

CRWMS/M&O

Calculation Cover Sheet

Complete only applicable items.

1. QA: L

Page: 1 Of: 32

2. Calculation Title RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIb			
3. Document Identifier (including Revision Number) B00000000-01717-0210-00078 REV 00			4. Total Pages 32
5. Total Attachments 2	6. Attachment Numbers - Number of pages in each I-11 pages, II-4 pages		
	Print Name	Signature	Date
7. Originator	Kevin G. Mon	<i>Kevin Mon</i>	JUL 01 1999
8. Checker	Peter K. Mast	<i>Peter K. Mast</i> PK MAST	<i>July 1, 1999</i>
9. Lead	Joon H. Lee	<i>Joon H. Lee</i>	<i>July 1, 1999</i>
10. Remarks Input thermal hydrologic history files (DTN: LL990301604242.081). Computer software (WAPDEG version 3.09 and Post308) are tracked by TBV-568. Uses DTN: MO9807MWDWAPDG.000 on Conceptual Model. Uses DTN: MO9810SPA00013.000 and MO9812MWDDSQ37.000 on Input assumptions and input data. Supporting electronic media = ACC: MOL.19990528.0283, DTN: MO9904MWDWAP78.003. For LA Design Selection.			
Revision History			
11. Revision No.	12. Description of Revision		
00	Initial Issue.		

CONTENTS

	Page
1. PURPOSE	3
2. METHOD.....	3
3. ASSUMPTIONS	4
4. USE OF COMPUTER SOFTWARE AND MODELS	15
4.1 SOFTWARE APPROVED FOR QA WORK	15
4.2 SOFTWARE ROUTINES	16
4.3 MODELS	16
5. CALCULATION.....	17
5.1 MKHISTORY INPUTS	17
5.2 WAPDEG INPUTS.....	18
5.3 POST308 INPUTS	23
6. RESULTS.....	24
7. REFERENCES	31
8. ATTACHMENTS	32

1. PURPOSE

The purpose of this calculation is to document the Waste Package Degradation (WAPDEG) version 3.09 (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*) simulations used to analyze degradation and failure of 2-cm thick titanium grade 7 corrosion resistant material (CRM) drip shields as well as degradation and failure of the waste packages over which they are placed. The waste packages are composed of two corrosion resistant materials (CRM) barriers. The outer barrier is composed of 2 cm of Alloy 22 and the inner barrier is composed of 1.5 cm of titanium grade 7. The WAPDEG simulation results are post-processed into tables of drip shield / waste package degradation time histories suitable for use as input into the Integrated Probabilistic Simulator for Environmental Systems (RIP) version 5.19.01 (Golder Associates 1998) computer code. This calculation supports Performance Assessment analysis of the License Application Design Selection (LADS) Enhanced Design Alternative IIIb. Additional details concerning the Enhanced Design Alternative IIIb are provided in a Design Input Request (CRWMS M&O 1999e. *Design Input Request for LADS Phase II EDA Evaluations*, Item 3).

2. METHOD

Temperature and relative humidity (RH) time histories at the drip shield / waste package surfaces are calculated elsewhere and provided as input to this WAPDEG simulation. These histories are pre-processed into a form suitable for use as input to the WAPDEG stochastic simulation code through the use of the pre-processor Mkhhistory (Attachment I). The stochastic simulation code WAPDEG (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*) is used to generate drip shield / waste package failure profiles. WAPDEG's inputs also include various temperature and relative humidity thresholds for corrosion initiation, corrosion models, and corrosion model parameter distributions. WAPDEG has the capability to model drip shield / waste package failure degradation either through localized corrosion processes (pitting or crevice corrosion), leading to small pinhole perforations, or through general corrosion processes leading to much larger "patch" perforations. In this calculation, the drip shields and the titanium inner barrier of the waste packages are assumed to only undergo general corrosion processes, which result in "patch" perforations (see Assumption 3.9 in Section 3). More detailed discussions of the WAPDEG conceptual model are given elsewhere (CRWMS M&O 1998a. *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document - Chapter 5, Waste Package Degradation Modeling and Abstraction*, pp. 5-27 to 5-29). The drip shield / waste package failure profiles calculated by WAPDEG consist of time-varying measures of the number of pit or patch penetrations on each drip shield / waste package. The WAPDEG post-processor, Post308 (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*, Appendix D), abstracts this information to produce one RIP input table (Golder Associates 1998, pp. 7-22 through 7-25) per WAPDEG simulation. The RIP input table contains:

- 1) The fraction of drip shields / waste packages failed versus time curve for the simulation,
- 2) The average number of pit penetrations per failed drip shield / waste package versus time curve, and
- 3) The average number of patch penetrations per failed drip shield / waste package versus time curve.

As mentioned earlier, in this calculation, the drip shields and the titanium inner barrier of the waste packages are assumed to only undergo general corrosion processes, which result in "patch" perforations. As a result, the above curves only reflect the results of "patch" perforations (i.e., the curve for RIP input Item 2 above, for instance, will indicate no pit penetrations for the drip shields).

Post308 has two main objectives:

- a) It reformats the WAPDEG output to conform to the RIP input format and,
- b) It decreases the number of points in each of the three curves discussed above to approximately 83 (or less depending on the data being processed) through a process of time averaging.

More detailed discussions of the WAPDEG version 3.09 and Post308 codes appear elsewhere (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*).

Waste package failures under dripping conditions were modeled by executing the WAPDEG code three times, as described in Section 3.0. The first WAPDEG simulation (using the input file NE1a5s5EDA3b-ds.inp) models 2-cm thick titanium grade 7 drip shield failures. The first breach curve resulting from this simulation was then used to create a distribution of dripping start times for the waste packages beneath the failed drip shields. This distribution is contained in the file NE1a5s5EDA3b-ds.cdf. A second WAPDEG simulation (using the input file NE1a5s5EDA3b-wp1.inp) was then performed for the outer (Alloy 22) barrier of the waste package failures using this dripping start time distribution. The results of the outer barrier simulation are then used to create a distribution of corrosion initiation times (contained in NE1a5s5EDA3b-wp1.cdf) for the titanium grade 7 inner barrier. A third WAPDEG simulation was then performed for the titanium grade 7 inner barrier of the waste packages using this distribution of corrosion initiation times. Under non-dripping conditions, the presence of the drip shield is irrelevant to waste package degradation modeling and only two WAPDEG simulations are necessary (using the input files NE0a5s6EDA3b-wp1.inp for the waste package outer barrier and NE0a5s6EDA3b-wp2.inp for the waste package inner barrier).

3. ASSUMPTIONS

No assumptions are made in executing Mkhhistory. The limitations on the Mkhhistory software routine and on the validity of the resulting output are discussed in detail in Attachment I.

For the calculations involved in attaining a post processed table for input into RIP, there are two steps to consider: 1) Execution of the WAPDEG code and; 2) Post processing of WAPDEG output for creation of tables for input to RIP. There are several assumptions necessary to consider for the WAPDEG simulations. With the exception of the different thermal hydrologic (time/temperature/relative humidity) histories and the assumptions noted below, the modeling assumptions used to model degradation of the drip shields and waste packages are identical to those used previously in the TSPA-VA REV 01 base case calculation (CRWMS M&O 1998d. *Creating Input Tables from WAPDEG for RIP*) (DTN: MO9810SPA00013.000) to model degradation of dual-barrier waste packages (i.e., a 10-cm carbon steel outer barrier around a 2-cm CRM inner barrier).

Although WAPDEG version 3.07 (CRWMS M&O 1998c. *Software Routine Report for WAPDEG (Version 3.07)*) was used in the TSPA-VA base case calculation and WAPDEG version 3.09 is used in the present calculation, the assumptions listed in the TSPA-VA REV 01 base case calculation are applicable to the present calculation (with the exception of those noted below). No additional assumptions pertaining to the use of the Post308 code are made in the calculation of the drip shield or waste package degradation profiles.

The WAPDEG input file NE1a5s5EDA3b-ds.inp is used to model degradation of a 2 cm titanium drip shield. The following assumptions are made for titanium grade 7 drip shield corrosion degradation modeling:

- 3.1 The variability in drip shield degradation is adequately characterized by modeling 400 drip shields. This assumption is made to be consistent with the number of waste packages simulated. This assumption is used in the WAPDEG input file, NE1a5s5EDA3b-ds.inp, in the fourth line (first value) after the last history file name.
- 3.2 The fraction of model parameter variance assigned to drip-shield-to-drip-shield variance is set at 0.35 (the second value on the third input line after the last thermal hydrologic "history" file name in the WAPDEG input file NE1a5s5EDA3a-ds.inp). The remainder of the model parameter variance is assigned to patch-to-patch variance between the patches on each drip shield. This is consistent with Assumption 3.12 in the TSPA-VA REV 01 base case calculation (CRWMS M&O 1998d. *Creating Input Tables from WAPDEG for RIP*, Section 3.0) in which the waste-package-to-waste-package fraction of model parameter variance is set to 0.35. It is expected that the same material and exposure environment variances appropriate for consideration in modeling of the waste packages would also be appropriate for consideration in modeling the drip shields and lead to the same variance partitioning.
- 3.3 The total drip shield surface area modeled is 30.22 m². This is based on the length of the 21 PWR (Pressurized Water Reactor) waste package type over which it is emplaced and drip shield dimensions provided (CRWMS M&O 1999b. *Design Input Transmittal For Waste Stream Information for LADS, Phase 2, EDAs*, Item 1 p. 3/34 Table 2 and Item 5 p. 1/2). The drip shields are assumed to have a "mail-box" (inverted U-shaped) configuration and to be placed over the waste packages with a gap between the drip shields and the waste packages to avoid direct contact. The length of the waste package is 5.325 m. The waste package total length includes two 0.225-m outer barrier extensions ("skirts"), one on each end (i.e., two of them), for lifting of the waste package (CRWMS M&O 1999d. *Design Input Transmittal For Skirt Dimensions for LADS, Phase 2, EDA Waste Packages*, Item 1 p. 1/1). The outer barrier extensions are not considered in corrosion modeling. The inner and outer radii of the curved portion of the drip shield (the drip shield is corrugated like a storm drain pipe) are 1.050 m and 1.220 m, respectively. The average of the drip shield inner and outer radii are used to define an effective radius to be used in determining the effective surface area of the drip shield. The function of the drip shield is to delay dripping water contact with the waste package surface until after drip shield failure. The breached drip shield area, through which dripping water can flow, is the modeling area of interest to this calculation. The most conservative assumption would be that dripping water can penetrate the drip shield through

its entire surface area. The least conservative assumption would be that dripping water could penetrate the drip shield only through the projected area above the waste package (i.e., a rectangular area defined by the waste package diameter multiplied by its length). The effective area used in this calculation is a realistic compromise between these two extreme approaches. The height of the drip shield side plates is 1.317 m. Thus, the drip shield surface area modeled (i.e., subject to corrosion degradation) is given by:

IR := 1.050m	OR := 1.220m	Inner (IR) and outer (OR) drip shield rad
L := 5.325m - 2·0.225m	L = 4.875 m	Waste package length - two skirts
SPH := 1.317m		Drip shield side plate height
$er := \frac{(IR + OR)}{2}$	er = 1.135 m	Effective Radius
Tot := 2·SPH·L + $\pi \cdot er \cdot L$	Tot = 30.22 m ²	Drip shield surface area modeled

This assumption is used only in determining the number of patches per waste package in Assumption 3.4.

- 3.4 The drip shield surface area was divided into 975 patches each 0.0310 m² in area. This patch size was chosen to be consistent with the patch size chosen in the TSPA-VA REV 01 base case calculation (CRWMS M&O 1998d. *Creating Input Tables from WAPDEG for RIP*, Section 3.0 Assumption 3.3). Continuing from the calculations presented in Assumption 3.3 above:

PS := 0.0310m ²	Patch Size
$\frac{Tot}{PS} = 975$	975 Patches/DS

This assumption is used in the WAPDEG input file NE1a5s5EDA3b-ds.inp in the fourth line (second value) after the last thermal hydrologic history file name.

- 3.5 The drip shields are 2-cm thick and are composed of titanium grade 7 (CRWMS M&O 1999e. *Design Input Request for LADS Phase II EDA Evaluations*, Item 3 p. 2). The current version of WAPDEG was developed to model a two-barrier waste package, with the outer barrier hard-wired to be a corrosion allowance material (CAM) of carbon steel, and the corrosion model parameters for the inner barrier able to be supplied by the user through the WAPDEG input file. In order to model the drip shield corrosion degradation process as a corrosion resistant material (CRM) with no CAM, it is required to assume that the drip shield has a very thin (1e-12 cm) “simulated” CAM and the CAM pit multiple (or localization factor) be set to a very large number (1e12) in the WAPDEG input file used. The effect is an immediate failure of the drip shield simulated CAM upon satisfaction of the relative humidity (RH) and temperature thresholds for corrosion initiation of the “simulated” CAM. This assumption is used in the WAPDEG input file NE1a5s5EDA3b-ds.inp on the second

input line after the last history file name (first value) and on the third input line after the [No Drip Model, CAM] and [Neutral Drip Model, CAM] input headers.

- 3.6 Corrosion of the drip shields is assumed not to occur until after they are emplaced and ventilation ceases 50 years after waste package emplacement (CRWMS M&O 1999c. *Design Input Request for LADS Phase II EDA Evaluations*, p. 4, "LADS Enhanced Design Alternatives" Table Row 9 Column 4). This is accomplished by using a 50-year corrosion delay time. The basis for this assumption is that it is not expected that the drip shields will be fabricated any significant period of time before their use and that during the ventilation period, any dripping water will be removed by air flow, and relative humidity in the emplacement drifts will be maintained at very low levels. This assumption is used in the WAPDEG input file NE1a5s5EDA3b-ds.inp on the nineteenth and twentieth input lines after the last history file name.
- 3.7 The temperature corrosion initiation threshold for the very thin simulated CAM outer barrier was assumed to be represented by the cumulative distribution function for titanium grade 7 as given in A22TiTh.cdf (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 1/3 Response 1). This assumption has the effect of delaying the initiation of corrosion of the titanium grade 7 drip shield until the temperature initiation threshold for corrosion of the simulated CAM is satisfied (since the CAM fails immediately upon satisfaction of the corrosion initiation thresholds). This assumption is based on the input received. This assumption is used in the WAPDEG input file NE1a5s5EDA3b-ds.inp on the first and second input lines after the [No Drip Model Features] header and on the first and second input lines after the [Neutral Drip Features].
- 3.8 The relative humidity corrosion initiation threshold for the very thin simulated CAM outer barrier was assumed to be represented by the cumulative distribution function for titanium grade 7 as given in A22TiRHth.cdf (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 1/3 Response 2). This assumption has the effect of delaying the initiation of corrosion of the titanium grade 7 until the relative humidity initiation threshold for corrosion of the simulated CAM is satisfied (since the CAM fails immediately upon satisfaction of the corrosion initiation thresholds). This assumption is used in the WAPDEG input file NE1a5s5EDA3b-ds.inp on the third and fourth input lines after the [No Drip Model Features] header and on the fifth and sixth input lines after the [Neutral Drip Features].
- 3.9 It is assumed that there is no localized corrosion (i.e., there is only general or "patch" corrosion) of the titanium grade 7 drip shields. This assumption is based on input received (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection*

Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading, Item 1 p. 2/3 Response 5). This assumption is used in the input file NE1a5s5EDA3b-ds.inp in the [No Drip Model, CRM] and [Neutral Drip Model, CRM] input segments by using the “CRMGeneralRateOnly” model.

- 3.10 The general corrosion rates used to model general corrosion degradation of the titanium grade 7 drip shields under dripping conditions are derived in Attachment II. In Attachment II, it is assumed that it is appropriate to derive the titanium grade 7 general corrosion rate cdfs (3 of them) used with the “CRMGeneralCorrosionRateOnly” model at the temperatures of 30°C (gTi15050.cdf), 60°C (gTi25050.cdf), and 120°C (gTi35050.cdf). The basis for this assumption is that these thermal conditions span the possible repository exposure conditions under which active general corrosion can occur based on the thermal hydrologic history files used and the temperature corrosion initiation threshold used (A22TiTh.cdf). This assumption is used throughout Attachment II.
- 3.11 In deriving the general corrosion rates used to model general corrosion degradation of the titanium grade 7 drip shields under dripping conditions, the total variance of the cdfs are assumed to be composed of 50% uncertainty and 50% variability, and it is assumed that the median general corrosion rate is at the 50th percentile of the uncertainty distribution. This assumption is based on input received (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading, Item 1 p. 1/3 Response 1).* This assumption is used throughout Attachment II.
- 3.12 The general corrosion rates used to model general corrosion degradation of the titanium grade 7 drip shields under dripping conditions are derived in Attachment II. In Attachment II, it is assumed that it is appropriate to derive the titanium grade 7 corrosion cdfs (3 of them) used with the “CRMGeneralCorrosionRateOnly” model at 201 equally spaced (in natural logarithm space) general corrosion rates between the minimum and maximum general corrosion rate for each temperature used (30°C, 60°C, and 120°C). Given that none of the general corrosion rate distributions span more than 5 orders of magnitude (see Attachment II), use of this assumption allows each decade of corrosion rates to be characterized by at least 40 cdf points. This assumption is used throughout Attachment II.
- 3.13 The general corrosion rates used to model general corrosion degradation of the titanium grade 7 drip shields under dripping conditions are derived in Attachment II. In Attachment II cumulative probability values were interpolated linearly between natural log general corrosion rate values. It is assumed that this interpolation methodology results in well approximated cumulative probability values. As mentioned in Assumption 3.12, each decade of corrosion rates is characterized by at least 40 cdf points. Given this density of points in the cdfs (i.e., the small size of the interval over which interpolation is occurring), the

corrosion rate values obtained are well approximated. This assumption is used in the variance splitting procedure (slnvar(x, p, wtu, qu)) in Attachment II.

The following assumptions are made for Alloy 22 waste package outer barrier degradation modeling:

The WAPDEG input file NE1a5s5EDA3b-wp1.inp is used to model the 2-cm thick Alloy 22 outer barriers of waste packages under 2-cm thick titanium grade 7 drip shields that are always dripped on. In this simulation the waste packages are not contacted by dripping water until the titanium grade 7 drip shields fail. The WAPDEG input file NE0a5s6EDA3b-wp1.inp is used to model the 2-cm thick Alloy 22 outer barriers of waste packages under 2-cm thick titanium grade 7 drip shields that are never dripped on (equivalent, for WAPDEG modeling purposes, to having no drip shields present). The assumptions used in modeling Alloy 22 waste package outer barrier degradation are identical to those used in the TSPA-VA REV 01 base case calculation (CRWMS M&O 1998d. *Creating Input Tables from WAPDEG for RIP*) (DTN: MO9810SPA00013.000) with the exception of those listed below.

- 3.14 The total waste package surface area modeled is 28.00 m^2 , or approximately 903 patches each with an area of 0.0310 m^2 . This is based on the 21 PWR (Pressurized Water Reactor) waste package dimensions provided (CRWMS M&O 1999b. *Design Input Transmittal For Waste Stream Information for LADS, Phase 2, EDAs*, Item 1 p. 4/34 Table 3). The length of the waste package is 5.325 m. The waste package total length includes two 0.225-m outer barrier extensions (“skirts”), one on each end (i.e., two of them), for lifting of the waste package. The extensions are not considered in corrosion modeling (See Assumption 3.3). Thus, the waste package surface area modeled (subject to corrosion) is given by the radial surface area and the area of the two end caps. The calculation below is a continuation of that presented in Assumptions 3.3 and 3.4:

$$\text{OD} := 1.574 \text{ m} \quad L = 4.875 \text{ m} \quad \text{Waste Package Outer Diameter and Length}$$

$$\text{WPA} := \pi \cdot \text{OD} \cdot L + 2 \cdot \pi \cdot \left(\frac{\text{OD}}{2} \right)^2 \quad \text{WPA} = 28.00 \text{ m}^2 \quad \text{Total Waste Package Area}$$

$$\frac{\text{WPA}}{\text{PS}} = 903 \quad 903 \text{ Patches/WP}$$

This assumption is used on the fourth input line (second value) in the WAPDEG input files NE1a5s5EDA3b-wp1.inp and NE0a5s6EDA3b-wp1.inp.

- 3.15 The NE1a5s5EDA3b-ds.cdf (a cdf of first breach times of the drip shields modeled) distribution is used as the “Distribution parameter(s)” for the “Distr for time range for ceramic protection” of the waste packages (this is perhaps better termed “the delay time for corrosion initiation” of the waste packages) in the WAPDEG input file NE1a5s5EDA3b-wp1.inp. The basis of this assumption is that dripping water can not contact a waste package underneath an intact drip shield. This distribution is read by the fourteenth and fifteenth lines after the last thermal hydrologic “history” file name in the WAPDEG input file

NE1a5s5EDA3b-wp1.inp. (No drip shield delay time is used in the input file NE0a5s6EDA3b-wp1.inp).

- 3.16 After failure of a titanium grade 7 drip shield (defined by the NE1a5s5EDA3b-ds.cdf), ten percent (10%) of the waste package surface area under the breached drip shield is assumed to be contacted by the dripping water. This assumption is made to incorporate the anticipated protection from dripping water contact that the drip shield provides subsequent to its initial (single patch) breach. In light of Assumptions 3.3 and 3.4, in which the entire surface area of the drip shield is considered in degradation modeling, this is a conservative assumption as the first breach of the drip shield may be on one of the side plates and not directly over the waste package. This assumption is used in the WAPDEG input file NE1a5s5EDA3b-wp1.inp on the tenth through thirteenth input lines after the last history file name. (No drip shield delay time is used in the input file NE0a5s6EDA3b-wp1.inp).
- 3.17 The current version of WAPDEG was developed to model a two-barrier waste package, with the outer barrier hard-wired to be a corrosion allowance material (CAM) of carbon steel, and the corrosion model parameters for the inner barrier able to be supplied by the user through the WAPDEG input file (*.inp, where "*" represents any file name prefix). In order to model a corrosion resistant material (CRM) with no CAM (corresponding to the single-barrier waste package), it is required that the "simulated" CAM thickness be set to a small number (1e-12 cm) and the CAM pit multiple (or roughness factor) to a large number (1e12) in the WAPDEG input file used. The effect is an immediate failure of the CAM upon satisfaction of the relative humidity (RH) and temperature thresholds for corrosion initiation. This assumption is used in the WAPDEG input files NE1a5s5EDA3b-wp1.inp and NE0a5s6EDA3b-wp1.inp on the second input line after the last history file name and on the third input line after the [No Drip Model, CAM] and [Neutral Drip Model, CAM] input headers.
- 3.18 The temperature corrosion initiation threshold for the very thin simulated CAM outer barrier was assumed to be represented by the cumulative distribution function A22TiTh.cdf (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 1/3 Response 3). This assumption has the effect of delaying the initiation of corrosion of the Alloy 22 until the temperature initiation threshold for corrosion of the simulated CAM is satisfied (since the CAM fails immediately upon satisfaction of the corrosion initiation thresholds). This assumption is based on that input. This assumption is used in the WAPDEG input files NE1a5s5EDA3b-wp1.inp and NE0a5s6EDA3b-wp1.inp on the first and second input lines after the [No Drip Model Features] and the [Neutral Drip Features] (if dripping occurs) headers.
- 3.19 The relative humidity corrosion initiation threshold for the very thin simulated CAM outer barrier was assumed to be represented by the cumulative distribution function A22TiRHth.cdf (CRWMS M&O 1999c. *Design Input Transmittal For License Application*

Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading, Item 1 p. 1/3 through 2/3 Response 4). This assumption has the effect of delaying the initiation of corrosion of the Alloy 22 until the relative humidity initiation threshold for corrosion of the simulated CAM is satisfied (since the CAM fails immediately upon satisfaction of the corrosion initiation thresholds). This assumption is used in the WAPDEG input files NE1a5s5EDA3b-wp1.inp and NE0a5s6EDA3b-wp1.inp on the third and fourth input lines after the [No Drip Model Features] header and on the fifth and sixth input lines after the [Neutral Drip Features] header (if dripping occurs).

- 3.20 General corrosion of the Alloy 22 waste package outer barrier under dripping is assumed to take place under mild electrochemical exposure conditions (pH range 3-10, 340 mV SHE). The basis for this assumption is several statements in the Engineered Materials Characterization Report (McCright 1998), among them: "Even if the salts present in the ground water concentrate on the warm metal surface, the net effect may produce an environment that is not highly aggressive." (p. 2-3). The absence of the CAM outer barrier (relative to the TSPA-VA design) also eliminates the possibility of tight crevice formation (a probable site for localized corrosion initiation) between the CAM and CRM barriers. This assumption is used in the WAPDEG input file NE1a5s5EDA3b-wp1.inp in the [Neutral Drip Model, CRM] input segment by using the "CRMGenrate+ArrheniusPit" model and corrosion rates from the gCx5050.cdf files (where x is the numeric 1, 2, and 3 corresponding to temperatures at 25, 50 and 100°C, respectively).
- 3.21 It is assumed that localized corrosion of Alloy 22 is possible in the presence of drips and if the temperature is above a critical temperature threshold for initiation. The critical threshold temperature is input to this calculation (file: A22LCTh.cdf) (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading, Item 1 p. 2/3 Response 6).* This assumption is based on that input. This assumption is used in the [Neutral Drip Features] input segment in the WAPDEG input file NE1a5s5EDA3b-wp1.inp on the third and fourth input lines following the [Neutral Drip Features] header.
- 3.22 For the 50 years before pre-closure ventilation ceases (see Assumption 3.6), it is assumed the waste package is not dripped upon. The basis for this assumption is that the repository is ventilated during this time (CRWMS M&O 1999e. *Design Input Request for LADS Phase II EDA Evaluations*, p. 4, "LADS Enhanced Design Alternatives" Table, Row 9 Column 4) and any seepage water in the emplacement drift is removed by the air flow. This assumption is used in defining the dripping initiation time on the fourteenth and fifteenth input lines after the last thermal hydrologic history file name in the WAPDEG input file NE1a5s5EDA3b-wp1.inp.

The following assumptions are made for titanium grade 7 waste package inner barrier degradation Modeling:

The WAPDEG input file NE1a5s5EDA3b-wp2.inp models the 1.5-cm thick titanium grade 7 inner barrier of a waste package (with a 2-cm thick Alloy 22 outer barrier) under a 2-cm thick titanium grade 7 drip shield that is always dripped on. In this simulation corrosion does not initiate until the outer barrier of the waste package experiences a patch breach and then the entire inner barrier surface begins to degrade. The WAPDEG input file NE0a5s6EDA3b-wp2.inp models a 1.5-cm thick titanium grade 7 inner barrier of a waste package (with a 2-cm thick Alloy 22 outer barrier) under a 2-cm thick titanium grade 7 drip shield that is never dripped on (equivalent, for WAPDEG modeling purposes, to having no drip shield present). The assumptions used in modeling the titanium grade 7 waste package inner barrier degradation are identical to those used in the TSPA-VA REV 01 base case calculation (CRWMS M&O 1998d, *Creating Input Tables from WAPDEG for RIP*) (DTN: MO9810SPA00013.000) with the exception of those listed below.

- 3.23 The same number of patches (903) were used to model the titanium grade 7 waste package inner barrier as were used to model the Alloy 22 waste package outer barrier (see Assumption 3.14). As the surface area of titanium grade 7 inner barrier is smaller than that of the Alloy 22 outer barrier, this assumption is equivalent to using a smaller patch size (the number of patches, not the patch area, is input to the WAPDEG code) to model degradation of the titanium grade 7 inner barrier. This assumption was made to be consistent with the modeling of the Alloy 22 waste package outer barrier. The assumption is conservative as a smaller patch size (or greater number of patches) leads to more conservative WAPDEG results (CRWMS M&O 1998a, *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document - Chapter 5, Waste Package Degradation Modeling And Abstraction*, p. F5-41 Figure 5-72). This assumption is used on the fourth input line (second value) in the WAPDEG input files NE1a5s5EDA3b-wp2.inp and NE0a5s6EDA3b-wp2.inp.
- 3.24 The NE1a5s5EDA3b-wp1.cdf (a cdf of first patch breach times of the Alloy 22 outer barriers of the waste packages) distribution is used as the "Distribution parameter(s)" for the "Distr for time range for ceramic protection" of the waste package inner barriers (this is perhaps better termed "the delay time for corrosion initiation" of the waste package inner barriers) in the WAPDEG input file NE1a5s5EDA3b-wp2.inp. The basis of this assumption is that dripping water can not contact the inner barrier of a waste package if the outer barrier of the waste package is intact. This assumption is also conservative as corrosion initiates upon the entire waste package inner barrier surface upon failure of the outer barrier. This distribution is read by the fourteenth and fifteenth lines after the last thermal hydrologic "history" file name in the WAPDEG input file NE1a5s5EDA3b-wp2.inp. (No drip shield delay time is used in the input file NE0a5s6EDA3b-wp2.inp).
- 3.25 After failure of the Alloy 22 outer barrier of the waste package (defined by the NE1a5s5EDA3b-wp1.cdf), ten percent (10%) of the waste package inner barrier surface area is assumed to be contacted by the dripping water. This assumption is based on the same rationale as used for Assumption 3.16 (the modeling of the Alloy 22 waste package outer

barrier). This assumption is used in the WAPDEG input file NE1a5s5EDA3b-wp2.inp on the tenth through thirteenth input lines after the last history file name. (No drip shield delay time is used in the input file NE1a5s6EDA3b-wp1.inp).

- 3.26 The current version of WAPDEG was developed to model a two-barrier waste package, with the outer barrier hard-wired to be a corrosion allowance material (CAM) of carbon steel, and the corrosion model parameters for the inner barrier able to be supplied by the user through the WAPDEG input file (*.inp, where "*" represents any file name prefix). In order to model a corrosion resistant material (CRM) with no CAM (corresponding to the single-barrier waste package), it is required that the "simulated" CAM thickness be set to a small number (1e-12 cm) and the CAM pit multiple (or roughness factor) be set to a large number (1e12) in the WAPDEG input file used. The effect is an immediate failure of the CAM upon satisfaction of the relative humidity (RH) and temperature thresholds for corrosion initiation (in reality these thresholds are very likely to have already been satisfied before the NE1a5s5EDA3b-wp2.inp and NE0a5s6EDA3b-wp2.inp WAPDEG simulations begin since these thresholds were applied in the NE1a5s5EDA3b-wp1.inp and NE0a5s6EDA3b-wp1.inp WAPDEG simulations). This assumption is used in the WAPDEG input files NE1a5s5EDA3b-wp2.inp and NE0a5s6EDA3b-wp2.inp on the second input line after the last history file name and on the third input line after the [No Drip Model, CAM] and [Neutral Drip Model, CAM] input headers.
- 3.27 The temperature corrosion initiation threshold for the very thin simulated CAM outer barrier was assumed to be represented by the cumulative distribution function for titanium grade 7 as given in A22TiTh.cdf (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 1/3 Response 3). This assumption has the effect of delaying the initiation of corrosion of the titanium inner barrier until the temperature initiation threshold for corrosion of the simulated CAM is satisfied (since the CAM fails immediately upon satisfaction of the corrosion initiation thresholds). This assumption is based on the input received. This assumption is used in the WAPDEG input files NE1a5s5EDA3b-wp2.inp and NE0a5s6EDA3b-wp2.inp on the first and second input lines after the [No Drip Model Features] and the [Neutral Drip Features] headers.
- 3.28 The relative humidity corrosion initiation threshold for the very thin simulated CAM outer barrier was assumed to be represented by the cumulative distribution function for titanium grade 7 as given in A22TiRHth.cdf (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 1/3 through 2/3 Response 4). This assumption has the effect of delaying the initiation of corrosion of the titanium inner barrier until the relative humidity initiation threshold for corrosion of the simulated CAM is satisfied (since the CAM fails immediately upon satisfaction of the corrosion initiation thresholds).

This assumption is used in the WAPDEG input files NE1a5s5EDA3b-wp2.inp and NE0a5s6EDA3b-wp2.inp on the third and fourth input lines after the [No Drip Model Features] header and on the fifth and sixth input lines after the [Neutral Drip Features] header (if dripping occurs).

- 3.29 It is assumed that there is no localized corrosion (i.e., there is only general or “patch” corrosion) of the titanium grade 7 waste package inner barrier. This assumption is based on input received (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 1/3 through 2/3 Response 7). This assumption is used in the input file NE1a5s5EDA3b-wp2.inp in the [No Drip Model, CRM] and [Neutral Drip Model, CRM] input segments by using the “CRMGeneralRateOnly” model.
- 3.30 The general corrosion rates used to model general corrosion degradation of the titanium grade 7 waste package inner barrier under dripping conditions are those derived in Attachment II for the titanium grade 7 drip shields and discussed in Assumptions 3.10 through 3.13. The basis for this assumption is that the exposure conditions at the inner barrier surface are not considered to differ in any significant way from those at the drip shield surface. This assumption is used in the input file NE1a5s5EDA3b-wp2.inp in the [Neutral Drip Model, CRM] input segments by using the “CRMGeneralRateOnly” model with the titanium grade 7 corrosion rate cdfs derived in Attachment II (files: gTi15050.cdf, gTi25050.cdf, and gTi35050.cdf).
- 3.31 The general corrosion rates used to model general corrosion degradation of the titanium grade 7 drip waste package inner barrier under non-dripping conditions are those used in the WAPDEG base case calculation (CRWMS M&O 1998d. *Creating Input Tables from WAPDEG for RIP*) (DTN: MO9810SPA00013.000) to model degradation of the Alloy 22 waste package inner barrier under non-dripping conditions. Corrosion rates for titanium grade 7 under no drip conditions are presently not available. General corrosion behavior of titanium grade 7 is expected to be similar to titanium grade 16. Corrosion rates for titanium grade 16 are available from the Long Term Corrosion Test Facility and are reported in Table 2.2-8 of the *Engineered Materials Characterization Report* (McCright 1998). The one year data available for Ti grade 16 indicates negligible corrosion rates under vapor conditions and is consistent with the corrosion rates reported for Alloy 22 under the same conditions. (Note that the six month corrosion data for titanium grade 16 are considered to be anomalous for reasons discussed in Section 2.2.7.1 of *Engineered Materials Characterization Report*). This assumption will have to be verified if titanium grade 7 is specified for the License Application Design. This assumption is used in the input file NE0a5s6EDA3b-wp2.inp in the [No Drip Model, CRM] input segment by using the “CRMGeneralRateOnly” model with the Alloy 22 non-dripping general corrosion rate cdfs (gnd17550.cdf, gnd27550.cdf, and gnd37550.cdf).

4. USE OF COMPUTER SOFTWARE AND MODELS

4.1 SOFTWARE APPROVED FOR QA WORK

The software used to perform the drip shield / waste package degradation simulations was WAPDEG version 3.09 (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*) (TBV-568) and its post processor, Post308 (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*, Appendix D) (TBV-568). The following has been obtained from the Software Configuration Secretary (SCS) relative to this software:

Software Name:	WAPDEG
Software Version:	3.09
CSCI Identifier:	30048 V3.09
Document Identifier:	30048-2999, REV 02
Media Identifier:	30048-M04-001, REV 02
Software Change Request:	LSBR 177

This software was obtained from the Software Configuration Manager in accordance with appropriate procedures. The WAPDEG simulations were executed on a DELL PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371) in the Windows NT 4.0 operating system. The post processing was accomplished on a DELL PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371) in the Windows NT 4.0 operating system.

WAPDEG version 3.09 is an appropriate tool for this application, because it was specifically designed to calculate waste package failure profiles (and the modeling process may be adapted to calculate drip shield failure profiles) in a manner consistent with the information requirements of the RIP code. Although there has been a Software Routine Report (SRR) prepared for version 3.09 of the WAPDEG code (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*), WAPDEG did not go through the complete qualification process required by QAP-SI-0 REV 04 when effective, so it is not to be considered qualified and has been designated "to be verified" (TBV-568). WAPDEG version 3.09 was used within the range of values for which it was validated in its Software Routine Report (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*).

Post308 is an appropriate tool for this application, because it is able to read WAPDEG output files and post-process them to make tables for input into RIP. Although all of the documentation necessary to fully qualify the Post308 code (as a software routine) has been included in the WAPDEG version 3.09 SRR (CRWMS M&O 1998b. *Software Routine Report for WAPDEG*

(Version 3.09), Appendix D), since WAPDEG version 3.09 did not go through the complete verification and validation process required by QAP-SI-0 REV 04 when effective, Post308 is not to be considered qualified and has been designated “to be verified” (TBV-568). Post308 was used within the range of values for which it was validated in its (equivalent of a) Software Routine Report (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*, Appendix D).

4.2 SOFTWARE ROUTINES

Mkhistory version 1.01 (Attachment I) was used to pre-process the thermal hydrologic time, temperature, and relative humidity “histories” into a format usable by the WAPDEG code.

Software Name: Mkhistory

Software Version: 1.01

Mkhistory was executed on a DELL PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371) in the Windows NT 4.0 operating system. Mkhistory version 1.01 has gone through the complete verification and validation process required by AP-SI.1Q REV 00 for a software routine and is thus a fully qualified software routine approved for use in quality affecting work. Mkhistory was used within the range of values tested and documented in Attachment I.

Mkhistory version 1.01 is an appropriate application because it is able to read input data and produce output files that can be used as input into WAPDEG.

4.3 MODELS

The WAPDEG conceptual model and computer software are used in this calculation. The data tracking numbers for this model’s inputs and outputs as well as the documentation sources for this model are contained in the TSPA-VA Technical Basis Document (CRWMS M&O 1998a. *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document - Chapter 5, Waste Package Degradation Modeling and Abstraction*) (DTN: MO9807MWDWAPDG.000), the TSPA-VA REV 01 base case calculation (CRWMS M&O 1998d. *Creating Input Tables from WAPDEG for RIP*) (DTN: MO9810SPA00013.000), and the WAPDEG version 3.09 Software Routine Report (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*). The specific model inputs and outputs relevant to this calculation have also been submitted to the data tracking system (CRWMS M&O 1999a. *Supporting Media for “RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIIb”*) (DTN: MO9904MWDWAP78.003) and are discussed further in the next section.

The WAPDEG computer model was selected for use in this calculation because it was specifically designed to calculate waste package failure profiles (and the modeling process may be adapted to calculate drip shield failure profiles) in a manner consistent with the information requirements of the RIP code.

5. CALCULATION

All inputs discussed in this section and all results discussed in the following section are included in the electronic media that supports this calculation (CRWMS M&O 1999a. *Supporting Media for "RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIIb"*) (DTN: MO9904MWDWAP78.003).

5.1 MKHISTORY INPUTS

Files containing the relative humidity and temperature histories at the surface of waste packages in the northeast (NE) region of the repository were provided as input to this calculation (Buscheck 1999) (DTN: LL990301604242.081). These histories are organized by bin numbers and model identifier with file names like NE_snf_mean_yy_noBF_85_c_j4_22_03_02_0_data, where NE denotes the northeast region of the potential repository, snf denotes commercial spent nuclear fuel, yy is a bin number, noBF denotes no backfill was used, 85 denotes an areal mass loading of 85 MTU/acre, and the numeric 22 indicates that these thermal hydrologic histories are applicable to "long-term average" climate conditions. The remainder of the file name designators are not relevant to this calculation.

The thermal hydrologic history files contain columns of ASCII numerical data. Column 1 contains the time (years), Column 2 the waste package surface temperature ($^{\circ}\text{C}$), Column 3 the relative humidity at the waste package surface (fraction), Column 4 the air mass fraction (X_{air}), Column 5 the liquid saturation in the invert (fraction), Column 6 the drift wall temperature ($^{\circ}\text{C}$), Column 7 the drift wall relative humidity (fraction), Column 8 the drip shield surface temperature ($^{\circ}\text{C}$), and Column 9 the drip shield surface relative humidity (fraction). In this calculation, a total of 16 thermal hydrologic history files are used, each distinguished by differing values of the thermal hydrologic history file bin number. Bin numbers (the yy discussed above) 00, 01, 10, 11, 12, 21, 22, 31, 32, 41, 42, 52, 61, 62, 71, and 91 are used in this calculation (i.e., NE_snf_mean_00_noBF_85_c_j4_22_03_02_0_data, NE_snf_mean_01_noBF_85_c_j4_22_03_02_0_data, . . . , etc.).

These thermal hydrologic history files were processed by the Mkhhistory software routine. The bulk (but not all) of Mkhhistory's processing is devoted to copying Columns 1, 2, and 3 (the columns containing the time, temperature and RH at the waste package surface) or Columns 1, 8, and 9 (the columns containing the time, temperature and RH at the drip shield surface) from the thermal hydrologic history files named in Column 1 of the Mkhhistory input file(s) to the file named in Column 2 of the Mkhhistory input file. Note that the first row of ASCII numerical data (corresponding to time equals 0 years) is not copied to the file named in Column 2 of the Mkhhistory input file as discussed in Attachment I. Two Mkhhistory input files were used, EDA3ds.mk, for the drip shield surface, and EDA3.mk for the waste package surface. The initial contents of the Mkhhistory input file EDA3.mk are:

16,9,3	number of files, columns, and columns to print
1,2,3	print specified columns
NE_snf_mean_00_noBF_85_c_j4_22_03_02_0_data	NEsnf00noBF85cj42203020.hst
NE_snf_mean_01_noBF_85_c_j4_22_03_02_0_data	NEsnf01noBF85cj42203020.hst

NE_snf_mean_10_noBF_85_c_j4_22_03_02_0_data	NESnf10noBF85cj42203020.hst
NE_snf_mean_11_noBF_85_c_j4_22_03_02_0_data	NESnf11noBF85cj42203020.hst
NE_snf_mean_12_noBF_85_c_j4_22_03_02_0_data	NESnf12noBF85cj42203020.hst
NE_snf_mean_21_noBF_85_c_j4_22_03_02_0_data	NESnf21noBF85cj42203020.hst
NE_snf_mean_22_noBF_85_c_j4_22_03_02_0_data	NESnf22noBF85cj42203020.hst
NE_snf_mean_31_noBF_85_c_j4_22_03_02_0_data	NESnf31noBF85cj42203020.hst
NE_snf_mean_32_noBF_85_c_j4_22_03_02_0_data	NESnf32noBF85cj42203020.hst
NE_snf_mean_41_noBF_85_c_j4_22_03_02_0_data	NESnf41noBF85cj42203020.hst
NE_snf_mean_42_noBF_85_c_j4_22_03_02_0_data	NESnf42noBF85cj42203020.hst
NE_snf_mean_52_noBF_85_c_j4_22_03_02_0_data	NESnf52noBF85cj42203020.hst
NE_snf_mean_61_noBF_85_c_j4_22_03_02_0_data	NESnf61noBF85cj42203020.hst
NE_snf_mean_62_noBF_85_c_j4_22_03_02_0_data	NESnf62noBF85cj42203020.hst
NE_snf_mean_71_noBF_85_c_j4_22_03_02_0_data	NESnf71noBF85cj42203020.hst
NE_snf_mean_91_noBF_85_c_j4_22_03_02_0_data	NESnf91noBF85cj42203020.hst

The first line of this Mkhhistory input file indicates that 16 thermal hydrologic history files (whose file names are listed in the first column of the Mkhhistory input file (starting on row 3)) are to be processed by Mkhhistory, these history files contain 9 columns of data, of which 3 will be extracted to the file name specified in the second column of the Mkhhistory input file. The second line of the Mkhhistory input file indicates that columns 1, 2, and 3 of the thermal hydrologic history files (whose file names are listed in the first column of the Mkhhistory input file (starting on row 3)) will be extracted to the file name specified in the second column of the Mkhhistory input file (i.e., data from NE_snf_mean_00_noBF_85_c_j4_22_03_02_0_data is to be copied to NESnf00noBF85cj42203020.hst, etc.). The above are the contents of EDA3.mk before execution of Mkhhistory (several data segments are appended to this file during Mkhhistory program execution as discussed in Attachment I. The thermal hydrologic history files before and after processing by Mkhhistory and the EDA3.mk and EDA3ds.mk files after execution of Mkhhistory are included in the electronic media supporting this calculation (CRWMS M&O 1999a. *Supporting Media for "RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIIb"*) (DTN: MO9904MWDWAP78.003).

Procedurally, the Mkhhistory program prompts the user for a list-file name (this is the Mkhhistory input file, i.e., EDA3.mk). The Mkhhistory program then prompts the user for the total number of waste packages to be considered. The user entered "0" to cause the default value of 1,000,000 waste packages to be used in order to retain the maximum possible six digits of accuracy for the fraction of waste packages represented by each thermal hydrologic history file.

5.2 WAPDEG INPUTS

WAPDEG version 3.09 requires several input files (*.inp, *.cdf, and *.hst files, see below) (DTN: MO9904MWDWAP78.003) and creates several output files (*.aux, *.bin, *.cam, *.crm, *.out, *.pat) (DTN: MO9904MWDWAP78.003). Post308 (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*, Appendix D) reads from the *.bin, *.pat, *.out files of the WAPDEG version 3.09 results and creates several output files (*.asc, *.dat, *.rip) (DTN: MO9904MWDWAP78.003). The *.rip files are used as input to RIP (Golder Associates 1998) and are the primary results of this calculation described in Section 6.0.

The *.cdf file names and other model parameters are contained in the WAPDEG input file for the particular simulation being executed. Specifically WAPDEG requires:

- 1) Thermal hydrologic history files containing the relative humidity (RH) and temperature (T) at the surface of the waste packages or drip shields (the *.hst files discussed above) (DTN: MO9904MWDWAP78.003)
- 2) Cumulative distribution functions (cdf) for the temperature threshold for the onset of corrosion. This threshold is used for the simulated outer barrier corrosion allowance material (CAM) of the drip shields and waste package barriers (file: A22TiTh.cdf) (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 1/3 Response 1 and 3).
- 3) Cumulative distribution functions for the RH threshold for the onset of corrosion for the simulated CAM outer barrier of the drip shields and waste package barriers (file: A22TiRHth.cdf) (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 1/3 Response 2 and 4).
- 4) Cumulative distribution functions for the titanium grade 7 drip shield and waste package inner barrier general corrosion rates (see Attachment II) at 30, 60, and 120°C (files: gTi15050.cdf, gTi25050.cdf, and gTi35050.cdf) (DTN: MO9904MWDWAP78.003).
- 5) Cumulative distribution functions for general corrosion rates under dripping water conditions for the Alloy 22 corrosion resistant material (CRM) outer barrier (files: gC*.cdf) (Bullard 1998) (DTN: MO9812MWDDSQ37.000).
- 6) Cumulative distribution functions for the Alloy 22 outer barrier and titanium grade 7 inner barrier of the waste packages general corrosion rates with no dripping water (CRWMS M&O 1998e. *Cumulative Distribution Functions for No Drip Corrosion Resistant Material General Corrosion Model*, Section 6) at 25, 50, and 100°C (files: gnd*.cdf) (DTN: MO9810SPA00013.000).
- 7) The cumulative distribution function for the titanium grade 7 drip shield failures to use as drip start times for the waste packages beneath the failed drip shields (file: NE1a5s5EDA3b-ds.cdf) (DTN: MO9904MWDWAP78.003) containing the first breach times from the WAPDEG simulation using the NE1a5s5EDA3b-ds.inp input file). This cdf is used as a drip initiation time distribution in the WAPDEG simulation using the NE1a5s5EDA3b-wp1.inp WAPDEG input file.
- 8) The cumulative distribution function for the Alloy 22 waste package outer barrier failures to use as corrosion initiation times for the titanium waste package inner barriers (for the dripping case, NE1a5s5EDA3b-wp1.cdf containing the first breach times from the WAPDEG simulation using the NE1a5s5EDA3b-wp1.inp input file; for the non-dripping case, NE0a5s6EDA3b-wp1.cdf containing the first breach times from the WAPDEG simulation using the NE0a5s6EDA3b-wp1.inp input file). This cdf is used as a corrosion initiation time distribution in the WAPDEG simulations using the NE1a5s5EDA3b-wp2.inp (dripping case) and NE0a5s6EDA3b-wp2.inp (non-dripping case) input files.
- 9) A cumulative distribution function for the temperature threshold for the initiation of localized corrosion of the Alloy 22 waste package outer barrier (file: A22LCTth.cdf) (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced*

Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading, Item 1 p. 2/3 Response 6).

- 10) The above file names and other model parameters are contained in the WAPDEG input file (*.inp) for the particular simulation being executed. For the simulation of the drip shield / waste package failure profiles, the other parameters used in the WAPDEG input file are identical to those discussed in the TSPA-VA REV 01 base case calculation (CRWMS M&O 1998d. *Creating Input Tables from WAPDEG for RIP*, Section 5.0) (DTN: MO9810SPA00013.000), with the exceptions noted above in Section 3.0.

Five WAPDEG input files were used to generate the RIP input tables for the License Application Design Selection Analyses: Enhanced Design Alternative IIIb. NE1a5s5EDA3b-ds.inp (for the drip shield under dripping conditions), NE1a5s5EDA3b-wp1.inp (for the waste package outer barrier under dripping conditions only after drip shield failure), NE1a5s5EDA3b-wp2.inp (for the waste package inner barrier under dripping conditions), NE0a5s6EDA3b-wp1.inp (for the waste package outer barrier under non-dripping conditions), and NE0a5s6EDA3b-wp2.inp (for the waste package inner barrier under non-dripping conditions). These input files are included in the electronic media supporting this calculation (CRWMS M&O 1999a. *Supporting Media for "RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIIb"*) (DTN: MO9904MWDWAP78.003).

The first two characters of the input file name indicate that the Northeast (NE) region of the potential repository (using its thermal hydrologic history files) is being simulated. The next character in the input file name (0 or 1) indicates, respectively, that a no-drip case is being simulated or the waste packages are subject to dripping throughout the simulation. The next two characters (a5) indicate that the file is for the base case infiltration. The next characters (s5 or s6) refer to the different uncertainty/variability splits and percentile of the uncertainty distribution used for the median of the titanium (drip shield and waste package inner barrier) and Alloy 22 (waste package outer barrier) general corrosion rate variability distributions. The classifications are as follows:

Uncertainty/Variability Splitting
(0.25 Uncertainty = 0.75 Variability, etc.)

		Uncertainty		
		0.25	0.50	0.75
Percentile	5th	s1	s2	s3
	50th	s4	s5	s6
	95th	s7	s8	s9

From the above table, it is apparent that the dripping input files (NE1a5s5EDA3b-ds.inp, NE1a5s5EDA3b-wp1.inp, and NE1a5s5EDA3b-wp2.inp) use a 50% uncertainty - 50% variability split and use the 50th percentile of the uncertainty distribution for the median of the general corrosion rate variability distributions. The non-dripping input files (NE0a5s6EDA3b-wp1.inp and NE0a5s6EDA3b-wp2.inp) use a 75% uncertainty - 25% variability split and use the 50th percentile

of the uncertainty distribution for the median of the general corrosion rate variability distributions. The characters (EDA3b) indicate that these input files are used in analyzing LA Design Selection Analyses: Enhanced Design Alternative IIb. For reference, below is shown the input file NE1a5s5EDA3b-ds.inp used in the WAPDEG simulation of the dripping exposure condition:

NE1a5s5EDA3b-ds.inp

snf, always drip, 100%, No Backfill, lta nominal i alpha mean
Uncertainty/Variability=50/50 drip, 50th Quantile
Ti Gr7 2 cm Drip Shield EDA3b

START OF PARAMETERS

3.09	Version number of code
16	Number of alternate histories
NESnf00noBF85cj42203020ds.hst	History file 1
10996, 0., 0.	packs/history, T std, RH std
NESnf01noBF85cj42203020ds.hst	History file 2
132147, 0., 0.	packs/history, T std, RH std
NESnf10noBF85cj42203020ds.hst	History file 3
2972, 0., 0.	packs/history, T std, RH std
NESnf11noBF85cj42203020ds.hst	History file 4
207353, 0., 0.	packs/history, T std, RH std
NESnf12noBF85cj42203020ds.hst	History file 5
35184, 0., 0.	packs/history, T std, RH std
NESnf21noBF85cj42203020ds.hst	History file 6
49526, 0., 0.	packs/history, T std, RH std
NESnf22noBF85cj42203020ds.hst	History file 7
155585, 0., 0.	packs/history, T std, RH std
NESnf31noBF85cj42203020ds.hst	History file 8
5568, 0., 0.	packs/history, T std, RH std
NESnf32noBF85cj42203020ds.hst	History file 9
206434, 0., 0.	packs/history, T std, RH std
NESnf41noBF85cj42203020ds.hst	History file10
983, 0., 0.	packs/history, T std, RH std
NESnf42noBF85cj42203020ds.hst	History file11
112040, 0., 0.	packs/history, T std, RH std
NESnf52noBF85cj42203020ds.hst	History file12
64191, 0., 0.	packs/history, T std, RH std
NESnf61noBF85cj42203020ds.hst	History file13
4913, 0., 0.	packs/history, T std, RH std
NESnf62noBF85cj42203020ds.hst	History file14
7860, 0., 0.	packs/history, T std, RH std
NESnf71noBF85cj42203020ds.hst	History file15
2620, 0., 0.	packs/history, T std, RH std
NESnf91noBF85cj42203020ds.hst	History file16
1637, 0., 0.	packs/history, T std, RH std
1.0e-12, 2.0	Thickness of outer, inner barriers (cm)
75., 0.35	% thick to fail CRM, frac variance to packs
400, 975, 3100, 3100	Number of packs, patches/pack, pits/patch
1.0, 1.e6, 1200	Bin start time & end time (y), and # of bins
1.e4, 5.e4, 1.e5, 1.e6	Output times (y) for cumul. pit penetrations
304058394, F, F	Random# seed, restart flag, ignore CAM variance
0.0, 0.0	Max temp, RH change over a time step (C, %RH)
180.0, 180.0	Angle defining top/bottom (degrees)
Fixed	Distribution for fraction top seeing drips
1.0	Distribution parameter(s)
Fixed	Distribution for fraction bottom seeing drips
1.0	Distribution parameter(s)
Fixed	Distribution for dripping start time

0.0	Distribution parameter(s)
Fixed	Distribution for dripping stop time
1000000.0	Distribution parameter(s)
T, F	Neutral(T/F) water initially, new water (T/F)
Fixed	Distr for time range for ceramic protection
50.0	Distribution parameter(s)
1.0	Package variance share
[No Drip Model, CAM]	This segment always required
CAMGeneral+PitMultiples	CAM corrosion model for no drips
Fixed	Distribution for pit multiple
1.0e12	Mean, StDev, Min, Max
[No Drip Model, CRM]	This segment always required
CRMGeneralRateOnly	CRM corrosion model for drips
3, 1.e+6	Number of dists (temps °C), max CRM rate
30.0	Temp appropriate for dist #1
File	Distribution type for #1
gTi15050.cdf	Distribution parameter (s)
60.0	Temp appropriate for dist #2
File	Distribution type for #2
gTi25050.cdf	Distribution parameter (mm/yr)
120.0	Temp appropriate for dist #3
File	Distribution type for #3
gTi35050.cdf	Distribution parameter (mm/yr)
[No Drip Features]	This segment always required
File	Distr for thermal protection temperature
A22TiTth.cdf	Distribution parameter(s)
File	Dist type for humid-air initiation
A22TiRHth.cdf	Distribution parameter(s)
Fixed	Dist type for humid-air/aqueous transition
100.	Distribution parameter(s)
0.0, 0.0	Galvanic protect depth %, % patches protected
0.0	Spalling depth as a % of thickness
Fixed	Dist for multiple for CAM corrosion rate
1.0	Distribution parameter(s)
Fixed	Dist for multiple for CRM corrosion rate
1.0	Distribution parameter(s)
1.0	Pack variance share for multiples
[Neutral Drip Model, CAM]	Required if any non-neutral drips can be seen
CAMGeneral+PitMultiples	CAM corrosion model for no drips
Fixed	Distribution for pit multiple
1.0e12	Mean, StDev, Min, Max
[Neutral Drip Model, CRM]	Required if any non-neutral drips can be seen
CRMGeneralRateOnly	CRM corrosion model for drips
3, 1.e+6	Number of dists (temps °C), max CRM rate
30.0	Temp appropriate for dist #1
File	Distribution type for #1
gTi15050.cdf	Distribution parameter (s)
60.0	Temp appropriate for dist #2
File	Distribution type for #2
gTi25050.cdf	Distribution parameter (mm/yr)
120.0	Temp appropriate for dist #3
File	Distribution type for #3
gTi35050.cdf	Distribution parameter (mm/yr)
[Neutral Drip Features]	Required if any non-neutral drips can be seen
File	Distr for thermal protection temperature
A22TiTth.cdf	Distribution parameter(s)
File	Dist type for CRM LC T init
A22LCTth.cdf	Distribution parameter
File	Dist type for humid-air initiation
A22TiRHth.cdf	Distribution parameter(s)
Fixed	Dist type for humid-air/aqueous transition

100.	Distribution parameter(s)
0.0, 0.0	Galvanic protect depth %, % patches protected
0.0	Spalling depth as a % of thickness
Fixed	Dist for multiple for CAM corrosion rate
1.0	Distribution parameter(s)
Fixed	Dist for multiple for CRM corrosion rate
1.0	Distribution parameter(s)
1.0	Pack variance share for multiples

Procedurally, the WAPDEG code was executed by typing the name of the executable (i.e., wap309) on the command line and entering the name of the WAPDEG input file (i.e., NE1a5s5EDA3b-ds.inp).

The “raw” output from a WAPDEG simulation consists of six files: a *.out file, *.pat file, *.bin file, *.crm file, *.cam file, and *.aux file (where “*” is the input file name prefix). The content and format of these files are discussed in the WAPDEG version 3.09 Software Routine Report (CRWMS M&O 1998b, Section 4.1). These files are also included in the electronic media supporting this calculation (CRWMS M&O 1999a. *Supporting Media for “RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIb”*) (DTN: MO9904MWDWAP78.003). Only the *.out (drip shield / waste package failure curves), *.pat (cumulative number of patch penetrations for each drip shield / waste package), and *.bin (cumulative number of pit penetrations for each drip shield / waste package (if any)) files are used by Post308 to create the RIP input tables.

5.3 POST308 INPUTS

The input files discussed above are used by WAPDEG to produce drip shield / waste package degradation profiles. The drip shield / waste package degradation profiles resulting from the WAPDEG simulations are then read by the post processor, Post308, which generates a table in a format appropriate for input into RIP (Golder Associates 1998. pp. 7-22 through 7-25). The RIP input table contains:

- 1) The fraction of drip shields / waste packages failed versus time curve for the simulation,
- 2) The average number of pit penetrations per failed drip shield / waste package versus time curve, and
- 3) The average number of patch penetrations per failed drip shield / waste package versus time curve.

As identified earlier in this calculation, the drip shields and waste package inner barriers are assumed to only undergo general corrosion processes, which result in “patch” perforations. As a result, the above curves only reflect the results of “patch” perforations for the titanium grade 7 layers (i.e., RIP input Item 2 above, for instance, will indicate no pit penetrations for the drip shields).

Procedurally, Post308 is executed in a Windows NT 4.0 MS-DOS prompt window within the same directory as the output files from WAPDEG (i.e., *.bin, *.pat, *.out). The program prompts the user for the particular filename prefix that is common to the WAPDEG simulation output files to be post processed. After the program post processes the WAPDEG output, it prompts the user to enter a file name for the RIP input table to be created. The RIP input tables were chosen to have the same prefix name as the corresponding WAPDEG input files with a *.rip extension. The output from the post

processor consists of three files; *.asc, *.dat, and *.rip. The content and format of these files are discussed in the WAPDEG version 3.09 Software Routine Report (CRWMS M&O 1998b, Appendix D). These files are also included in the electronic media supporting this calculation (CRWMS M&O 1999a. *Supporting Media for "RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIIb"*) (DTN: MO9904MWDWAP78.003).

6. RESULTS

Since unqualified inputs were used in the development of the results presented in this section, they should be considered TBV. This document will not directly support any construction, fabrication, or procurement activity, and therefore, the inputs and outputs are not required to be procedurally controlled as TBV. However, any use of the data from this analysis for inputs into documents supporting construction, fabrication, or procurement is required to be controlled as TBV in accordance with appropriate procedures. Furthermore, this calculation makes use of software (WAPDEG version 3.09 and Post308) that is unqualified (TBV-568).

All input and output files relevant to this calculation are included in the electronic media supporting this calculation (CRWMS M&O 1999a. *Supporting Media for "RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIIb"*) (DTN: MO9904MWDWAP78.003). For brevity, only selected files are reproduced in hardcopy form within this section.

The primary outputs of Mkhhistory are the *.hst files used as input to WAPDEG. For reference, the contents of NESnf00noBF85cj42203020.hst are:

1.000000	96.180000	0.452550
1.500000	100.990000	0.477310
2.000000	103.970000	0.492840
3.000000	109.020000	0.517740
4.000000	112.430000	0.531440
5.000000	114.800000	0.535520
6.000000	116.730000	0.542480
7.000000	118.210000	0.547360
8.000000	119.040000	0.552390
9.000000	119.780000	0.548740
10.000000	120.070000	0.548910
11.000000	120.180000	0.550070
12.000000	120.090000	0.552870
15.000000	118.480000	0.490130
20.000000	114.220000	0.544470
25.000000	109.350000	0.604580
26.000000	108.350000	0.613090
27.000000	107.410000	0.619300
30.000000	104.670000	0.636770
35.000000	102.840000	0.655810
40.000000	98.290000	0.671410
50.000000	130.100000	0.512230
51.000000	151.890000	0.230600
52.000000	155.330000	0.178810
55.000000	153.890000	0.173190
60.000000	148.120000	0.200690
65.000000	139.330000	0.252470
70.000000	125.240000	0.374630
75.000000	112.700000	0.551380

76.000000	111.080000	0.571820
77.000000	109.860000	0.577250
80.000000	106.230000	0.591310
90.000000	103.990000	0.612050
100.000000	102.050000	0.629720
101.000000	101.840000	0.630730
105.000000	101.050000	0.635040
110.000000	100.070000	0.640450
120.000000	98.000000	0.651040
130.000000	95.750000	0.660620
140.000000	93.460000	0.670880
160.000000	90.250000	0.687380
180.000000	88.510000	0.700430
200.000000	87.040000	0.714310
220.000000	86.000000	0.722940
250.000000	84.480000	0.735500
300.000000	82.410000	0.754120
350.000000	80.640000	0.768910
400.000000	79.140000	0.781300
450.000000	77.850000	0.792030
500.000000	76.610000	0.802220
550.000000	75.440000	0.811660
600.000000	74.380000	0.820000
700.000000	72.500000	0.834660
800.000000	70.720000	0.847270
900.000000	69.170000	0.858650
1000.000000	67.770000	0.867440
1100.000000	66.710000	0.874390
1200.000000	65.680000	0.880170
1300.000000	64.580000	0.887690
1400.000000	63.430000	0.893790
1500.000000	62.220000	0.901490
1600.000000	61.410000	0.904460
1800.000000	59.900000	0.911360
2000.000000	58.350000	0.918190
2200.000000	57.240000	0.922190
2500.000000	55.630000	0.927390
3000.000000	53.680000	0.931980
3500.000000	52.230000	0.933480
4000.000000	51.000000	0.937380
4500.000000	50.010000	0.937000
5000.000000	49.150000	0.939390
6000.000000	47.510000	0.940830
7000.000000	46.140000	0.941100
8000.000000	44.870000	0.944410
10000.000000	42.660000	0.945530
15000.000000	37.880000	0.952080
20000.000000	34.540000	0.958980
30000.000000	29.790000	0.968960
40000.000000	27.190000	0.976110
50000.000000	25.690000	0.979990
60000.000000	24.570000	0.984570
80000.000000	23.270000	0.988390
100000.000000	22.590000	0.991700
120000.000000	22.270000	0.992800
150000.000000	21.850000	0.994590
200000.000000	21.530000	0.995960
300000.000000	21.260000	0.997210
400000.000000	21.150000	0.997780
500000.000000	21.080000	0.998070
600000.000000	21.040000	0.998280

700000.000000	21.020000	0.998410
800000.000000	21.000000	0.998540
900000.000000	20.990000	0.998620

The other outputs of Mkhhistory are appended to the EDA3.mk file and consist of the history file input segment (i.e., all the text in the input file lines from “16 |Number of alternate histories” to “2620, 0., 0. |packs/history, T std, RH std” in the WAPDEG input files used), documentation of the sum of the fraction and total number of waste packages represented by each history, and a text segment that could be used to graph all of the histories processed. These files are contained in the electronic media supporting this calculation (CRWMS M&O 1999a. *Supporting Media for “RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIIb”*).

For reference the RIP input table NE1a5s5EDA3b-wp2.rip (DTN: MO9904MWDWAP78.003) is shown below.

```
! From wapdeg file: NE1a5s5EDA3b-wp2
! From wapdeg version: 3.09
! Postprocessor: post308
! NE1a5s5EDA3b-wp2.inp
!
! snf, always drip, 10%, No Backfill, lta nominal i alpha mean
! Uncertainty/Variability=50/50 drip, 50th Quantile
! Ti Gr7 1.5 cm WP - EDA3b
!
! START OF PARAMETERS
2
3 83
1 2 3
0.0000
156674.1070
168036.2097
186233.3961
200747.9395
216300.5197
227790.6937
235780.1260
242671.7310
251199.7414
258527.7673
263026.7992
266072.5060
269153.4804
272270.1308
278624.4268
285101.8268
288403.1503
291742.7014
295120.9227
298538.2619
301995.1720
305492.1113
309029.5433
312607.9367
316227.7660
319889.5110
323593.6569
327340.6949
```

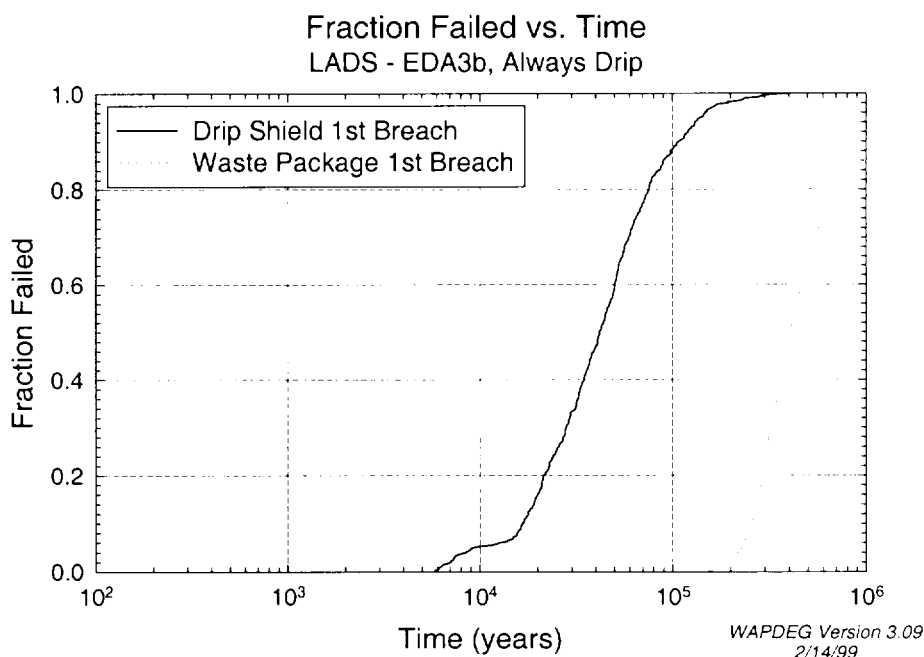
331131.1215		
334965.4392		
338844.1561		
342767.7865		
346736.8505		
350751.8740		
354813.3892		
358921.9346		
363078.0548		
367282.3005		
371535.2291		
375837.4043		
380189.3963		
384591.7820		
389045.1450		
393550.0755		
398107.1706		
402717.0343		
407380.2778		
412097.5191		
419282.9434		
426579.5188		
431519.0768		
436515.8322		
441570.4474		
449269.7683		
457088.1896		
462381.0214		
467735.1413		
473151.2590		
487007.8675		
501187.2336		
506990.7083		
512861.3840		
518800.0389		
527845.9522		
540141.0639		
549540.8739		
559122.7912		
572146.4341		
582103.2178		
592252.8994		
609563.8284		
630985.2221		
649392.3908		
664518.6828		
676082.9754		
687871.3091		
703893.8902		
728678.5362		
763020.0976		
862363.8731		
971708.4452		
1000000.0000		
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0066	0.0000	1.8270
0.0181	0.0000	2.4113
0.0288	0.0000	2.7536
0.0387	0.0000	3.4038
0.0490	0.0000	4.0471

0.0635	0.0000	4.2378
0.0748	0.0000	4.1982
0.0863	0.0000	4.5464
0.1017	0.0000	4.8616
0.1155	0.0000	4.9588
0.1263	0.0000	4.9305
0.1340	0.0000	5.0577
0.1402	0.0000	5.1174
0.1516	0.0000	5.8844
0.1698	0.0000	6.2556
0.1780	0.0000	6.4323
0.1895	0.0000	6.3985
0.2045	0.0000	6.3215
0.2167	0.0000	6.3791
0.2279	0.0000	6.5483
0.2477	0.0000	6.4704
0.2561	0.0000	6.7160
0.2666	0.0000	6.8841
0.2837	0.0000	6.7930
0.2926	0.0000	6.9035
0.2986	0.0000	7.1665
0.3037	0.0000	7.3910
0.3102	0.0000	7.6955
0.3193	0.0000	8.0018
0.3355	0.0000	8.0333
0.3464	0.0000	8.1913
0.3541	0.0000	8.5224
0.3669	0.0000	8.6541
0.3770	0.0000	8.9193
0.3913	0.0000	9.0151
0.4042	0.0000	9.1655
0.4145	0.0000	9.4206
0.4187	0.0000	9.7633
0.4283	0.0000	9.9643
0.4430	0.0000	10.0964
0.4493	0.0000	10.4169
0.4676	0.0000	10.4413
0.4752	0.0000	10.7644
0.4783	0.0000	11.2578
0.4927	0.0000	11.4562
0.5047	0.0000	11.7537
0.5101	0.0000	12.1642
0.5204	0.0000	12.7675
0.5398	0.0000	13.0500
0.5479	0.0000	13.3236
0.5549	0.0000	13.6068
0.5623	0.0000	13.8794
0.5729	0.0000	14.3395
0.5855	0.0000	14.7902
0.5947	0.0000	15.0458
0.6061	0.0000	15.3402
0.6126	0.0000	15.7407
0.6213	0.0000	16.7485
0.6429	0.0000	17.4257
0.6507	0.0000	17.7745
0.6584	0.0000	18.0788
0.6650	0.0000	18.3900
0.6735	0.0000	18.9266
0.6843	0.0000	19.7518
0.7001	0.0000	20.0931
0.7084	0.0000	20.6518

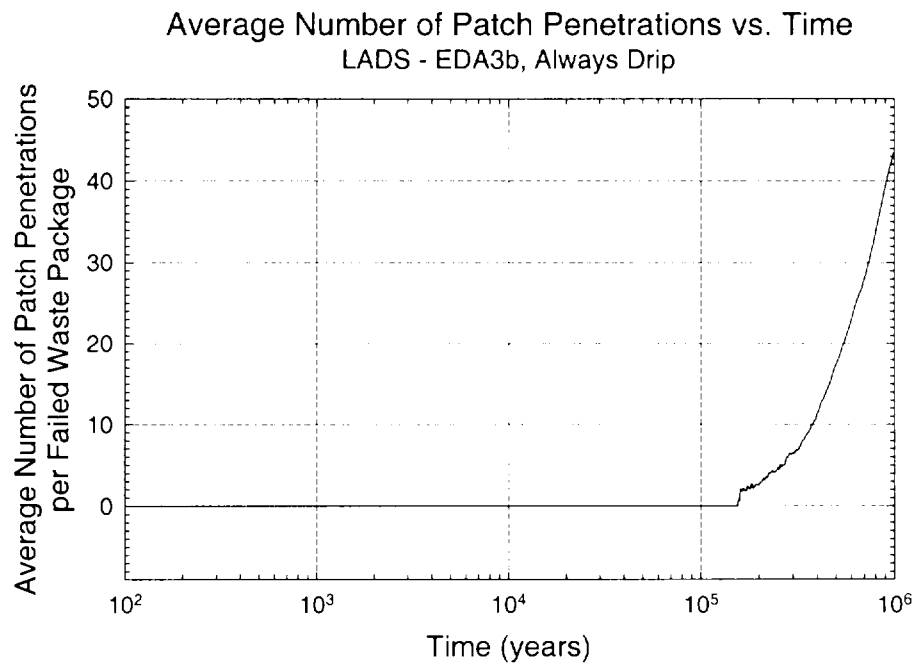
0.7204	0.0000	21.4239
0.7302	0.0000	21.9416
0.7406	0.0000	22.4752
0.7489	0.0000	23.6015
0.7601	0.0000	24.8899
0.7736	0.0000	25.7308
0.7876	0.0000	26.3554
0.7997	0.0000	26.6903
0.8038	0.0000	27.4024
0.8142	0.0000	28.1962
0.8242	0.0000	29.5653
0.8345	0.0000	31.4916
0.8428	0.0000	37.2917
0.8556	0.0000	42.6232
0.8575	0.0000	43.3557

The RIP input table consists of a column of times in years (the first single column of data) followed by three columns consisting of the fraction of waste packages failed, the number of pit penetrations per failed waste package, and the number of patch penetrations per failed waste package. These last three columns all share the same time grid (the first single column of data).

Presented below is a graph (derived from the NE1a5s5EDA3b-ds.dat (for the drip shields) and NE1a5s5EDA3b-wp2.dat (for the waste packages) files) of the first breach (patch) curves for the drip shields and waste packages. There is no localized corrosion allowed of the drip shields and waste package inner barriers. Hence the first breach curve of the drip shields and waste packages is equivalent to their first patch curve.



Presented below is a graph of the average number of patch penetrations per failed waste package (derived from the NE1a5s5EDA3b-wp2.asc file):



The first breach curve for the waste package and the average number of patch penetrations per failed waste package curve are also represented in the RIP input table, NE1a5s5EDA3b-wp2.rip.

7. REFERENCES

1. Bullard, B. E. 1998. *Alloy 22 Dripping General Corrosion Rate Cumulative Distribution Functions*. Las Vegas, Nevada: CRWMS M&O. DTN: MO9812MWDDSQ37.000.
2. Buscheck, T.A. 1999. *LADS Phase II Multiscale TH Calculation for EDA III*. Livermore, California: Lawrence Livermore National Laboratory. DTN: LL990301604242.081.
3. CRWMS M&O 1999a. *Supporting Media for "RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIIb"*. 210-78r0.exe. Windows Self-extracting archive. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990528.0283. DTN: MO9904MWDWAP78.003.
4. CRWMS M&O 1999b. *Design Input Transmittal For Waste Stream Information for LADS, Phase 2, EDAs*. Input Tracking No. PA-WP-99142.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990315.0047.
5. CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*. Input Tracking No. PA-WP-99089.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990219.0501.
6. CRWMS M&O 1999d. *Design Input Transmittal For Skirt Dimensions for LADS, Phase 2, EDA Waste Packages*. Input Tracking No. PA-WP-99148.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990316.0175.
7. CRWMS M&O 1999e. *Design Input Request for LADS Phase II EDA Evaluations*. Input Tracking No. LAD-SSR-99112.R. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990209.0147.
8. CRWMS M&O 1998a. *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document - Chapter 5, Waste Package Degradation Modeling And Abstraction*. B00000000-01717-4301-00005 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0005. DTN: MO9807MWDWAPDG.000.
9. CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*. CSCI: 30048 V3.09. DI: 30048-2999 REV 02. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981012.0224.
10. CRWMS M&O 1998c. *Software Routine Report for WAPDEG (Version 3.07)*. CSCI: 30048 V3.07. DI: 30048-2999 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980715.0166.

11. CRWMS M&O 1998d. *Creating Input Tables from WAPDEG for RIP*. B000000000-01717-0210-00013 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981110.0431. DTN: MO9810SPA00013.000.
12. CRWMS M&O 1998e. *Cumulative Distribution Functions for No Drip Corrosion Resistant Material General Corrosion Model*. B000000000-01717-0210-00012 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980715.0174. DTN: MO9810SPA00013.000.
13. Golder Associates 1998. *RIP Integrated Probabilistic Simulator for Environmental Systems, Theory Manual and User's Guide*. Redmond, Washington: Golder Associates, Inc. TIC: 238560.
14. McCright, R. D. 1998. *Engineered Materials Characterization Report. Volume 3. Revision 1.1 Corrosion Data and Modeling: Update for Viability Assessment*. UCRL-ID-119564. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980806.0177.

8. ATTACHMENTS

Attachment Number	Title
I	Mkhistory
II	Titanium Grade 7 General Corrosion Rates

ATTACHMENT I - MKHISTORY

CONTENTS

	Page
1. GENERAL DESCRIPTION.....	I-2
2. DESCRIPTION OF CODE AND ALGORITHMS USED.....	I-2
3. DESCRIPTION OF TEST CASE.....	I-5
3.1 TEST CASE INPUT.....	I-6
4. RANGE OF INPUT PARAMETER VALUES OVER WHICH RESULTS WERE VERIFIED	I-7
4.1 IDENTIFICATION OF LIMITATIONS ON SOFTWARE ROUTINE OR VALIDITY	I-7
5. REFERENCE LIST OF ALL DOCUMENTATION RELEVANT TO THE QUALIFICATION	I-7
6. COMPUTER LISTING OF SOURCE CODE.....	I-8

1. GENERAL DESCRIPTION

The software routine Mkhhistory was written to create "time-history" files for the temperature and relative humidity, typically applicable to the waste package surface, drip shield surface, or drift wall, which are used as input to the stochastic waste package degradation simulator WAPDEG (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*). Although Version 3.09 of the WAPDEG code is referenced here, the output from Mkhhistory Version 1.01 could be used by any version of WAPDEG created to date. Mkhhistory was developed and tested in the Windows NT 4.0 operating system. This code was developed to enhance traceability of data manipulation and to minimize potential error induced by human data manipulation. The details of the "time-history" file format are discussed in (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*, p. 28). Mkhhistory also:

- 1) produces a text file segment (containing the history file names and fraction of the total number of waste packages to which each history is to be applied) suitable for importation into a WAPDEG input (*.inp) file (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*, p. 28).
- 2) prints, to both the screen and an output file, the fractions of the total number of waste packages to which each history is to be applied as well as the products of these fractions with the total number of waste packages, i.e., the number of waste packages to which each history is to be applied.
- 3) creates a columnar file of time, temperature, and relative humidity data for each history file processed for use in graphing the data.

Mkhhistory is a FORTRAN program 206 lines in extent. It conforms to the FORTRAN 90 standard and is thus highly portable. Mkhhistory has been compiled with Digital FORTRAN 5.0 in the Windows/PC environments. Mkhhistory is designed to run independently of any other software application.

All input and output files discussed in this document are included in the accompanying electronic media (CRWMS M&O 1999a. *Supporting Media for "RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIIb"*, \Attachment-I directory) (DTN: MO9904MWDWAP78.003).

2. DESCRIPTION OF CODE AND ALGORITHMS USED

The bulk of Mkhhistory's coding is devoted to reading values from text files of a certain format (see below) and writing these values to other text files with no calculations performed, i.e., reformatting of data values. Mkhhistory does perform a few very simple calculations:

- 1) it multiplies the fraction of the total number of waste packages to which each history is to be applied by a user input total number of waste packages to obtain the number of waste packages to which each history is to be applied.

- 2) it sums the fraction of the total number of waste packages and the number of waste packages to which each history is to be applied.

Mkhistory first asks the user to enter the name of a file which lists the files to be processed (the “list-file” name) and the number of waste packages. The list-file used for testing of Mkhistory (mktest.mk) is shown below:

```
6,7,3          |number of files, columns, and columns to print
1,2,3          |print specified columns
CC_dhlw_mean_02_sand_BF_j_22_03_data    CCdhlw02sandBFj2203.hst
CC_dhlw_mean_12_sand_BF_j_22_03_data    CCdhlw12sandBFj2203.hst
CC_dhlw_mean_22_sand_BF_j_22_03_data    CCdhlw22sandBFj2203.hst
CC_dhlw_mean_32_sand_BF_j_22_03_data    CCdhlw32sandBFj2203.hst
CC_dhlw_mean_42_sand_BF_j_22_03_data    CCdhlw42sandBFj2203.hst
CC_dhlw_mean_52_sand_BF_j_22_03_data    CCdhlw52sandBFj2203.hst
```

mktest.mk’s first line contains an integer representing the number of files to be processed (six in this case), the number of columns of data in each file to be processed (seven in this case), and the number of columns to print to the output file(s) (three in this case). The next input line contains the column numbers (from the files to be processed) that are to be read and printed to the output file(s). The maximum number of files to be processed is 999 in Mkhistory (see Section 4.1). The next input lines (number-of-files-to-be-processed of them) consist of two columns of text strings; the first column contains the name of the text file to be processed, and the second column contains the file name to which the corresponding processed results are written. For example, the contents of CC_dhlw_mean_02_sand_BF_j_22_03_data are:

```
file: CC_dhlw_mean_02_sand_BF_j_22_03_data
RH bin 0 of 9
temperature bin 2 of 2
zone 6 of 6: Center Center (CC)
```

```
12/97 PA property set
line load
sand backfill
1X LTA infiltration (42.06 mm/yr avg infiltration)
area of zone CC = 788649.0 (m^2)
fraction of zone CC represented by data set = 0.333864
area of repository represented by data set = 263301.50 (m^2)
```

time(years)	temp(C)	RH	Xair	Sliquid	dw T	dw RH
0.0	18.04	1.000000	0.985620	0.908230	18.039000	0.998080
1.0	165.35	0.378930	0.985570	0.987270	131.580002	0.945950
1.5	170.97	0.354500	0.985570	0.983260	137.630005	0.850510
2.0	179.22	0.272290	0.985570	0.972670	146.990005	0.611240
2.5	188.60	0.172870	0.985570	0.907560	157.190002	0.365880
3.0	198.94	0.097367	0.985570	0.745310	167.990005	0.196260
.
.
.

The contents of the corresponding file (CCdhlw02sandBFj2203.hst) containing the processed results are:

1.000000	165.350000	0.378930
1.500000	170.970000	0.354500
2.000000	179.220000	0.272290
2.500000	188.600000	0.172870
3.000000	198.940000	0.097367
.	.	.
.	.	.
.	.	.

with similar results for the remaining 5 files specified in mktest.mk. As can be seen from these files, no calculations are performed in creating CCdhlw02sandBFj2203.hst, only reformatting of data. Mkhhistory scans the file to be processed for a line that starts with "time"; skips the next line; then reads Columns 1, 2, and 3 from CC_dhlw_mean_02_sand_BF_j_22_03_data and echoes them to CCdhlw02sandBFj2203.hst.

CCdhlw02sandBFj2203.hst is a file with a format suitable for use as a WAPDEG time, temperature, relative humidity "history" file (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*, p. 28).

As mentioned above, Mkhhistory asks the user for the total number of waste packages. If the value entered is less than or equal to zero or greater than 1,000,000, the total number of waste packages is defaulted to 1,000,000. Mkhhistory scans the text file to be processed (i.e., CC_dhlw_mean_02_sand_BF_j_22_03_data) for a line starting with "area of zone," goes to the next line, then reads a real number (starting at Column 46). This is the fraction of the total number of waste packages to which the history file is to be applied. The user-input total number of waste packages then multiplies this real number and a WAPDEG input file segment is appended to the list-file (i.e., mktest.mk). If the total number of waste packages were chosen to be 1,000,0000, the following segment would be appended to mktest.mk:

6	Number of alternate histories
CCdhlw02sandBFj2203.hst	History file 1
333864, 0., 0.	packs/history, T std, RH std
CCdhlw12sandBFj2203.hst	History file 2
148505, 0., 0.	packs/history, T std, RH std
CCdhlw22sandBFj2203.hst	History file 3
17580, 0., 0.	packs/history, T std, RH std
CCdhlw32sandBFj2203.hst	History file 4
21975, 0., 0.	packs/history, T std, RH std
CCdhlw42sandBFj2203.hst	History file 5
290073, 0., 0.	packs/history, T std, RH std
CCdhlw52sandBFj2203.hst	History file 6
187913, 0., 0.	packs/history, T std, RH std

Here, the product of the user-input total number of waste packages and the fraction of the total number of waste packages to which each history is to be applied (i.e., 333864) appears as the first value on the line following the file name containing the processed WAPDEG time, temperature, relative humidity data. This value is rounded to the nearest whole integer. This text segment can be readily imported into a WAPDEG input file (CRWMS M&O 1998b. *Software Routine Report for WAPDEG (Version 3.09)*, p. 28) for use in analyses.

Mkhhistory also appends to the list-file the fraction of the total number of waste packages to which each history is to be applied and the results of the calculation of the product of the user-input total

number of waste packages and the fraction of the total number of waste packages to which each history is to be applied. Mkhhistory also sums these fractions and products for visual verification by the user that the fractions sum to approximately 1 and the products sum to the user-input total number of waste packages, i.e.:

```
History File 1      0.333864      333864
History File 2      0.148505      148505
History File 3      0.017580       17580
History File 4      0.021975       21975
History File 5      0.290073      290073
History File 6      0.187913      187913
Totals are:         0.999910 and   999910
Running mkhistory version 1.01
Using list-file: mktest.mk
```

Also, to facilitate further traceability, the Mkhhistory version number and list-file name are appended to the list-file, as shown above.

Mkhhistory also appends to the list-file a text segment that is convenient for graphing the time history of the temperature and relative humidity for each processed file, i.e., a text segment like the one below is appended to the list-file.

```
h001c01      h001c02      h001c03      h002c01      h002c02      h002c03      . . .
1.000000     165.350000     0.378930     1.000000     170.040000     0.390000     . . .
1.500000     170.970000     0.354500     1.500000     176.780000     0.347130     . . .
2.000000     179.220000     0.272290     2.000000     186.340000     0.245050     . . .
2.500000     188.600000     0.172870     2.500000     196.470000     0.134700     . . .
3.000000     198.940000     0.097367     3.000000     206.950000     0.079447     . . .
. . .         . . .         . . .         . . .         . . .         . . .
. . .         . . .         . . .         . . .         . . .         . . .
```

The hxxxxyy column label signifies that the data was extracted from column yy of the xxxth file processed by Mkhhistory. Effectively, the list-file serves as an input and output file as information is appended to it.

3. DESCRIPTION OF TEST CASE

Because Mkhhistory is a very simple program that performs few calculations, relatively simple testing is performed to verify the program execution and results. The testing approach involves comparing the results of executing Mkhhistory with the list-file mktest.mk and comparing the results with hand calculations and visual inspection. Execution of the list-file mktest.mk and verification of its output by comparison with the files on the accompanying electronic media (CRWMS M&O 1999a. *Supporting Media for "RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIIb"*, \Attachment-I\hand directory) (DTN: MO9904MWDWAP78.003) are considered sufficient installation and checkout steps for successful first use of Mkhhistory on a new platform, operating system or new user's location.

3.1 TEST CASE INPUT

The test case involves the use of the list-file mktest.mk, the listing of which is shown below:

6,7,3	number of files, columns, and columns to print
1,2,3	print specified columns
CC_dhlw_mean_02_sand_BF_j_22_03_data	CCdhlw02sandBFj2203.hst
CC_dhlw_mean_12_sand_BF_j_22_03_data	CCdhlw12sandBFj2203.hst
CC_dhlw_mean_22_sand_BF_j_22_03_data	CCdhlw22sandBFj2203.hst
CC_dhlw_mean_32_sand_BF_j_22_03_data	CCdhlw32sandBFj2203.hst
CC_dhlw_mean_42_sand_BF_j_22_03_data	CCdhlw42sandBFj2203.hst
CC_dhlw_mean_52_sand_BF_j_22_03_data	CCdhlw52sandBFj2203.hst

After reading mktest.mk, Mkhhistory will read the 6 text files to be processed (the file names in the first column of mktest.mk) and extract the specified columns from the files to be processed, and echo their contents to the output files (the file names in the second column of mktext.mk).

Comparison of these output files with the text files to be processed shows that the data in Columns 1, 2, and 3 of the 7 data columns in the text files to be processed have been correctly reformatted (copied) to the output files. Furthermore, the data in Columns 1, 2 and, 3 of the 7 data columns in the text files to be processed have been correctly copied to the end of the list-file, mktest.mk. From these visual inspections, one can conclude that the data reformatting by Mkhhistory is being correctly executed.

Visual inspection may also be used to verify that the fraction of the total number of waste packages to which the corresponding history file is to be applied has been correctly copied to the list-file (in the second column in the third text segment in mktest.mk) and that multiplication by the user-input total number of waste packages (1,000,000 in this case) has been correctly executed (this product is shown in the third column in the third text segment in mktext.mk). Visual inspection can also be used to verify the contents of the second text segment of mktest.mk, the "Number of alternate histories," has been correctly copied from the first line of the first text segment in mktest.mk; the processed filenames have been correctly copied from the second column of the first text segment in mktest.mk; and the "packs/history" have been correctly calculated as shown in the third column in the third text segment in mktext.mk.

The values requiring hand calculation verification are the sum of the fractions of the total number of waste packages to which each history file is to be applied and the sum of the products of the user-input total number of waste packages (1,000,000 in this case) and the fraction of the total number of waste packages to which each history is to be applied. These values appear on line one (1) of the fourth text segment in the list-file mktest.mk ("Totals are: . . ."). The values quoted agree with hand calculations. It is up to the Mkhhistory user's discretion as to whether the totals obtained (0.99991000 . . . and 999910) are acceptably close enough to the user's desired values (typically 1.00. . . and the user-input total number of waste packages (1,000,000 in this case)).

4. RANGE OF INPUT PARAMETER VALUES OVER WHICH RESULTS WERE VERIFIED

As Mkhistry does very few calculations, the valid range of input parameters is largely determined by the limitations discussed in the next section. Mkhistry has been executed with list-files specifying as many as 40 text files to be processed. Assuming the text files to be processed are correctly formatted, as discussed previously (Section 2.1) and in the next section, and the limitations discussed in the next section are not violated, Mkhistry will execute properly.

4.1 IDENTIFICATION OF LIMITATIONS ON SOFTWARE ROUTINE OR VALIDITY

- 4.1.1 The list-file name must be less than 40 characters, i.e., only the first 40 characters of the name will be read.
- 4.1.2 The total number of text files to be processed (and hence the number of processed files produced) by Mkhistry is limited to 999.
- 4.1.3 The total number of rows of data (rows appearing after the line beginning with "time") in any text file to be processed must be less than 500.
- 4.1.4 The file name of each text file to be processed must be no more than 128 characters and the file name of each created history file must be no more than 30 characters, i.e., the history file names that appears in the WAPDEG input file segment (appended to the list-file) is limited to 30 characters.
- 4.1.5 The total number of waste packages (user-input) can be an integer no greater than 1,000,000 and no less than 1. If the user enters a value greater than 1,000,000 or less than 1, a default value of 1,000,000 is assumed.
- 4.1.6 Each text file to be processed must contain a line starting with "area of zone" immediately followed by a line containing a real value at column 46. The real value is to occupy a field width of 9 spaces and 6 digits will appear after the decimal place (i.e., this value is read with the FORTRAN format statement "format(45x, f9.6)."
- 4.1.7 The line starting with "area of zone" and its following line must be followed (not necessarily immediately) by a line starting with "time" which is followed with the columnar data.

5. REFERENCE LIST OF ALL DOCUMENTATION RELEVANT TO THE QUALIFICATION

CRWMS M&O 1999a. *Supporting Media for "RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IIIb"*. 210-78r0.exe. Windows Self-extracting archive. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990528.0283. DTN: MO9904MWDWAP78.003.

6. COMPUTER LISTING OF SOURCE CODE

```

PROGRAM mkhistory
C
C  This program reads a list of drift-scale thermal
C  hydrologic model result files with matching history
C  file names; produces the history files; creates the
C  WAPDEG history file segment; and creates a listing
C  of all the histories suitable for graphing
C  purposes.
C
C  NH is the maximum number of histories to be read
C  NR is the maximum number of rows in a history file
C  NC is the maximum number of columns in a history file
C  NP is the default maximum number of waste packages
C  NLINE is the length of a line read
C
      IMPLICIT NONE
      INTEGER NH, NR, NC, NP, NLINE
      PARAMETER (NH = 999, NR = 500, NC = 50)
      PARAMETER (NP = 1000000, NLINE = 160)
      INTEGER listfid, datafid, hstyfid, numpack, numhst
      INTEGER i, j, k, nrows(NH), ifrac(NH), totalifrac
      INTEGER numcol, npcol, pcol(NC)

      DOUBLE PRECISION dat(NC,NR,NH)

      DOUBLE PRECISION frac(NH), totalfrac
      character ver*10, line*NLINE
      character listfl*40, datafl*NLINE(NH), hstyfl*NLINE(NH)
C
C  Initialize values
C
      3000 format(A160)
      ver = '1.01'
      listfid = 31
      datafid = 32
      hstyfid = 33
      ifrac = -999
      frac = -999.99
      totalifrac = 0
      totalfrac = 0.D0
C
C  Get the names of the data files to post process and the history
C  files to create
C
      write(*,*) 'Enter the list-file name:'
      read (*,*) listfl
      write(*,*) 'Enter the total number of waste packages:'
      read (*,*) numpack
C
C  Default numpack to get all significant digits from fractions
C
      if ((numpack .le. 0) .OR. (numpack .ge. NP)) then
        numpack = NP

```



```

        write(*,*) 'Number of waste packages defaulted to:', numpack
    end if
    write(*,*)
c
c The first line of the list-file should contain the number
c of file names that will follow (less than NH), the number
c of columns in each file, and the number of columns to reprint.
c The second line should contain the list of column numbers to
c reprint.
c
    OPEN (listfid, FILE = listfl, STATUS = 'OLD')
    read (listfid,*) numhst,numcol,npcol
    if (numhst .gt. NH) then
        write(*,*) 'Error: Number of histories too many'
        write(*,*) 'Increase NH and recompile'
        STOP
    end if
    if (numcol .gt. NC) then
        write(*,*) 'Error: Number of columns too many'
        write(*,*) 'Increase NC and recompile'
        STOP
    end if
    read (listfid,*) (pcol(i),i=1,npcol)
c
c Read the file names and then open each file.
c Get the fraction of waste packages in the line after the
c phase 'area of zone' in the 46 position
c Read in the data columns after the line starting with
c the time label
c
    do i = 1, numhst
        read(listfid,3000) line
        CALL getfilenames(line, NLINE, datafl(i), hstyfl(i))
        OPEN (datafid, FILE = datafl(i), STATUS = 'OLD')
        read(datafid,3000) line
        do while (line(1: 4) .NE. 'time')
            read (datafid, 3000) line
            if (line(1:12) .EQ. 'area of zone') then
                read(datafid, 2005) frac(i)
2005         format(45x,f9.6)
            end if
        end do
        j = 1
        do while (j .le. NR)
            read(datafid,*, end = 101) (dat(k,j,i),k=1,numcol)
            j = j+1
        end do
101     continue
        nrows(i) = j-1
        CLOSE(datafid)
    end do
c
c Create history files and history segment for WAPDEG input file
c First row (time = 0) is not printed
c
    write(listfid,*)
    write(listfid,2002) numhst
2002 format(I3,27x,'|Number of alternate histories')
    do i = 1, numhst
        OPEN (hstyfid, FILE = hstyfl(i))
        do j = 2, nrows(i)

```

```

        write(hstyfid,2012) (dat(pcol(k),j,i),k=1,npcol)
    end do
    write(hstyfid,*)
    write(listfid,2007) hstyfl(i), i
2007   format(A30,'|History file',I3)
        ifrac(i) = int(numpack*frac(i) + 0.5)
        write(listfid,2008) ifrac(i)
2008   format(I9,',', 0., 0.',13x,'|packs/history, T std, RH std')
        CLOSE(hstyfid)
    end do
    write(listfid,*)
c
c   Print fraction information (to the screen and list-file)
c
    do i = 1, numhst
        write(*,2009) i, frac(i), ifrac(i)
        write(listfid,2009) i, frac(i), ifrac(i)
        totalifrac = totalifrac + ifrac(i)
        totalfrac = totalfrac + frac(i)
2009   format(1x,'History File',I3,1x,f15.6,5x,I9)
    end do
c
    write(*,2010) totalfrac,totalifrac
    write(*,*) 'Running mkhistory version '//ver
    write(*,*) 'Using list-file: '//listfl
c
    write(listfid,2010) totalfrac,totalifrac
    write(listfid,*) 'Running mkhistory version '//ver
    write(listfid,*) 'Using list-file: '//listfl
2010 format(1x,'Totals are:',5x,f15.6,' and ',I9)
c
c   Create listing for graphing purposes (column widths of 16)
c
    write(listfid,2011) (('h',i,'c',pcol(k),k=1,npcol),i=1,numhst)
2011 format(198(9x,A1,I3.3,A1,I2.2))
    do j = 2, nrows(1)
        write(listfid,2012) ((dat(pcol(k),j,i),k=1,npcol),i=1,numhst)
2012   format(198(1x,f15.6))
    end do
c
c   Pause program before completing
c
    write(*,*) 'Press return to continue'
    read (*,*)
    CLOSE(listfid)
    END !PROGRAM mkhistory
c
c *****
c
    SUBROUTINE getfilenames(line, linesize, datafl, hstyfl)
c
c   Find the positions in line where the file names are.
c   Input : line, linesize
c   Output: datafl, hstyfl
c   Local : i, starthst, endhst, startdat, enddat
c
c   Arguments
c
    IMPLICIT NONE
    character line*(*), datafl*(*), hstyfl*(*)
    integer linesize

```

```

C
C Local variables
C
C     integer i, starthst, endhst, startdat, enddat
C
C Find the positions in line where the file names are.
C
C     i = 1
C     do while (line(i:i) .eq. ' ')
C         i = i + 1
C     end do
C     startdat = i
C     do while (line(i:i) .ne. ' ')
C         i = i + 1
C     end do
C     enddat = i - 1
C     do while (line(i: i) .eq. ' ')
C         i = i + 1
C     end do
C     starthst = i
C     do while ((line(i: i) .ne. ' ') .and. (i .le. linesize))
C         i = i + 1
C     end do
C     endhst = i - 1
C     datafl = line(startdat:enddat)
C     hstyfl = line(starthst:endhst)
C     RETURN
C     END      !SUBROUTINE getfilenames
C
C *****
C

```

Attachment II - TITANIUM GRADE 7 GENERAL CORROSION RATES

This worksheet documents the creation of the general corrosion rate cumulative distribution functions applicable to a titanium grade 7 alloy at 30, 60, and 120°C. The corrosion rate distributions are defined by Model B of a recent communication on titanium corrosion models (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 1 of 3 Response 1). The function $r(T)$ below models the median corrosion rate (mm/yr) at temperature, T (°C). The variation around this median corrosion rate is specified as a normal distribution truncated at $\pm 3s$, with 50% uncertainty and 50% variability. s is the given model standard deviation of the general corrosion rate distributions.

Cumulative distribution function (cdf) tables (with 201 entries) of the full corrosion rate distributions are created below. Then cdf tables are created and printed out that represent just variability centered at the median corrosion rate due to uncertainty.

$$r(T) := 10^{-6} \cdot \exp \left(2.4070 - \frac{118.91}{T + 273.15} + 0.37673 \cdot 10^{-2.7} + 0.9449 \cdot 0 + 1.0239 \cdot 1 \right)$$

$$s := 1.7146$$

$$N := 200 \quad i := 0..N$$

$$z_i := -3 + \frac{i}{N} \cdot 6$$

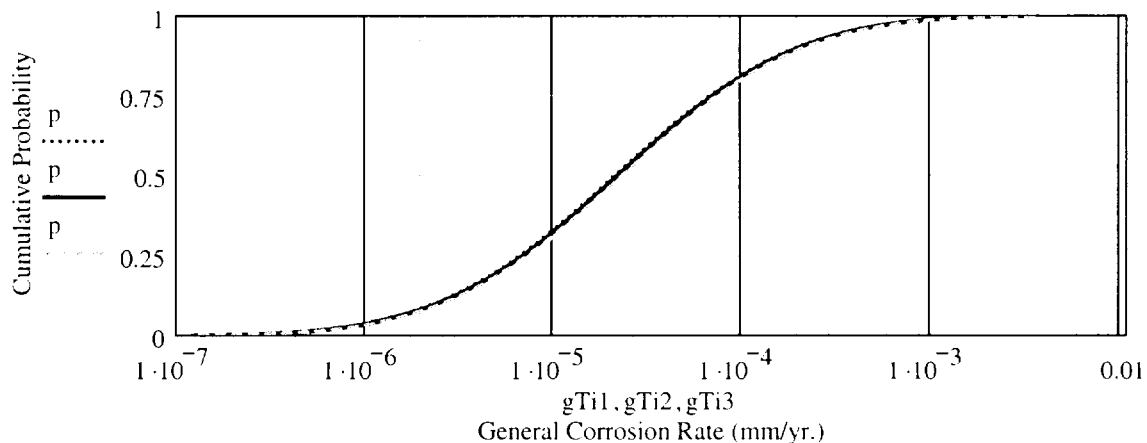
$$p := \frac{\text{cnorm}(z) - \text{cnorm}(-3)}{\text{cnorm}(3) - \text{cnorm}(-3)}$$

$$gTi1 := r(30) \cdot \exp(s \cdot z)$$

$$gTi2 := r(60) \cdot \exp(s \cdot z)$$

$$gTi3 := r(120) \cdot \exp(s \cdot z)$$

- Note, all vectors are of size (N+1).
- The z-values range from -3 to +3 with a spacing of 0.03.
- p is a vector of probabilities corresponding to the z-values for a standard normal distribution truncated at ± 3 standard deviations.
- The vector gTi_x (where x may be 1, 2, or 3) are general corrosion rates (mm/yr) with standard deviation, s , corresponding to the p -values for temperatures 30, 60, and 120°C, respectively.



Range of values:

$$\min(\text{gTi1}) = 1.2192 \cdot 10^{-7}$$

$$\text{median}(\text{gTi2}) = 2.1644 \cdot 10^{-5}$$

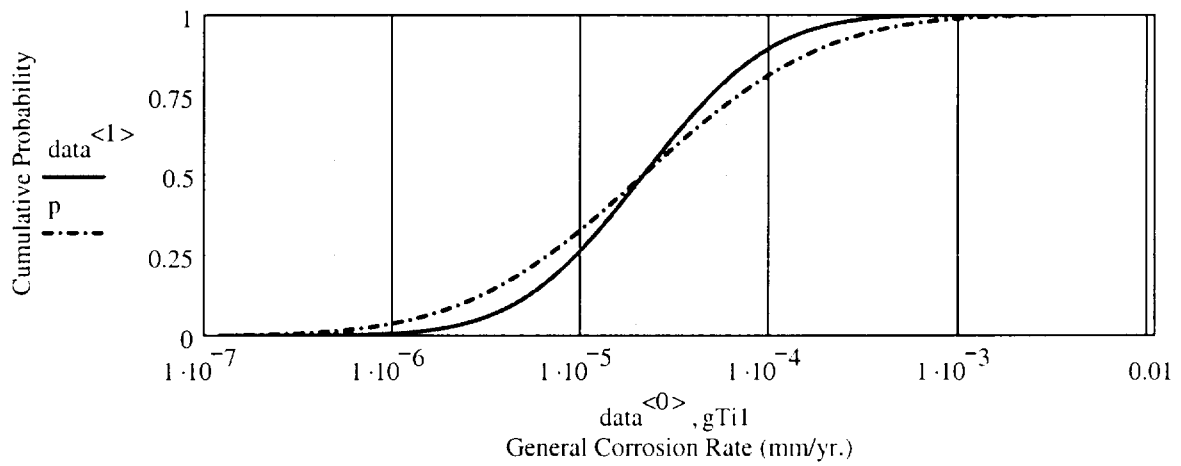
$$\max(\text{gTi3}) = 3.9167 \cdot 10^{-3}$$

The function, `slnvar(x,p,wtu,qu)`, below partitions the variance of the discrete univariate distribution given by the cdf table of rate values in `x` and cumulative probabilities in `p`. By matching probability values we create a table of standard normal score values matched with natural log rate values. This table is then used to lookup rate values that correspond to the Gaussian variance partitioning of the standard normal for the given uncertain variability (`wtu`) and quantile (`qu`) both expressed as fractions. Note, `slnvar` is an acronym: split ln (natural log) variance.

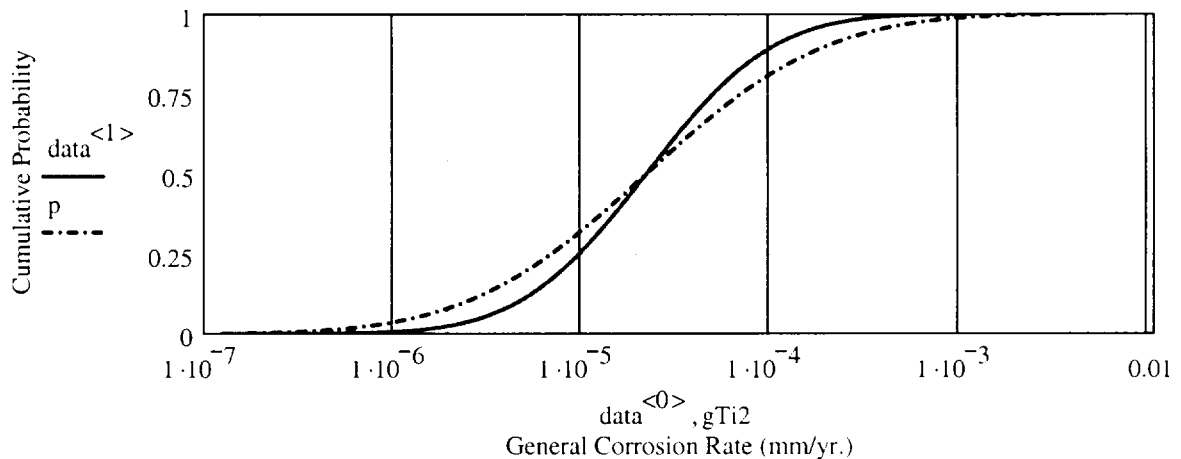
<code>slnvar(x, p, wtu, qu) :=</code>	<code>wtv ← 1 - wtu</code> <code>zu ← √wtu · qnorm(qu, 0, 1)</code> <code>for i ∈ 0..length(x) - 1</code> <div style="border-left: 1px solid black; padding-left: 10px; margin-left: 20px;"> <code>z_i ←</code> <div style="display: inline-block; vertical-align: middle;"> $-\infty$ if $p_i = 0$ ∞ if $p_i = 1$ $qnorm(p_i, 0, 1)$ otherwise </div> </div> <code>lnx_i ← ln(x_i)</code> <div style="border-left: 1px solid black; padding-left: 10px; margin-left: 20px;"> <code>zv_i ←</code> <div style="display: inline-block; vertical-align: middle;"> $-\infty$ if $p_i = 0$ ∞ if $p_i = 1$ $(zu + z_i \cdot \sqrt{wtv})$ otherwise </div> </div> <code>for i ∈ (0..length(x) - 1)</code> <code>xv_i ← exp(linterp(z, lnx, zv_i))</code> <code>augment(xv, p)</code>	<ul style="list-style-type: none"> • <code>wtv</code> is the fraction of the variance that represents variability. • <code>zu</code> is the standard normal score value that corresponds with the given quantile. • Values of <code>z</code> and <code>lnx</code> make up the lookup table. • The probability values zero and one are mapped specifically to remove the appearances of infinity, precision is only good to prob ~ 10⁻¹³. • <code>zv</code> are the standard normal values with mean <code>zu</code> and variance <code>wtv</code> that corresponds with the variability distribution. • Return matrix of rates and cumulative probabilities.
---------------------------------------	---	---

By changing the file names below for each set of uncertainty and quantile values the cdf files are produced by the file print functions in Mathcad.

```
filnam := "gTi15050.cdf"
data := slnvar(gTi1, p, 0.50, 0.50)
WRITEPRN(filnam) := (rows(data) cols(data) )
APPENDPRN(filnam) := data
```



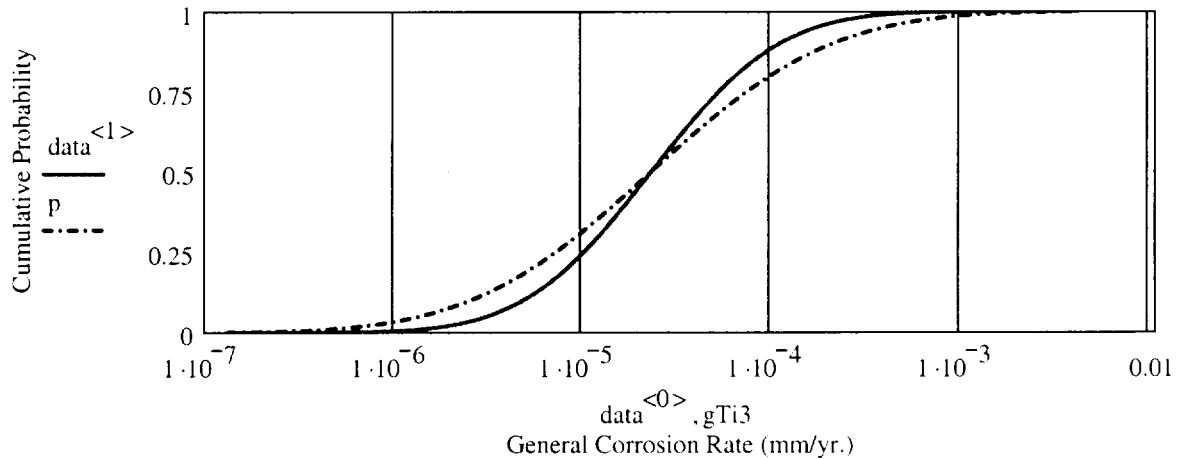
```
filnam := "gTi25050.cdf"
data := slnvar(gTi2, p, 0.50, 0.50)
WRITEPRN(filnam) := (rows(data) cols(data) )
APPENDPRN(filnam) := data
```



```

filnam := "gTi35050.cdf"
data := slnvar(gTi3,p,0.50,0.50)
WRITEPRN(filnam) := (rows(data) cols(data) )
APPENDPRN(filnam) := data

```



References

CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*. Input Tracking No. PA-WP-99089.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990219.0501.