MOL.19990201.0089

CRWMS/M&O

Calculation Cover Sheet

Complete only applicable items.

1. QA: L

Page: 1 Of: 27

2. Calculation Title			
RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IV			MOL.19990201.0089
3. Document Identifier (including Revision Number) B00000000-01717-0210-00072 REV 00			4. Total Pages 27
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	Kevin Mon	JUN 28 1999
8. Checker	Peter K. Mast	[signature] for PK Mast	June 28 1999
9. Lead	Joon H. Lee	[signature]	June 29, 1999

10. Remarks

Input thermal hydrologic history files (DTN: LL990301704242.082).
Computer software (WAPDEG version 3.09 and Post308) are tracked by TBV-568.

Uses DTN: MO9807MWDWAPDG.000 on Conceptual Model.
Uses DTN: MO9810SPA00013.000 on Input assumptions and input data.
Supporting electronic media = ACC: MOL.19990201.0090, DTN: MO9904MWDWAP72.002.

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 10
   4.1 SOFTWARE APPROVED FOR QA WORK 10
   4.2 SOFTWARE ROUTINES 12
   4.3 MODELS 12
5. CALCULATION 12
   5.1 MKHISTORY INPUTS 13
   5.2 WAPDEG INPUTS 14
   5.3 POST308 INPUTS 19
6. RESULTS 19
7. REFERENCES 26
8. ATTACHMENTS 27

1. PURPOSE

The purpose of this calculation is to document 1) 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 (that are placed over single-layer waste packages composed of a 30-cm thick A-516 carbon steel corrosion allowance material (CAM)) as well as degradation and failure of the waste packages themselves, and 2) post-processing of these results 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 IV. Additional details concerning the Enhanced Design Alternative IV 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 Mkhistory (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 / 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 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 / waste packages are assumed to only undergo general corrosion processes, which result in "patch" perforations. As a result, for the drip shields, 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 the 2-cm thick titanium grade 7 drip shields were modeled by executing the WAPDEG code twice, as described in Section 3.0. The first WAPDEG simulation (using the input file NE1a5s5EDA4-ds.inp) is used to model degradation of the 2-cm thick titanium grade 7 drip shields. 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 NE1a5s5EDA4-ds.cdf. A second WAPDEG simulation (using the input file NE1a5s5EDA4-wp.inp) was then performed to model waste package degradation and failure using this dripping start time distribution.

3. ASSUMPTIONS

No assumptions are made in executing Mkhistory. The limitations on the Mkhistory 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 NE1a5s5EDA4-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, NE1a5s5EDA4-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 NE1a5s5EDA4-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 34.15 m^2. 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. 2/2). 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 5.635 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 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 1.100 m and 1.270 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 1.432 m. Thus, the drip shield surface area modeled (subject to corrosion) is given by:

$IR := 1.100 m \qquad OR := 1.270 m$ Inner (IR) and outer (OR) drip shield rad

$L := 5.635 m - 2 \cdot 0.225 m \qquad L = 5.185 m$ Waste package length - two skirts

$SPH := 1.432 m$ Drip shield side plate height

$er := \frac{(IR + OR)}{2} \qquad er = 1.185 m$ Effective Radius

$Tot := 2 \cdot SPH \cdot L + \pi \cdot er \cdot L \qquad Tot = 34.15 m^2$ 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 1,102 patches each 0.0310 m^2 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:

$PS := 0.0310 m^2$ Patch Size

$\frac{Tot}{PS} = 1102$ 1102 Patches/DS

This assumption is used in the WAPDEG input file, NE1a5s5EDA4-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*, p. 4 "LADS Enhanced Design Alternatives" Table Note 8). The current version of WAPDEG was developed to model a two-barrier waste package: the outer barrier is hard-wired to be a corrosion allowance material (CAM) of carbon steel, and the corrosion model parameters for the inner barrier are 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) is 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, NE1a5s5EDA4-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/or [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 1999e. *Design*

Input Request for LADS Phase II EDA Evaluations, p. 4 "LADS Enhanced Design Alternatives" Table Row 9 Column 5). This is accomplished by using a 50-year 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, NE1a5s5EDA4-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 A22TiTth.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, NE1a5s5EDA4-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 drip shield 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, NE1a5s5EDA4-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, NE1a5s5EDA4-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 drip shield corrosion 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 (A22TiTth.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 corrosion rate is at the 50^{th} 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 WAPDEG input file NE1a5s5EDA4-wp.inp is used to model a single-barrier 30-cm thick A-516 carbon steel waste packages under 2-cm thick titanium grade 7 drip shields that are always dripped on. In this simulation the waste package is not contacted by dripping water until the drip shields fail (note that the CAM humid-air and aqueous corrosion degradation models used in this calculation do not depend on the presence or absence of dripping water as discussed in Assumption 3.14). The assumptions used in modeling A-516 carbon steel waste package 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.

The following assumptions are made for A-516 carbon steel waste package degradation modeling.

3.14 The file NE1a5s5EDA4-ds.cdf (a cdf of first breach times of the drip shields modeled) 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 NE1a5s5EDA4-wp.inp. The basis of this assumption is that dripping water can not contact a waste package underneath an intact drip shield. This assumption is of no consequence to degradation modeling as the WAPDEG CAM corrosion degradation models do not depend on the presence or absence of dripping water (CRWMS M&O 1998a. *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document - Chapter 5, Waste Package Degradation Modeling and Abstraction*, Section 5.5.5.1 pp. 5-34 through 5-35 and Section 5.6.4.1 p. 5-40). This distribution is read by the fourteenth and fifteenth lines after the last thermal hydrologic "history" file name.

3.15 After failure of a titanium grade 7 drip shield (defined by the NE1a5s5EDA4-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 that the combined drip shield (which is now considered to be breached) and backfill provide with regard to water contact with the waste packages. This assumption is used in the second WAPDEG input file, NE1a5s5EDA4-wp.inp, on the tenth through thirteenth input lines after the last history file name. This assumption is of no consequence to degradation modeling as the WAPDEG CAM corrosion degradation models do not depend on the presence or absence of dripping water (CRWMS M&O 1998a. *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document - Chapter 5, Waste Package Degradation Modeling and Abstraction*, Section 5.5.5.1 pp. 5-34 through 5-35 and Section 5.6.4.1 p. 5-40).

3.16 The waste packages are 30-cm thick (first value on third input line after the last thermal hydrologic history file name) and are composed of A-516 carbon steel. The current version of WAPDEG was developed to model a two-barrier waste package: the outer barrier is hard-wired to be a corrosion allowance material (CAM) of carbon steel, and the corrosion model parameters for the inner barrier are supplied by the user through the WAPDEG input file. In order to model the carbon steel single barrier waste package corrosion degradation process as a CAM with no corrosion resistant material (CRM) inner barrier, it is assumed that the waste package has a very thin (1e-12 cm) "simulated" CRM (the second value on the third input line after the last thermal hydrologic "history" file name) and the CRM corrosion rate is set to 100 mm/yr (the values of the "Distribution Parameter(s)" for the CRMGeneralRateOnly model used in the [No Drip, CRM] and [Neutral Drip, CRM] input headers. These two inputs combine to assure immediate failure of the simulated CRM upon CAM outer layer failure. This assumption is used in the WAPDEG input files, NE1a5s5EDA4-wp.inp and NE0a5s6EDA4-wp.inp, as the second value on the third input line after the last thermal hydrologic history file name.

3.17 The total waste package surface area modeled is 39.40 m^2 or 1271 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, EDA*s, Item 1 p. 4/34 Table 4). The length of the waste package is 5.635 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:

$OD := 2.024 \cdot m \qquad L = 5.185\,m$		Waste Package Outer Diameter and Length
$WPA := \pi \cdot OD \cdot L + 2 \cdot \pi \cdot \left(\frac{OD}{2}\right)^2$	$WPA = 39.4\,m^2$	Total Waste Package Area
$\frac{WPA}{PS} = 1.271 \cdot 10^3$		1271 Patches/WP

This assumption is used on the fourth input line (second value) in the WAPDEG input file NE1a5s5EDA4-wp.inp.

3.17 For the 50 years before drip shield emplacement (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 period (CRWMS M&O 1999e. *Design Input Request for LADS Phase II EDA Evaluations*. p. 4 "LADS Enhanced Design Alternatives" Table Row 9 Column 5) and any seepage water into the emplacement drift is removed by the air flow. This assumption is used in defining the dripping initiation time on lines 14 and 15 of the WAPDEG input file, NE1a5s5EDA4-wp.inp.

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 has not gone through the complete qualification process required by QAP-SI-0 REV 04 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 the Post308 code 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 has not gone through the complete qualification process required by QAP-SI-0 REV 04, 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 Revision 1 (see Attachment I) 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 IV)* (DTN: MO9904MWDWAP72.002) 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 IV)* (DTN: MO9904MWDWAP72.002).

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: LL990301704242.082). These histories are organized by bin numbers and model identifier with file names like NE_snf_mean_yy_sandBF_85_c_j4_22_03_02_001_data, where NE denotes the northeast region of the potential repository, snf denotes commercial spent nuclear fuel, yy is a bin number, sandBF denotes quartz sand backfill, 85 denotes an areal mass loading of 85 MTU, 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 (°C), Column 3 the relative humidity at the waste package surface (fraction), Column 4 the air mass fraction (Xair), Column 5 the liquid saturation in the invert (fraction), Column 6 the drift wall temperature (°C), Column 7 the drift wall relative humidity (fraction), Column 8 the drip shield surface temperature (°C), and Column 9 the drip shield surface relative humidity (fraction). In this calculation, a total of 21 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, 02, 10, 11, 12, 20, 21, 22, 31, 32, 40, 41, 42, 51, 52, 60, 61, 62, 71, and 72 are used in this calculation (i.e., NE_snf_mean_00_sandBF_85_c_j4_22_03_02_001_data, NE_snf_mean_01_sandBF_85_c_j4_22_03_02_001_data, . . ., etc.).

These thermal hydrologic history files were processed by the Mkhistory software routine. The bulk (but not all) of Mkhistory'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 Mkhistory input file(s) to the file named in Column 2 of the Mkhistory 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 Mkhistory input file as discussed in Attachment I. Two Mkhistory input files were used, EDA4ds.mk, for the drip shield surface, and EDA4.mk for the waste package surface. The initial contents of the Mkhistory input file EDA4.mk are:

```
21,9,3                            |number of files, columns, and columns to print
1,2,3                             |print specified columns
NE_snf_mean_00_sandBF_85_c_j4_22_03_02_001_data   NEsf00sBF85cj4220302001.hst
NE_snf_mean_01_sandBF_85_c_j4_22_03_02_001_data   NEsf01sBF85cj4220302001.hst
NE_snf_mean_02_sandBF_85_c_j4_22_03_02_001_data   NEsf02sBF85cj4220302001.hst
NE_snf_mean_10_sandBF_85_c_j4_22_03_02_001_data   NEsf10sBF85cj4220302001.hst
NE_snf_mean_11_sandBF_85_c_j4_22_03_02_001_data   NEsf11sBF85cj4220302001.hst
NE_snf_mean_12_sandBF_85_c_j4_22_03_02_001_data   NEsf12sBF85cj4220302001.hst
NE_snf_mean_20_sandBF_85_c_j4_22_03_02_001_data   NEsf20sBF85cj4220302001.hst
NE_snf_mean_21_sandBF_85_c_j4_22_03_02_001_data   NEsf21sBF85cj4220302001.hst
NE_snf_mean_22_sandBF_85_c_j4_22_03_02_001_data   NEsf22sBF85cj4220302001.hst
NE_snf_mean_31_sandBF_85_c_j4_22_03_02_001_data   NEsf31sBF85cj4220302001.hst
NE_snf_mean_32_sandBF_85_c_j4_22_03_02_001_data   NEsf32sBF85cj4220302001.hst
NE_snf_mean_40_sandBF_85_c_j4_22_03_02_001_data   NEsf40sBF85cj4220302001.hst
```

```
NE_snf_mean_41_sandBF_85_c_j4_22_03_02_001_data   NEsf41sBF85cj4220302001.hst
NE_snf_mean_42_sandBF_85_c_j4_22_03_02_001_data   NEsf42sBF85cj4220302001.hst
NE_snf_mean_51_sandBF_85_c_j4_22_03_02_001_data   NEsf51sBF85cj4220302001.hst
NE_snf_mean_52_sandBF_85_c_j4_22_03_02_001_data   NEsf52sBF85cj4220302001.hst
NE_snf_mean_60_sandBF_85_c_j4_22_03_02_001_data   NEsf60sBF85cj4220302001.hst
NE_snf_mean_61_sandBF_85_c_j4_22_03_02_001_data   NEsf61sBF85cj4220302001.hst
NE_snf_mean_62_sandBF_85_c_j4_22_03_02_001_data   NEsf62sBF85cj4220302001.hst
NE_snf_mean_71_sandBF_85_c_j4_22_03_02_001_data   NEsf71sBF85cj4220302001.hst
NE_snf_mean_72_sandBF_85_c_j4_22_03_02_001_data   NEsf72sBF85cj4220302001.hst
```

The first line of this Mkhistory input file indicates that 21 thermal hydrologic history files (whose file names are listed in the first column of the Mkhistory input file (starting on Row 3)) are to be processed by Mkhistory, 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 Mkhistory input file. The second line of the Mkhistory 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 Mkhistory input file (starting on Row 3)) will be extracted to the file name specified in the second column of the Mkhistory input file (i.e., data from NE_snf_mean_00_sandBF_85_c_j4_22_03_02_001_data is to be copied to NEsf00sBF85cj4220302001.hst, etc.). The above are the contents of EDA4.mk before execution of Mkhistory (several data segments are appended to this file during Mkhistory program execution as discussed in Attachment I). The thermal hydrologic history files before and after processing by Mkhistory and the EDA4.mk and EDA4ds.mk files after execution of Mkhistory 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 IV)* (DTN: MO9904MWDWAP72.002).

Procedurally, the Mkhistory program prompts the user for a list-file name (this is the Mkhistory input file, i.e., EDA4.mk). The Mkhistory 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: MO9904MWDWAP72.002) and creates several output files (*.aux, *.bin, *.cam, *.crm, *.out, *.pat) (DTN: MO9904MWDWAP72.002). 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: MO9904MWDWAP72.002). 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: MO9904MWDWAP72.002)

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 (file: A22TiTth.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,* p. 1/3 Response 1 and 3) and for the actual 30-cm thick single barrier waste packages (file: TThresh.cdf) (CRWMS M&O 1998e. *Cumulative Distribution Functions for the Temperature Threshold for the Onset of Carbon Steel Corrosion*) (DTN: MO9810SPA00013.000).
3) Cumulative distribution functions for the RH threshold for the onset of corrosion for the simulated CAM outer barrier of the drip shields (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) and the actual 30-cm thick single barrier waste packages (file: HARH.cdf and AQRH.cdf) (CRWMS M&O 1998f. *Cumulative Distribution Functions for the Relative Humidity Thresholds for the Onset of Carbon Steel Corrosion*) (DTN: MO9810SPA00013.000).
4) Cumulative distribution functions for the titanium grade 7 drip shield general corrosion rates (see Attachment II) at 30, 60, and 120°C (files: gTi15050.cdf, gTi25050.cdf, and gTi35050.cdf) (DTN: MO9904MWDWAP72.002).
5) 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: NE1a5s5EDA4-ds.cdf containing the first breach times from the WAPDEG simulation using the NE1a5s5EDA4-ds.inp input file). This cdf is used as a drip initiation time distribution in the WAPDEG simulation using the NE1a5s5EDA4-wp.inp input file (DTN: MO9904MWDWAP72.002).
6) 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.
7) Although the WAPDEG input files for this simulation list another input cdf (file: A22LCTth.cdf on the fifth input line after the [Neutral Drip Features] header) (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) for the temperature threshold for localized corrosion initiation under dripping conditions, this file is not used in any way within the calculation as localized corrosion is not allowed to occur (see Assumption 3.9).

Two WAPDEG input files were used to generate the RIP input tables for the License Application Design Selection Analyses: Enhanced Design Alternative IV; NE1a5s5EDA4-ds.inp (for the drip shield under dripping conditions) and NE1a5s5EDA4-wp.inp (for the waste packages under dripping or no dripping conditions, see Assumption 3.14). 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 IV)* (DTN: MO9904MWDWAP72.002).

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 is not relevant to this calculation. The next two characters (a5) indicate that the file is for the base case infiltration. The next characters (s5) refer to the different uncertainty/variability splits and percentile of the uncertainty distribution used for the median of the titanium general corrosion rate 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 input files (NE1a5s5EDA4-ds.inp and NE1a5s5EDA4-wp.inp) use a 50% uncertainty - 50% variability split and use the 50th percentile of the uncertainty distribution for the median of the titanium general corrosion rate variability distributions. The characters (EDA4) indicate that these input files are used in analyzing LADS Enhanced Design Alternative IV. For reference, below is shown the input file NE1a5s5EDA4-ds.inp used in the WAPDEG simulation of the dripping exposure condition:

```
NE1a5s5EDA4-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 EDA4

START OF PARAMETERS
3.09                            |Version number of code
 21                             |Number of alternate histories
NEsf00sBF85cj4220302001ds.hst   |History file  1
      868, 0., 0.               |packs/history, T std, RH std
NEsf01sBF85cj4220302001ds.hst   |History file  2
    47724, 0., 0.               |packs/history, T std, RH std
NEsf02sBF85cj4220302001ds.hst   |History file  3
    77368, 0., 0.               |packs/history, T std, RH std
NEsf10sBF85cj4220302001ds.hst   |History file  4
     1490, 0., 0.               |packs/history, T std, RH std
NEsf11sBF85cj4220302001ds.hst   |History file  5
   100707, 0., 0.               |packs/history, T std, RH std
NEsf12sBF85cj4220302001ds.hst   |History file  6
   164570, 0., 0.               |packs/history, T std, RH std
NEsf20sBF85cj4220302001ds.hst   |History file  7
```

```
     1114, 0., 0.                 |packs/history, T std, RH std
 NEsf21sBF85cj4220302001ds.hst    |History file  8
     65385, 0., 0.                |packs/history, T std, RH std
 NEsf22sBF85cj4220302001ds.hst    |History file  9
    127121, 0., 0.                |packs/history, T std, RH std
 NEsf31sBF85cj4220302001ds.hst    |History file 10
     13943, 0., 0.                |packs/history, T std, RH std
 NEsf32sBF85cj4220302001ds.hst    |History file 11
     29692, 0., 0.                |packs/history, T std, RH std
 NEsf40sBF85cj4220302001ds.hst    |History file 12
       524, 0., 0.                |packs/history, T std, RH std
 NEsf41sBF85cj4220302001ds.hst    |History file 13
     42142, 0., 0.                |packs/history, T std, RH std
 NEsf42sBF85cj4220302001ds.hst    |History file 14
    100969, 0., 0.                |packs/history, T std, RH std
 NEsf51sBF85cj4220302001ds.hst    |History file 15
     12797, 0., 0.                |packs/history, T std, RH std
 NEsf52sBF85cj4220302001ds.hst    |History file 16
     28248, 0., 0.                |packs/history, T std, RH std
 NEsf60sBF85cj4220302001ds.hst    |History file 17
        74, 0., 0.                |packs/history, T std, RH std
 NEsf61sBF85cj4220302001ds.hst    |History file 18
     29683, 0., 0.                |packs/history, T std, RH std
 NEsf62sBF85cj4220302001ds.hst    |History file 19
    124180, 0., 0.                |packs/history, T std, RH std
 NEsf71sBF85cj4220302001ds.hst    |History file 20
      8618, 0., 0.                |packs/history, T std, RH std
 NEsf72sBF85cj4220302001ds.hst    |History file 21
     22778, 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, 1102, 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
```

The "No Backfill" statement in the header lines (these are "comment" lines having no effect on the actual parameters used in degradation modeling) for both input files (NE1a5s5EDA4-ds.inp and NE1a5s5EDA4-wp.inp) is in error as backfill was modeled in producing the thermal hydrologic history files. 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 input file, i.e., NE1a5s5EDA4-ds.inp for the drip shields or NE1a5s5EDA4-wp.inp for the waste packages for dripping conditions.

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 IV)* (DTN: MO9904MWDWAP72.002). 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 / waste packages are assumed to only undergo general corrosion processes, which result in "patch" perforations. As a result, for the drip shields, 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).

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 IV)* (DTN: MO9904MWDWAP72.002).

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 IV)* (DTN: MO9904MWDWAP72.002). For brevity, only selected files are reproduced in hardcopy form within this section.

The primary outputs of Mkhistory are the *.hst files used as input to WAPDEG. For reference, the contents of NEsf00sBF85cj4220302001.hst (DTN: MO9904MWDWAP72.002) are:

```
  1.000000     99.420000     0.459720
  1.500000    103.730000     0.483220
  2.000000    106.820000     0.499350
  3.000000    111.800000     0.523120
  4.000000    114.870000     0.536050
  5.000000    116.990000     0.538010
  6.000000    118.360000     0.543180
  7.000000    119.000000     0.547860
  8.000000    119.240000     0.552350
  9.000000    119.250000     0.554920
 10.000000    119.230000     0.558410
 11.000000    118.440000     0.485400
 12.000000    117.540000     0.496430
 15.000000    114.360000     0.535310
 20.000000    107.970000     0.592630
 25.000000    103.820000     0.618530
 26.000000    102.740000     0.622520
 27.000000    101.630000     0.625670
 30.000000    100.250000     0.637310
 35.000000     95.200000     0.651300
 40.000000     91.270000     0.663140
 50.000000    135.460000     0.371970
 51.000000    203.130000     0.084984
 52.000000    204.730000     0.046821
 55.000000    196.920000     0.058679
 60.000000    179.840000     0.099831
 65.000000    153.630000     0.171260
 70.000000    144.030000     0.182970
 75.000000    140.160000     0.191880
 76.000000    139.260000     0.193570
 77.000000    138.930000     0.195320
 80.000000    135.890000     0.200230
 90.000000    129.580000     0.213940
100.000000    124.180000     0.225580
101.000000    123.840000     0.226300
105.000000    122.610000     0.230650
110.000000    121.140000     0.236080
120.000000    118.280000     0.246960
130.000000    115.630000     0.257800
140.000000    112.930000     0.313720
160.000000    108.430000     0.330700
180.000000    105.680000     0.341670
200.000000    102.860000     0.353350
```

220.000000	100.980000	0.361270
250.000000	98.310000	0.377420
300.000000	94.690000	0.401820
350.000000	91.740000	0.416630
400.000000	89.260000	0.430430
450.000000	87.130000	0.456350
500.000000	85.130000	0.479970
550.000000	83.230000	0.501870
600.000000	81.590000	0.521120
700.000000	78.680000	0.554670
800.000000	76.010000	0.583330
900.000000	73.780000	0.607970
1000.000000	71.810000	0.629910
1100.000000	70.400000	0.645870
1200.000000	69.010000	0.662530
1300.000000	67.570000	0.678410
1400.000000	66.070000	0.696110
1500.000000	64.500000	0.714650
1600.000000	63.570000	0.722740
1800.000000	61.820000	0.740520
2000.000000	60.000000	0.759200
2200.000000	58.810000	0.769510
2500.000000	57.060000	0.784090
3000.000000	55.040000	0.797120
3500.000000	53.600000	0.803090
4000.000000	52.330000	0.810630
4500.000000	51.340000	0.813960
5000.000000	50.460000	0.817990
6000.000000	48.800000	0.825680
7000.000000	47.370000	0.831640
8000.000000	46.020000	0.839470
10000.000000	43.710000	0.848470
15000.000000	38.610000	0.879700
20000.000000	35.150000	0.897280
30000.000000	30.240000	0.928380
40000.000000	27.530000	0.945090
50000.000000	25.990000	0.955800
60000.000000	24.820000	0.965420
80000.000000	23.440000	0.976130
100000.000000	22.720000	0.982120
120000.000000	22.380000	0.984660
150000.000000	21.940000	0.988890
200000.000000	21.610000	0.992400
300000.000000	21.330000	0.995030
400000.000000	21.210000	0.996210
500000.000000	21.140000	0.996820
600000.000000	21.100000	0.997260
700000.000000	21.070000	0.997530
800000.000000	21.050000	0.997710
900000.000000	21.040000	0.997890

The other outputs of Mkhistory are appended to the EDA4.mk file and consist of the history file input segment (i.e., all the text in the input file lines from "21 |Number of alternate histories" to "22778, 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 IV).

For reference the RIP input table NE1a5s5EDA4-wp.rip (DTN: MO9904MWDWAP72.002) is shown below.

```
! From wapdeg file: NE1a5s5EDA4-wp
! From wapdeg version: 3.09
! Postprocessor: post308
! NE1a5s5EDA4-wp.inp
!
! snf, always drip, 10%, No Backfill, lta nominal i alpha mean, 11/19/98
! Uncertainty/Variability=50/50 drip, 50th Quantile
! 30 cm carbon steel
!
! START OF PARAMETERS
 2
 3   83
 1    2    3
          0.0000
      15134.6125
      17126.0760
      19839.7400
      20774.7582
      21628.1408
      22649.4449
      23442.2882
      23713.7371
      23988.3292
      24266.1010
      24689.2101
      25264.2957
      26002.7445
      26607.2506
      27071.1806
      27542.2870
      27861.2117
      28183.8293
      28675.2489
      29174.2701
      29512.0923
      29853.8262
      30199.5172
      30726.0827
      31260.7937
      31622.7766
      31988.9511
      32359.3657
      32734.0695
      33113.1121
      33690.4798
      34475.2318
      35075.1874
      35481.3389
      35892.1935
      36307.8055
      36728.2300
```

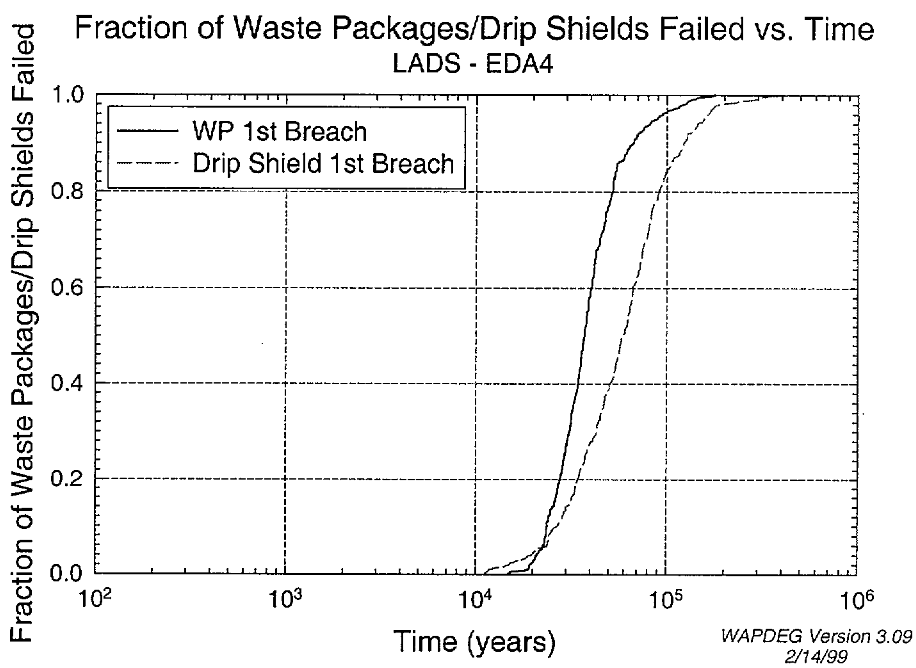
37153.5229		
37583.7404		
38018.9396		
38459.1782		
38904.5145		
39355.0075		
39810.7171		
40271.7034		
40738.0278		
41209.7519		
41686.9383		
42169.6503		
42657.9519		
43151.9077		
43651.5832		
44157.0447		
44668.3592		
45185.5944		
45708.8190		
46238.1021		
46773.5141		
47315.1259		
47863.0092		
48417.2368		
48977.8819		
49831.8712		
50992.6046		
52180.3750		
53088.4444		
53703.1796		
54325.0331		
54954.0874		
56236.6171		
58892.1708		
61662.2245		
65330.3708		
69186.1538		
72453.1986		
77645.2912		
85151.4141		
92807.6861		
106093.9342		
123804.7842		
153725.0777		
1000000.0000		
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0070	0.0000	5.6073
0.0229	0.0000	10.4025
0.0355	0.0000	10.0581
0.0468	0.0000	10.7680
0.0593	0.0000	12.4876
0.0801	0.0000	12.0227
0.0986	0.0000	10.7509
0.1098	0.0000	10.7463
0.1204	0.0000	11.2516
0.1280	0.0000	12.3758
0.1380	0.0000	14.0840
0.1466	0.0000	17.1244
0.1644	0.0000	18.7320
0.1790	0.0000	19.7818

0.1922	0.0000	21.1778
0.2019	0.0000	21.8327
0.2127	0.0000	22.4812
0.2268	0.0000	23.9438
0.2426	0.0000	25.2640
0.2576	0.0000	25.7113
0.2647	0.0000	27.1874
0.2789	0.0000	27.6488
0.2923	0.0000	29.2494
0.3025	0.0000	31.6108
0.3167	0.0000	32.4634
0.3383	0.0000	32.4519
0.3472	0.0000	33.8696
0.3547	0.0000	35.5391
0.3662	0.0000	36.6872
0.3770	0.0000	39.3139
0.3988	0.0000	42.4933
0.4173	0.0000	44.7726
0.4362	0.0000	45.5796
0.4542	0.0000	46.6334
0.4698	0.0000	48.0891
0.4849	0.0000	49.6659
0.4997	0.0000	50.9392
0.5176	0.0000	52.0252
0.5273	0.0000	54.1260
0.5440	0.0000	55.2535
0.5568	0.0000	57.1003
0.5773	0.0000	58.0622
0.5833	0.0000	60.6920
0.5967	0.0000	62.3909
0.6074	0.0000	64.4088
0.6213	0.0000	66.1448
0.6380	0.0000	67.8847
0.6553	0.0000	69.4916
0.6683	0.0000	71.5368
0.6806	0.0000	73.5711
0.6827	0.0000	76.9277
0.6875	0.0000	79.8922
0.6925	0.0000	82.9458
0.7068	0.0000	85.0869
0.7151	0.0000	87.7552
0.7173	0.0000	91.3695
0.7241	0.0000	94.3188
0.7322	0.0000	97.3722
0.7503	0.0000	98.5418
0.7587	0.0000	101.3043
0.7675	0.0000	103.7382
0.7742	0.0000	108.4184
0.7872	0.0000	113.9177
0.8050	0.0000	118.8657
0.8260	0.0000	121.4790
0.8340	0.0000	124.3072
0.8433	0.0000	126.6049
0.8553	0.0000	128.5996
0.8609	0.0000	135.1511
0.8670	0.0000	149.4878
0.8817	0.0000	161.7972
0.8968	0.0000	176.9269
0.9113	0.0000	192.3130
0.9226	0.0000	205.0010
0.9339	0.0000	225.9823

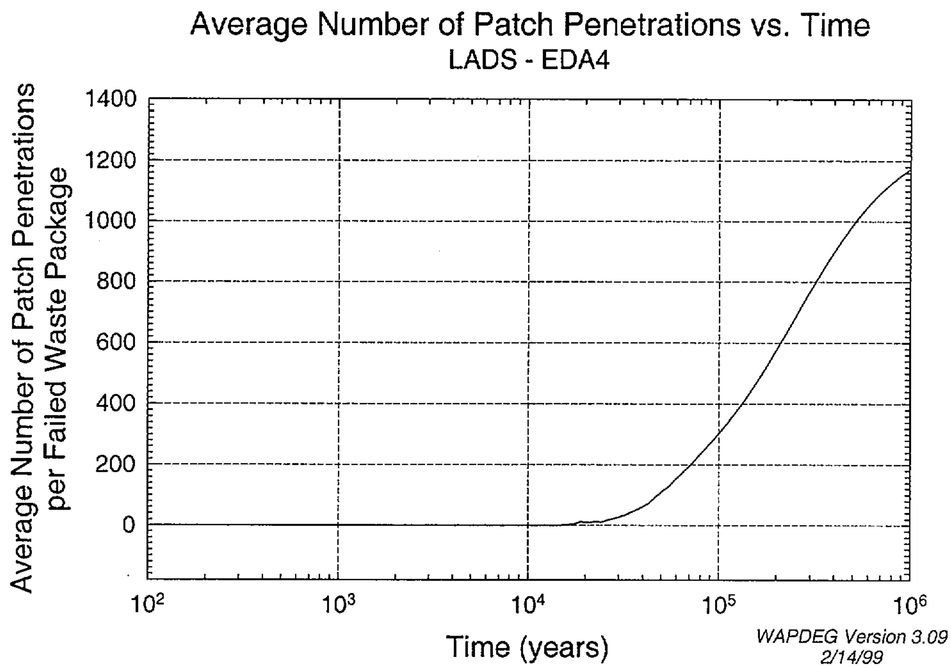
0.9468	0.0000	252.9025
0.9582	0.0000	278.4609
0.9697	0.0000	322.4406
0.9823	0.0000	376.1079
0.9951	0.0000	459.3605
1.0000	0.0000	1170.9500

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). Again, the "No Backfill" statement in the header lines (these are "comment" lines copied directly from the WAPDEG input files) for both RIP input table files (NE1a5s5EDA4-ds.rip and NE1a5s5EDA4-wp.rip) is in error as backfill was modeled in producing the thermal hydrologic history files.

Presented below is a graph (derived from the NE1a5s5EDA4-wp.dat file) of the first breach curve (equivalent to the first patch curve as no localized corrosion was modeled for the carbon steel barrier) for the waste packages:



Below is shown a graph of the average number of failed patches per failed waste package (derived from the NE1a5s5EDA4-wp.asc file):



The first breach curve for the waste package and the average number of patches per failed waste package curves are also represented in the RIP input table, NE1a5s5EDA4-wp.rip.

7. REFERENCES

1. Buscheck, T.A. 1999. *LADS Phase II Multiscale TH Calculation for EDA IV.* Livermore, California: Lawrence Livermore National Laboratory. DTN: LL990301804242.082.

2. CRWMS M&O 1999a. *Supporting Media for RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IV.* 210-72r0.exe. Windows self-extracting archive. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990201.0090. DTN: MO9904MWDWAP72.002.

3. 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.

4. 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.

5. 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.

6. 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.

7. 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.

8. 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.

9. 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.

10. CRWMS M&O 1998d. *Creating Input Tables from WAPDEG for RIP.* B00000000-01717-0210-00013 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981110.0431. DTN: MO9810SPA00013.000.

11. CRWMS M&O 1998e. *Cumulative Distribution Functions for the Temperature Threshold for the Onset of Carbon Steel Corrosion.* B00000000-01717-0210-00015 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980603.0253. DTN: MO9810SPA00013.000.

12. CRWMS M&O 1998f. *Cumulative Distribution Functions for the Relative Humidity Thresholds for the Onset of Carbon Steel Corrosion.* B00000000-01717-0210-00016 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980603.0257. 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.

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 Mkhistory 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 1998. *Software Routine Report for WAPDEG (Version 3.09)*). Although Version 3.09 of the WAPDEG code is referenced here, the output from Mkhistory Version 1.01 could be used by any version of WAPDEG created to date. Mkhistory 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 1998. *Software Routine Report for WAPDEG (Version 3.09)*, p. 28). Mkhistory 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 1998. *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.

Mkhistory is a FORTRAN program 206 lines in extent. It conforms to the FORTRAN 90 standard and is thus highly portable. Mkhistory has been compiled with Digital FORTRAN 5.0 in the Windows/PC environments. Mkhistory 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 1999. *Supporting Media for RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IV*, \Attachment-I directory) (DTN: MO9904MWDWAP72.002).

2. DESCRIPTION OF CODE AND ALGORITHMS USED

The bulk of Mkhistory'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. Mkhistory 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. Mkhistory 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 1998. *Software Routine Report for WAPDEG (Version 3.09)*, p. 28).

As mentioned above, Mkhistory 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. Mkhistory 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 1998. *Software Routine Report for WAPDEG (Version 3.09)*, p. 28) for use in analyses.

Mkhistory 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. Mkhistory 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 Mkhistory version number and list-file name are appended to the list-file, as shown above.

Mkhistory 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 h*xxx*c*yy* column label signifies that the data was extracted from column *yy* of the *xxx*th file processed by Mkhistory. Effectively, the list-file serves as an input and output file as information is appended to it.

3. DESCRIPTION OF TEST CASE

Because Mkhistory 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 Mkhistory 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 1999. *Supporting Media for RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IV*, \Attachment-I\hand directory) (DTN: MO9904MWDWAP72.002) are considered sufficient installation and checkout steps for successful first use of Mkhistory 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, Mkhistory 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 Mkhistory 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 Mkhistory 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 Mkhistory does very few calculations, the valid range of input parameters is largely determined by the limitations discussed in the next section. Mkhistory 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, Mkhistory 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 Mkhistory 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 1999. *Supporting Media for RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative IV.* 210-72r0.exe. Windows self-extracting archive. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990201.0090. DTN: MO9904MWDWAP72.002..

CRWMS M&O 1998. *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.

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
      integer i, starthst, endhst, startdat, enddat
c
c  Find the positions in line where the file names are.
c
      i = 1
      do while (line(i:i) .eq. ' ')
        i = i + 1
      end do
      startdat = i
      do while (line(i:i) .ne. ' ')
        i = i + 1
      end do
      enddat = i - 1
      do while (line(i: i) .eq. ' ')
        i = i + 1
      end do
      starthst = i
      do while ((line(i: i) .ne. ' ') .and. (i .le. linesize))
        i = i + 1
      end do
      endhst = i - 1
      datafl = line(startdat:enddat)
      hstyfl = line(starthst:endhst)
      RETURN
      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 1999. Design Input Transmittal - *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 and 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 ±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.

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

$s := 1.7146$

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

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

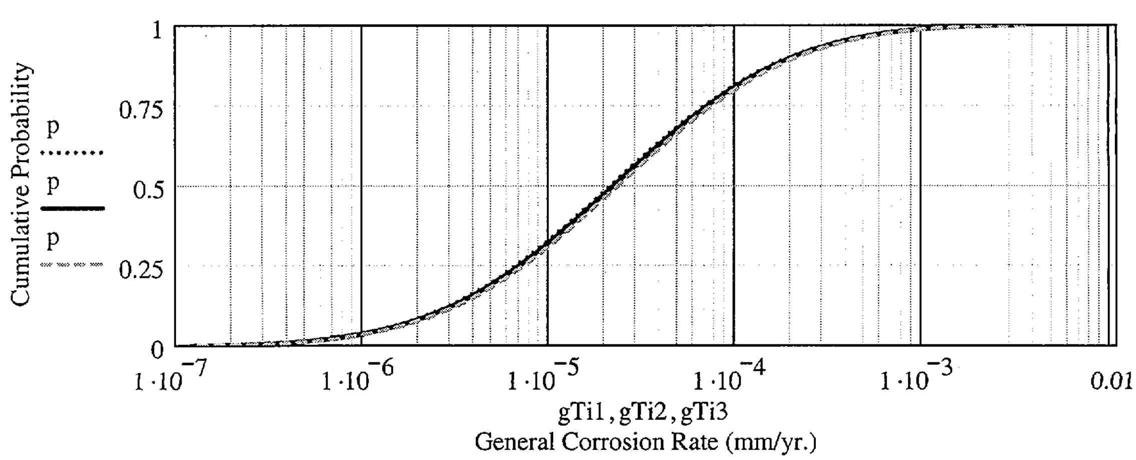
$p := \frac{\text{cnorm}(z) - \text{cnorm}(-3)}{\text{cnorm}(3) - \text{cnorm}(-3)}$

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

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

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

- 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 gTix (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:

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

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

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

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.

```
slnvar(x, p, wtu, qu) := | wtv ← 1 − wtu
                         | zu ← √wtu · qnorm(qu, 0, 1)
                         | for i ∈ 0 .. length(x) − 1
                         |    | z_i ← | −∞ if p_i = 0
                         |    |       | ∞ if p_i = 1
                         |    |       | qnorm(p_i, 0, 1) otherwise
                         |    | lnx_i ← ln(x_i)
                         |    | zv_i ← | −∞ if p_i = 0
                         |    |        | ∞ if p_i = 1
                         |    |        | (zu + z_i · √wtv) otherwise
                         | for i ∈ (0 .. length(x) − 1)
                         |    xv_i ← exp(linterp(z, lnx, zv_i))
                         | augment(xv, p)
```

• wtv is the fraction of the variance that represents variability.
• zu is the standard normal score value that corresponds with the given quantile.
• Values of z and lnx 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}.
• zv are the standard normal values with mean zu and variance wtv that corresponds with the variability distribution.
• Return matrix of rates and cumulative probabilities.

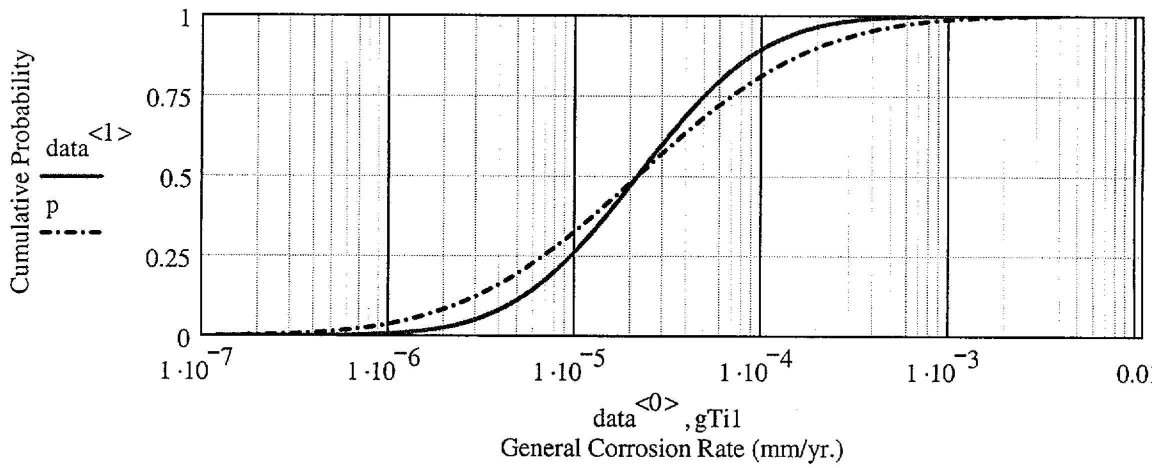
By changing the file names below for each set of uncertainty and quantile values the cdf files are produced by the file print functions in Mathcad.

filnam := "gTi15050.cdf"

data := slnvar(gTi1, p, 0.50, 0.50)

WRITEPRN(filnam) := (rows(data) cols(data))

APPENDPRN(filnam) := data

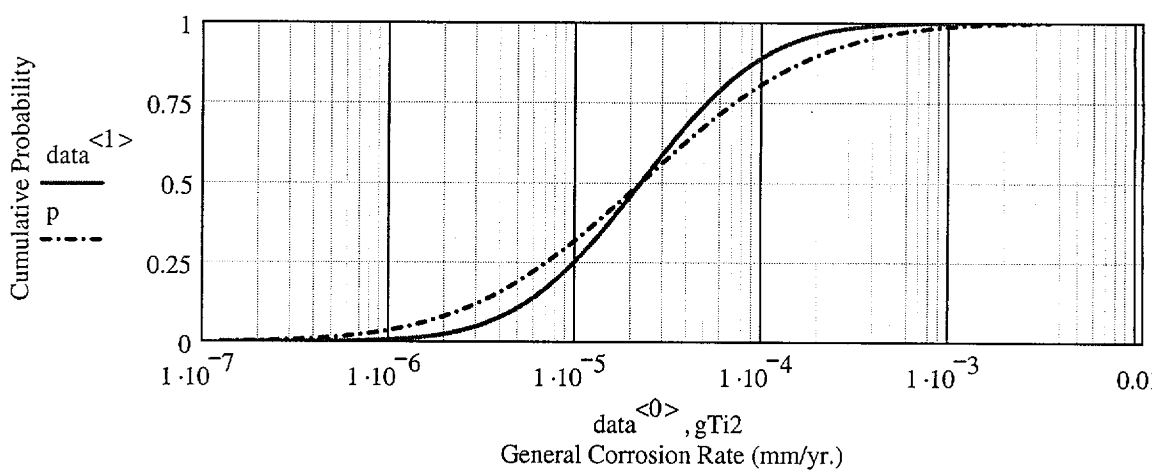


filnam := "gTi25050.cdf"

data := slnvar(gTi2, p, 0.50, 0.50)

WRITEPRN(filnam) := (rows(data) cols(data))

APPENDPRN(filnam) := data

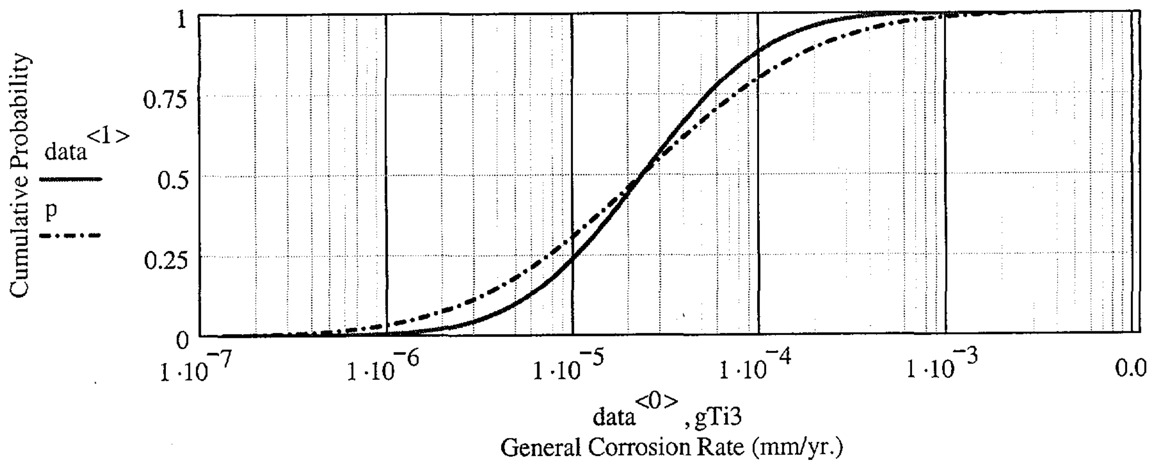


filnam := "gTi35050.cdf"

data := slnvar(gTi3, p, 0.50, 0.50)

WRITEPRN(filnam) := (rows(data) cols(data))

APPENDPRN(filnam) := data



References

CRWMS M&O 1999. *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.