	Fraction of top surface area subject to SCC	fraction
416	1	Fraction of side surface area subject to SCC	fraction
417	0	Fraction of bottom surface area subject to SCC	fraction
418	8	File Index for Lookup Table [KI (col1) vs depth (col2)]	WDKISCCM.fil

Row	Value	Parameter Description	Comments
419	9	File Index for Lookup Table [stress (col1) vs depth (col2)]	WDStressM.fil
420	1000	Barrier Variance Share Distribution Index (A, n)	Fixed
421	1	Parameter 1	
422	0	Parameter 2	
423	0	Parameter 3	
424	0	Parameter 4	
425	1000	Patch Variance Share Distribution Index (A, n)	Fixed
426	0	Parameter 1	
427	0	Parameter 2	
428	0	Parameter 3	
429	0	Parameter 4	
430	1000	A Distribution Index (velocity = A (KI)**n)	Fixed
431	Abar_SCC	Parameter 1	
432	0	Parameter 2	
433	0	Parameter 3	
434	0	Parameter 4	
435	1000	n Distribution Index	Fixed
436	nbar_SCC	Parameter 1	
437	0	Parameter 2	
438	0	Parameter 3	
439	0	Parameter 4	
440	1000	Incipient Crack Size Distribution Index	Fixed
441	0.05	Parameter 1	mm
442	0	Parameter 2	
443	0	Parameter 3	
444	0	Parameter 4	
445	0	Sample Type	
446	1000	Barrier Variance Share Distribution Index (for thresholds)	Fixed
447	1	Parameter 1	fraction
448	0	Parameter 2	
449	0	Parameter 3	
450	0	Parameter 4	
451	1000	Stress Threshold Distribution Index (Incipient)	Fixed
452	Stress_Thresh_SCC	Parameter 1	MPa
453	0	Parameter 2	
454	0	Parameter 3	
455	0	Parameter 4	
456	1000	KI Threshold Distribution Index (Incipient)	Fixed
457	KI_Thresh_SCC	Parameter 1	MPa*sqrt(m)
458	0	Parameter 2	
459	0	Parameter 3	
460	0	Parameter 4	
461	1000	Stress Threshold Distribution Index (MFD)	Fixed
462	-600	Parameter 1	MPa
463	0	Parameter 2	
464	0	Parameter 3	
465	0	Parameter 4	
466	1000	KI Threshold Distribution Index (MFD)	Fixed
467	KI_Thresh_SCC	Parameter 1	MPa*sqrt(m)
468	0	Parameter 2	
469	0	Parameter 3	
470	0	Parameter 4	
471	0	Immediate Failure Flag (-1 or 0 for true or false)	FALSE
472	0	Number of Localized Corrosion Modes Initiated (0, 1, or 2)	

Row	Value	Parameter Description	Comments
473	1	Number of Corrosion Modes Accelerated (0, 1, 2, or 3)	
474	1	General Corrosion Accelerated	
475	1000	Barrier Variance Share Distribution Index	Fixed
476	1	Parameter 1	fraction
477	0	Parameter 2	
478	0	Parameter 3	
479	0	Parameter 4	
480	1000	Acceleration Factor	Fixed
481	2 (2.5)	Parameter 1	20/10 (25/10)
482	0	Parameter 2	
483	0	Parameter 3	
484	0	Parameter 4	
485	0	Sample Type	
486	0	Number of Thresholds Reduced (0, 1, or 2)	
487	10	**MIC Event Index**	
488	1	Barrier Type	**A22 OB**
489	2	Number of Water Conditions	
490	1	Condition Number	**DSInside**
491	2	Condition Number	**DSOutside**
492	1	Fraction of surface area subject to MIC	
493	0	Use SCC patches first?	
494	1000	Barrier Variance Share Distribution Index	Fixed
495	1	Parameter 1	fraction
496	0	Parameter 2	
497	0	Parameter 3	
498	0	Parameter 4	
499	1000	MIC RHcrit Distribution Index	Fixed
500	0.9	Parameter 1	fraction
501	0	Parameter 2	
502	0	Parameter 3	
503	0	Parameter 4	
504	0	Sample Type (only one variable so not used, but must be specified)	
505	0	Immediate Failure Flag (- 1 or 0 for true or false)	FALSE
506	0	Number of Localized Corrosion Modes Initiated (0, 1, or 2)	
507	1	Number of Corrosion Modes Accelerated (0, 1, 2, or 3)	
508	1	Corrosion Mode Number (1, 2, or 3)	General Corrosion Accelerated
509	1000	Barrier Variance Share Distribution Index	Fixed
510	1	Parameter 1	fraction
511	0	Parameter 2	
512	0	Parameter 3	
513	0	Parameter 4	
514	1000	Acceleration Factor Distribution Index	Fixed
515	MIC_A22	Parameter 1	
516	0	Parameter 2	
517	0	Parameter 3	
518	0	Parameter 4	
519	0	Sample Type	
520	0	Number of Thresholds Reduced (0, 1, or 2)	
521	10	**MIC Event Index**	
522	2	Barrier Type	**A22 IB**
523	2	Number of Water Conditions	
524	1	Condition Number	**DSInside**

Row	Value	Parameter Description	Comments
525	2	Condition Number	**DSOutside**
526	1	Fraction of surface area subject to MIC	
527	0	Use SCC patches first?	
528	1000	Barrier Variance Share Distribution Index	Fixed
529	1	Parameter 1	fraction
530	0	Parameter 2	
531	0	Parameter 3	
532	0	Parameter 4	
533	1000	MIC RHcrit Distribution Index	Fixed
534	0.9	Parameter 1	fraction
535	0	Parameter 2	
536	0	Parameter 3	
537	0	Parameter 4	
538	0	Sample Type (only one variable so not used, but must be specified)	
539	0	Immediate Failure Flag (- 1 or 0 for true or false)	FALSE
540	0	Number of Localized Corrosion Modes Initiated (0, 1, or 2)	
541	1	Number of Corrosion Modes Accelerated (0, 1, 2, or 3)	
542	1	Corrosion Mode Number (1, 2, or 3)	General Corrosion Accelerated
543	1000	Barrier Variance Share Distribution Index	Fixed
544	1	Parameter 1	fraction
545	0	Parameter 2	
546	0	Parameter 3	
547	0	Parameter 4	
548	1000	Acceleration Factor Distribution Index	Fixed
549	MIC_A22	Parameter 1	
550	0	Parameter 2	
551	0	Parameter 3	
552	0	Parameter 4	
553	0	Sample Type	
554	0	Number of Thresholds Reduced (0, 1, or 2)	
555	WDSeed_CSNF (WDSeed_CDSP)	**Seed for the random number generator**	
556	NumBins	Number of bins for reporting penetrations with time	
557	BinStart	Bin Start Time	
558	0	Number of summary times for reporting penetrations	
559	0	Do Subset of Total Package Logical	FALSE
560	1	Number of First Package	
561	1	Number of Last Package	
562	SimTime	Simulation Time	
563	11	Number of Output files	
564	0	Generate OUT file logical	
565	0	Generate AUX file logical	
566	0	Generate PIT file logical	
567	0	Generate CRK file logical	
568	0	Generate PAT file logical	
569	0	Generate THK file logical	
570	0	Generate EVN file logical	
571	0	Generate DET file logical	
572	0	Generate INA file logical	
573	0	Generate OUA file logical	
574	0	Generate PDZ file logical	

Row	Value	Parameter Description	Comments
575	*(rows 575 to 699 are not referenced and contain zeros)*		
.	.		
.	.		
.	.		
699	0		
700	SCC_Outer_Lid.Output1		
701	SCC_Middle_Lid.Output1		
702	0		
703	0		
704	*(rows 704 to 2000 are not referenced and contain zeros)*		
.	.		
.	.		
.	.		
2000	0		

ATTACHMENT II
OTHER SUPPORTING FILES

The Integrated Waste Package Degradation (IWPD) Model uses several external files which must accompany the GoldSim Model file in which it is run. The first of these is the WD4DLL.WAP file listed in Table II-1. Note that the line numbers and the column headings in Table II-1 are not part of the WD4DLL.WAP file, but are included for clarity.

Table II-1. Contents of WD4DLL.WAP file.

Line	File Name
1	WDenv_00_07wheader.ou
2	WDenv_00wh.ou
3	EMPTY
4	WDKIinO.fil
5	WDKIinM.fil
6	WDKISCCO.fil
7	WDStressO.fil
8	WDKISCCM.fil
9	WDStressM.fil
10	WDCWDNDO_CSNF.cdf
11	WDCWDSizeO_CSNF.cdf
12	WDCWDNDM_CSNF.cdf
13	WDCWDSizeM_CSNF.cdf
14	WDCWDNDO_CDSP.cdf
15	WDCWDSizeO_CDSP.cdf
16	WDCWDNDM_CDSP.cdf
17	WDCWDSizeM_CDSP.cdf
18	WDlnRGC.cdf

WDenv_00_07wheader.ou and WDenv_00wh.ou are used only in this report. It is expected that another file will actually be used in the TSPA Model.

There is a dummy filename in position 3.

The contents of WDKIinO.fil are reproduced below.

```
! KIinO.fil
! Laser peened Outer lid DIRS: 161234, Table 8-5
!
#  1  2
#  50
#  1.0
! KI (MPA*m½)  depth (mm)
-5.6943         0.3988
-6.4965         0.8001
-6.1528         1.1989
-5.1372         1.6002
-3.6697         1.9990
-1.8824         2.4003
0.1212          2.7991
2.2821          3.2004
4.5533          3.5992
6.8939          3.9980
9.2702          4.3993
11.6543         4.7981
14.0165         5.1994
16.3364         5.5982
```

```
18.6024         5.9995
20.8003         6.3983
22.9177         6.7970
24.9441         7.1984
26.9023         7.5971
28.8612         7.9985
30.7287         8.3972
32.5008         8.7986
34.1745         9.1973
35.7479         9.5987
37.2200         9.9974
38.4530         10.3962
39.5674         10.7975
40.5636         11.1963
41.4432         11.5976
42.2086         11.9964
42.8627         12.3977
43.4439         12.7965
43.9342         13.1978
44.3269         13.5966
44.6272         13.9954
44.8409         14.3967
44.9743         14.7955
45.0329         15.1968
45.0208         15.5956
44.9464         15.9969
44.8182         16.3957
44.6449         16.7945
44.4361         17.1958
44.2112         17.5946
43.9968         17.9959
43.7750         18.3947
43.5578         18.7960
43.3569         19.1948
43.1853         19.5961
43.0560         19.9949
```

The contents of WDKIinM.fil are reproduced below.

```
! KIinM.fil
! As-Welded Middle Lid DIRS: 161234, Table 8-5
!
#  1  2
#  50
#  1.0
! KI (MPa*m½)   depth (mm)
7.5754          0.1593
10.9665         0.3203
13.7144         0.4797
16.1330         0.6407
18.3358         0.8000
20.3775         0.9593
22.3816         1.1203
24.3197         1.2797
26.1726         1.4407
27.9459         1.6000
29.6433         1.7593
31.2668         1.9203
32.8922         2.0797
34.5292         2.2407
36.1060         2.4000
37.6220         2.5593
39.0762         2.7203
40.4676         2.8797
41.8264         3.0407
43.2168         3.2000
44.5479         3.3593
45.8181         3.5203
47.0265         3.6797
48.1718         3.8407
```

```
49.2531        4.0000
50.3451        4.1593
51.3729        4.3203
52.3351        4.4797
53.2313        4.6407
54.0602        4.8000
54.8214        4.9593
55.4811        5.1203
56.0586        5.2797
56.5637        5.4407
56.9965        5.6000
57.3567        5.7593
57.6444        5.9203
57.7587        6.0797
57.6946        6.2407
57.5522        6.4000
57.3322        6.5593
57.0353        6.7203
56.6626        6.8797
56.1419        7.0407
55.3276        7.2000
54.4422        7.3593
53.4878        7.5203
54.6294        7.6797
56.2191        7.8407
57.7865        8.0000
```

The files WDKISCCO.fil, WDStressO.fil, WDKISCCM.fil, WDStressM.fil, WDCWDNDO_CSNF.cdf, WDCWDSizeO_CSNF.cdf, WDCWDNDM_CSNF.cdf, WDCWDSizeM_CSNF.cdf, WDCWDNDO_CDSP.cdf, WDCWDSizeO_CDSP.cdf, WDCWDNDM_CDSP.cdf, and WDCWDSizeM_CDSP.cdf are all files which are produced at run-time and change their contents for each realization of the IWPD Model.

The contents of WDlnRGC.cdf are reproduced below (column1 is the natural logarithm of the general corrosion rate, column 2 is the cumulative probability values, column 3 is the general corrosion rate in mm/yr (not used but provided for illustration)).

```
125  ! WDlnRGC.cdf - CDF for Ln[Rate (mm/yr)] for Alloy 22
      -16.961712197361             1e-015   4.3015204214735e-008
      -16.606332266861             1e-014   6.1370764287394e-008
      -16.250919072358             1e-013   8.7561969415836e-008
      -15.895446698814             1e-012   1.2493819039048e-007
      -15.539869004983             1e-011   1.7828739590043e-007
      -15.184103757973             1e-010   2.5446468878913e-007
      -14.828004150476             1e-009   3.6331189726815e-007
      -14.471307289094             1e-008   5.1902837174783e-007
      -14.113539817716             1e-007   7.4227962051286e-007
      -13.753841023008             1e-006   1.0636108004554e-006
      -13.390617861005             1e-005    1.529426298765e-006
      -13.020824635104             0.0001   2.2137456007201e-006
      -12.638272586363              0.001   3.2453979309883e-006
      -12.228771288622               0.01   4.8877851647675e-006
      -12.095541575836               0.02   5.5843552467729e-006
      -12.014176485059               0.03   6.0577235210094e-006
       -11.95450274756               0.04   6.4302139435167e-006
      -11.906896320413               0.05   6.7437371027708e-006
      -11.867014466231               0.06   7.0181250237782e-006
      -11.832515828457               0.07   7.2644655516632e-006
      -11.801989899202               0.08   7.4896394493125e-006
      -11.774519377179               0.09   7.6982357619692e-006
      -11.749473240538                0.1   7.8934816984425e-006
      -11.726398285935               0.11   8.0777411437344e-006
      -11.704957708673               0.12     8.25280257971e-006
```

-11.684894157232	0.13	8.4200553404489e-006
-11.666006404304	0.14	8.5806026817397e-006
-11.648134015655	0.15	8.7353371663517e-006
-11.631146932008	0.16	8.8849925752487e-006
-11.614938185062	0.17	9.0301806512331e-006
-11.599418678305	0.18	9.1714177309772e-006
-11.584513366555	0.19	9.3091444514342e-006
-11.570158406341	0.2	9.4437405995513e-006
-11.556298994738	0.21	9.5755364846527e-006
-11.542887705779	0.22	9.7048217747851e-006
-11.529883192646	0.23	9.8318524528176e-006
-11.51724916292	0.24	9.9568563577574e-006
-11.504953560484	0.25	1.0080037647227e-005
-11.492967905824	0.26	1.0201580427299e-005
-11.481266759108	0.27	1.0321651732614e-005
-11.46982727947	0.28	1.0440403994467e-005
-11.458628860377	0.29	1.0557977101684e-005
-11.447652825708	0.3	1.0674500134987e-005
-11.43688217469	0.31	1.0790092837602e-005
-11.42630136642	0.32	1.0904866871379e-005
-11.415896136709	0.33	1.1018926897439e-005
-11.405653341471	0.34	1.1132371512535e-005
-11.39556082205	0.35	1.1245294066247e-005
-11.385607288762	0.36	1.1357783379422e-005
-11.375782219648	0.37	1.1469924380546e-005
-11.366075771986	0.38	1.1581798673867e-005
-11.356478704522	0.39	1.1693485050718e-005
-11.346982308768	0.4	1.1805059953714e-005
-11.337578347973	0.41	1.1916597901966e-005
-11.328259002589	0.42	1.2028171884343e-005
-11.319016821266	0.43	1.2139853726833e-005
-11.309844676534	0.44	1.225171443934e-005
-11.300735724457	0.45	1.2363824546659e-005
-11.29168336764	0.46	1.2476254407934e-005
-11.282681221066	0.47	1.2589074528536e-005
-11.273723080277	0.48	1.2702355868114e-005
-11.264802891481	0.49	1.2816170148356e-005
-11.255914723223	0.5	1.2930590163975e-005
-11.247052739247	0.51	1.3045690100432e-005
-11.238211172251	0.52	1.3161545861962e-005
-11.229384298222	0.53	1.3278235413665e-005
-11.220566411044	0.54	1.3395839141646e-005
-11.21175179711	0.55	1.3514440235511e-005
-11.202934709625	0.56	1.3634125097966e-005
-11.194109342302	0.57	1.3754983786796e-005
-11.185269802139	0.58	1.3877110495173e-005
-11.176410080918	0.59	1.4000604077062e-005
-11.167524025069	0.6	1.4125568625509e-005
-11.15860530346	0.61	1.4252114112813e-005
-11.149647372663	0.62	1.4380357103089e-005
-11.140643439142	0.63	1.4510421549568e-005
-11.131586417741	0.64	1.4642439691204e-005
-11.12246888575	0.65	1.4776553065942e-005
-11.113283031688	0.66	1.4912913661378e-005
-11.104020597771	0.67	1.5051685227771e-005
-11.094672814858	0.68	1.5193044783627e-005
-11.085230328375	0.69	1.5337184350634e-005
-11.075683113423	0.7	1.5484312963077e-005
-11.066020376864	0.71	1.5634659007344e-005
-11.05623044364	0.72	1.5788472960683e-005
-11.046300623925	0.73	1.5946030615688e-005
-11.036217056846	0.74	1.610763689963e-005
-11.025964525342	0.75	1.6273630427313e-005

-11.015526235268	0.76	1.6444388965399e-005
-11.004883549816	0.77	1.6620336038545e-005
-10.994015667647	0.78	1.6801948978702e-005
-10.982899229434	0.79	1.6989768816026e-005
-10.971507832438	0.8	1.7184412544673e-005
-10.959811425593	0.81	1.7386588486316e-005
-10.947775547458	0.82	1.7597115745295e-005
-10.935360354661	0.83	1.7816949143246e-005
-10.922519366853	0.84	1.8047211604704e-005
-10.909197821533	0.85	1.8289236847896e-005
-10.895330481956	0.86	1.8544626601422e-005
-10.880838661918	0.87	1.8815328738574e-005
-10.865626102186	0.88	1.9103746273212e-005
-10.849573116212	0.89	1.9412893170728e-005
-10.832528043575	0.9	1.9746623493742e-005
-10.814294357166	0.91	2.0109979829965e-005
-10.794610437982	0.92	2.0509744608982e-005
-10.773116302859	0.93	2.0955355687502e-005
-10.74929553616	0.94	2.1460521153888e-005
-10.722365979358	0.95	2.2046295397764e-005
-10.69105213255	0.96	2.2747572249932e-005
-10.653038849576	0.97	2.3628927628531e-005
-10.603337771639	0.98	2.4832984417707e-005
-10.526951407683	0.99	2.6804214973517e-005
-10.325849053552	0.999	3.2774851685675e-005
-10.174589906086	0.9999	3.8126922194693e-005
-10.053211136624	0.99999	4.3047296134484e-005
-9.9518237288526	0.999999	4.7640670996241e-005
-9.8647635039768	0.9999999	5.1974179853622e-005
-9.7884780416973	0.99999999	5.6094205379008e-005
-9.7205916556578	0.999999999	6.0034470302955e-005
-9.6594369250961	0.9999999999	6.3820447508563e-005
-9.603798439259	0.99999999999	6.7471960981027e-005
-9.552764757972	0.999999999999	7.1004680683796e-005
-9.5056107132096	0.9999999999999	7.4433033708262e-005
-9.4614083903465	0.99999999999999	7.7796945354491e-005
-9.4189122120715	1	8.1174271693367e-005