

Calculation Cover Sheet

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CONTENTS

	Page
1. PURPOSE	3
2. METHOD	3
3. ASSUMPTIONS	4
4. USE OF COMPUTER SOFTWARE AND MODELS	12
4.1 SOFTWARE APPROVED FOR QA WORK	12
4.2 SOFTWARE ROUTINES	13
4.3 MODELS	13
5. CALCULATION	14
5.1 MKHISTORY INPUTS	14
5.2 WAPDEG INPUTS	15
5.3 POST308 INPUTS	19
6. RESULTS	20
7. REFERENCES	28
8. ATTACHMENTS	29

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 waste packages composed of a 2-cm thick Alloy 22 corrosion resistant material (CRM) as the outer barrier and an unspecified material to provide structural support as the inner barrier) 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. Performance credit of the inner barrier material is not taken in this calculation. This calculation supports Performance Assessment analysis of the License Application Design Selection (LADS) Enhanced Design Alternative V. Additional details concerning the Enhanced Design Alternative V 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 are assumed to only undergo general corrosion processes, which result in "patch" perforations (see Assumption 3.9 in Section 3). More detailed discussions of the WAPDEG conceptual model are given elsewhere (CRWMS M&O 1998a, *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document - Chapter 5, Waste Package Degradation Modeling and Abstraction*, pp. 5-27 to 5-29). The drip shield / waste package failure profiles calculated by WAPDEG consist of time-varying measures of the number of pit or patch penetrations on each drip shield / waste package. The WAPDEG post-processor, Post308 (CRWMS M&O 1998b, *Software Routine Report for WAPDEG (Version 3.09), Appendix D*), abstracts this information to produce one RIP input table (Golder Associates 1998, pp. 7-22 through 7-25) per WAPDEG simulation. The RIP input table contains:

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

As mentioned earlier, in this calculation, the drip shields 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 dripping conditions were modeled by executing the WAPDEG code twice, as described in Section 3.0. The first WAPDEG simulation (using the input file NE1a5s5EDA5-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 NE1a5s5EDA5-ds.cdf. A second WAPDEG simulation (using the input file NE1a5s5EDA5-wp.inp) was then performed to model waste package degradation and failure using this dripping start time distribution. Under non-dripping conditions, the presence of the drip shield is irrelevant to waste package degradation modeling and only one WAPDEG simulation is necessary (using the input file NE0a5s6EDA5-wp.inp)

3. ASSUMPTIONS

No assumptions are made in executing Mkhhistory. The limitations on the Mkhhistory software routine and on the validity of the resulting output are discussed in detail in Attachment 1.

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 NE1a5s5EDA5-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, NE1a5s5EDA3a-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 NE1a5s5EDA5-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 29.91 m². This is based on the length of the 21 PWR (Pressurized Water Reactor) waste package type over which it is emplaced and drip shield dimensions provided (CRWMS M&O 1999b *Design Input Transmittal For Waste Stream Information for LADS, Phase 2, EDAs*, Item 1 p. 3/34 Table 2 and Item 5 p. 1/2). The drip shields are assumed to have a "mail-box" (inverted U-shaped) configuration and to be placed over the waste packages with a gap between the drip shields and the waste packages to avoid direct contact. The length of the waste package is 5.275 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 1.050 m and 1.220 m, respectively. The average of the drip shield inner and outer radii are used to define an effective radius to be used in determining the effective surface area of the drip shield. The function of the drip shield is to delay dripping water contact with the waste package surface until after drip shield failure. The breached drip shield area, through which dripping water can flow, is the modeling area of interest to this calculation. The most conservative assumption would be that dripping water can penetrate the drip shield through its entire surface area. The least conservative assumption would be that dripping water could penetrate the drip shield only through the projected area above the waste package (i.e., a rectangular area defined by the waste package diameter multiplied by its length). The effective area used in this calculation is a realistic compromise between these two extreme approaches. The height of the drip shield side plates is 1.317 m. Thus, the drip shield surface area modeled (subject to corrosion) is given by:

IR := 1 050 m	OR := 1 220 m	Inner (IR) and outer (OR) dnp shield rad
L := 5 275 m - 2 0 225 m	L = 4 825 m	Waste package length - two skirts
SPIH := 1 317 m		Dnp shield side plate height
$er := \frac{(IR + OR)}{2}$	er = 1 135 m	Effective Radius
Tot := 2 SPIH L + π er L	Tot = 29 91 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 dnp shield surface area was divided into 965 patches each 0.0310 m² in area. This patch size was chosen to be consistent with the patch size chosen in the TSPA-VA REV 01 base case calculation (CRWMS M&O 1998d, *Creating Input Tables from WAPDEG for RIP* Section 3.0, Assumption 3.3). Continuing from the calculations presented in Assumption 3.3 above:

PS = 0.0310 m ²	Patch Size
$\frac{Tot}{PS} = 965$	965 Patches/DS

This assumption is used in the WAPDEG input file NE1a5s5EDA5-ds.inp in the fourth line (second value) after the last thermal hydrologic history file name.

- 3.5 The dnp 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, with the outer barrier hard-wired to be a corrosion allowance material (CAM) of carbon steel, and the corrosion model parameters for the inner barrier able to be supplied by the user through the WAPDEG input file. In order to model the drip shield corrosion degradation process as a corrosion resistant material (CRM) with no CAM, it is required to assume that the drip shield has a very thin (1e-12 cm) "simulated" CAM and the CAM pit multiple (or localization factor) 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 NE1a5s5EDA5-ds.inp on the second input line after the last history file name (first value) and on the third input line after the [No Dnp Model, CAM] and [Neutral Dnp Model, CAM] input headers.

- 3 6 Corrosion of the drip shields is assumed not to occur until after they are emplaced and ventilation ceases 75 years after waste package emplacement (CRWMS M&O 1999f *Design Input Request For Performance Assessment (PA) For Enhanced Design Alternative (EDA), Option V*, Attachment I p. 2). This is accomplished by using a 76-year corrosion delay time (the extra year was added to assure corrosion does not initiate). 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. The same emplacement scenario (drip shields emplaced 75 years after waste package emplacement) is used in generating the thermal hydrologic history files used in this calculation (Buscheck 1999) (DTN LL990301804242 083). This assumption is used in the WAPDEG input file NE1a5s5EDA5-ds.inp on the nineteenth and twentieth input lines after the last history file name.
- 3 7 The temperature corrosion initiation threshold for the very thin simulated CAM outer barrier was assumed to be represented by the cumulative distribution function for titanium grade 7 as given in A22TiTh.cdf (CRWMS M&O 1999c, *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 1/3 Response 1). This assumption has the effect of delaying the initiation of corrosion of the titanium grade 7 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 NE1a5s5EDA5-ds.inp on the first and second input lines after the [No Drip Model Features] header and on the first and second input lines after the [Neutral Drip Features].
- 3 8 The relative humidity corrosion initiation threshold for the very thin simulated CAM outer barrier was assumed to be represented by the cumulative distribution function for titanium grade 7 as given in A22TiRHth.cdf (CRWMS M&O 1999c, *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 1/3 Response 2). This assumption has the effect of delaying the initiation of corrosion of the titanium grade 7 until the relative humidity initiation threshold for corrosion of the simulated CAM is satisfied (since the CAM fails immediately upon satisfaction of the corrosion initiation thresholds). This assumption is used in the WAPDEG input file NE1a5s5EDA5-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 NE1a5s5EDA5-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 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 (A22TiTh.cdf). This assumption is used throughout Attachment II.
- 3.11 In deriving the general corrosion rates used to model general corrosion degradation of the titanium grade 7 drip shields under dripping conditions, the total variance of the cdfs are assumed to be composed of 50% uncertainty and 50% variability, and it is assumed that the median corrosion rate is at the 50th percentile of the uncertainty distribution. This assumption is based on input received (CRWMS M&O 1999c, *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading, Item 1 p. 1/3 Response 1*). This assumption is used throughout Attachment II.
- 3.12 The general corrosion rates used to model general corrosion degradation of the titanium grade 7 drip shields under dripping conditions are derived in Attachment II. In Attachment II, it is assumed that it is appropriate to derive the titanium grade 7 corrosion cdfs (3 of them) used with the "CRMGeneralCorrosionRateOnly" model at 201 equally spaced (in natural logarithm space) general corrosion rates between the minimum and maximum general corrosion rate for each temperature used (30°C, 60°C, and 120°C). Given that none of the general corrosion rate distributions span more than 5 orders of magnitude (see Attachment II), use of this assumption allows each decade of corrosion rates to be characterized by at least 40 cdf points. This assumption is used throughout Attachment II.
- 3.13 The general corrosion rates used to model general corrosion degradation of the titanium grade 7 drip shields under dripping conditions are derived in Attachment II. In Attachment II cumulative probability values were interpolated linearly between natural log general corrosion rate values. It is assumed that this interpolation methodology results in well approximated cumulative probability values. As mentioned in Assumption 3.12, each decade of corrosion rates is characterized by at least 40 cdf points. Given this density of points in the cdfs (i.e., the small size of the interval over which interpolation is occurring), the

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

The following assumptions are made for Alloy 22 Waste Package Degradation Modeling

The WAPDEG input file NE1a5s5EDA5-wp.inp is used to model waste packages under a 2-cm thick titanium grade 7 drip shields that are always dripped on. As mentioned in Section 1.0, the waste package design considered in the present calculation is a 2-cm thick Alloy 22 outer barrier and an inner barrier with a reasonable thickness to provide structural support. Design specifications for the inner barrier are not available. In the present calculation, credit for the inner barrier performance is not taken. In this simulation the waste package is not contacted by dripping water until the drip shield fails. The WAPDEG input file NE0a5s6EDA5-wp.inp is used to model waste packages under a 2-cm thick titanium grade 7 drip shields that are never dripped on (equivalent, for WAPDEG modeling purposes, to having no drip shields present). The assumptions used in modeling Alloy 22 waste package degradation are identical to those used in the TSPA-VA REV 01 base case calculation (CRWMS M&O 1998d, *Creating Input Tables from WAPDEG for RIP*) (DTN MO9810SPA00013.000) with the exception of those listed below.

- 3.14 The total waste package surface area modeled is 27.55 m² or approximately 889 patches each with an area of 0.0310 m². This is based on the 21 PWR (Pressurized Water Reactor) waste package dimensions provided (CRWMS M&O 1999b, *Design Input Transmittal For Waste Stream Information for LADS, Phase 2 EDAs*, Item 1 p. 3/34 Table 2). The length of the waste package is 5.275 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 (i.e., subject to corrosion degradation) 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.

$OD := 1.564 \text{ m}$	$L = 4.825 \text{ m}$	Waste Package Outer Diameter and Length
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$WPA := \pi \cdot OD \cdot L + 2 \pi \cdot \frac{OD^2}{4}$	$WPA = 27.55 \text{ m}^2$	Total Waste Package Area
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$\frac{WPA}{PS} = 888.701$	889 Patches/WP
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This assumption is used on the fourth input line (second value) in the WAPDEG input files NE1a5s5EDA5-wp.inp and NE0a5s6EDA5-wp.inp.

- 3.15 The NE1a5s5EDA5-ds.cdf (a cdf of first breach times of the drip shields modeled) distribution is used as the “Distribution parameter(s)” for the “Distr. for time range for ceramic protection” of the waste packages (this is perhaps better termed “the delay time for corrosion initiation” of the waste packages) in the WAPDEG input file NE1a5s5EDA5-

wp.inp. The basis of this assumption is that dripping water cannot contact a waste package underneath an intact drip shield. This distribution is read by the fourteenth and fifteenth lines after the last thermal hydrologic "history" file name. (No drip shield delay time is used in the input file NE0a5s6EDA5-wp.inp).

- 3.16 After failure of a titanium grade 7 drip shield (defined by the NE1a5s5EDA5-ds.cdf), ten percent (10%) of the waste package surface area under the breached drip shield is assumed to be contacted by the dripping water. This assumption is made to incorporate the anticipated protection from dripping water contact that the drip shield provides subsequent to its initial (single patch) breach. In light of Assumptions 3.3 and 3.4, in which the entire surface area of the drip shield is considered in degradation modeling, this is a conservative assumption as the first breach of the drip shield may be on one of the side plates and not directly over the waste package. This assumption is used in the WAPDEG input file NE1a5s5EDA5-wp.inp on the tenth through thirteenth input lines after the last history file name. (No drip shield delay time is used in the input file NE0a5s6EDA5-wp.inp)
- 3.17 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 (*.inp, where "*" represents any file name prefix). In order to model a corrosion resistant material (CRM) with no CAM (corresponding to the single-barrier waste package), it is required that the "simulated" CAM thickness be set to a small number (1e-12 cm) and the CAM pit multiple (or roughness factor) is set to a large number (1e12), in the WAPDEG input file used. The effect is an immediate failure of the CAM upon satisfaction of the relative humidity (RH) and temperature thresholds for corrosion initiation. This assumption is used in the WAPDEG input files NE1a5s5EDA5-wp.inp and NE0a5s6EDA5-wp.inp on the second input line after the last history file name and on the third input line after the [No Drip Model, CAM] and [Neutral Drip Model, CAM] input headers.
- 3.18 The temperature corrosion initiation threshold for the very thin simulated CAM outer barrier was assumed to be represented by the cumulative distribution function 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 3). This assumption has the effect of delaying the initiation of corrosion of the Alloy 22 until the temperature initiation threshold for corrosion of the simulated CAM is satisfied (since the CAM fails immediately upon satisfaction of the corrosion initiation thresholds). This assumption is based on the input received. This assumption is used in the WAPDEG input files NE1a5s5EDA5-wp.inp and NE0a5s6EDA5-wp.inp on the first and second input lines after the [No Drip Model Features] and the [Neutral Drip Features] headers.
- 3.19 The relative humidity corrosion initiation threshold for the very thin simulated CAM outer barrier was assumed to be represented by the cumulative distribution function

A22TiRHth.cdf (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*. Item 1 p. 1/3 Response 4). This assumption has the effect of delaying the initiation of corrosion of the Alloy 22 until the relative humidity initiation threshold for corrosion of the simulated CAM is satisfied (since the CAM fails immediately upon satisfaction of the corrosion initiation thresholds). This assumption is used in the WAPDEG input files NE1a5s5EDA5-wp.inp and NE0a5s6EDA5-wp on the third and fourth input lines after the [No Drip Model Features] header and on the fifth and sixth input lines after the [Neutral Drip Features] header (if dripping occurs).

- 3.20 General corrosion of the single Alloy 22 barrier under dripping is assumed to take place under mild electrochemical exposure conditions (pH range 3-10, 340 mV SHE). The basis for this assumption is several statements in the Engineered Materials Characterization Report (McCright 1998), among them: "Even if the salts present in the ground water concentrate on the warm metal surface, the net effect may produce an environment that is not highly aggressive." (p. 2-3). The absence of the CAM outer barrier (relative to the TSPA-VA design) also eliminates the possibility of tight crevice formation (a probable site for localized corrosion initiation) between the CAM and CRM barriers. This assumption is used in the WAPDEG input file NE1a5s5EDA5-wp.inp in the [Neutral Drip Model, CRM] input segment by using the "CRMGenerate+ArrheniusPit" model and corrosion rates from the gCx5050.cdf files (where x is the numeric 1, 2, and 3 corresponding to temperatures at 25, 50 and 100°C, respectively).
- 3.21 It is assumed that localized corrosion of Alloy 22 is possible in the presence of drips and if the temperature is above a critical temperature threshold for initiation. The critical threshold temperature is input to this calculation (file: A22LCTth.cdf) (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*. Item 1 p. 2/3 Response 6). This assumption is based on that input. This assumption is used in the [Neutral Drip Features] input segment in the WAPDEG input file NE1a5s5EDA5-wp.inp and on the third and fourth input lines following the [Neutral Drip Features] header.
- 3.22 For the 75 years before pre-closure ventilation ceases (see Assumption 3.6), it is assumed the waste package is not dripped upon. The basis for this assumption is that the repository is ventilated during this time period (CRWMS M&O 1999f. *Design Input Request For Performance Assessment (PA) For Enhanced Design Alternative (EDA), Option V*, Attachment I p. 2), 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 the fourteenth and fifteenth input lines after the last thermal hydrologic history file name in the WAPDEG input file NE1a5s5EDA5-wp.inp.

4. USE OF COMPUTER SOFTWARE AND MODELS

4.1 SOFTWARE APPROVED FOR QA WORK

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

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

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

4.2 SOFTWARE ROUTINES

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

Software Name	Mkhistory
Software Version:	1.01

Mkhistory was executed on a DELL PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371) in the Windows NT 4.0 operating system. Mkhistory version 1.01 has gone through the complete verification and validation process required by AP-SI.1Q 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 V*) (DTN MO9904MWDWAP73.001) 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 V*) (DTN: MO9904MWDWAP73.001).

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: LL990301804242.083). These histories are organized by bin numbers and model identifier with file names like NE_snf_mean_yy_noBF_150_c_j4_27_03e_05_0_data, where NE denotes the northeast region of the potential repository, snf denotes commercial spent nuclear fuel, yy is a bin number, noBF denotes no backfill was used, 150 denotes an areal mass loading of 150 MTU/acre, and the numeric 27 indicates that these thermal hydrologic histories are applicable to "long-term average" climate conditions. The remainder of the file name designators are not relevant to this calculation.

The thermal hydrologic history files contain columns of ASCII numerical data. Column 1 contains the time (years), Column 2 the waste package surface temperature ($^{\circ}\text{C}$), Column 3 the relative humidity at the waste package surface (fraction), Column 4 the air mass fraction (X_{air}), Column 5 the liquid saturation in the invert (fraction), Column 6 the drift wall temperature ($^{\circ}\text{C}$), Column 7 the drift wall relative humidity (fraction), Column 8 the drip shield surface temperature ($^{\circ}\text{C}$), and Column 9 the drip shield surface relative humidity (fraction). In this calculation, a total of 8 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) 01, 02, 12, 22, 32, 42, 52, and 62 are used in this calculation (i.e., NE_snf_mean_01_noBF_150_c_j4_27_03e_05_0_data, NE_snf_mean_02_noBF_150_c_j4_27_03e_05_0_data, . . . , etc.).

These thermal hydrologic history files were processed by the Mkhistor software routine. The bulk (but not all) of Mkhistor'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 Mkhistor input file(s) to the file named in Column 2 of the Mkhistor 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 Mkhistor input file as discussed in Attachment I. Two Mkhistor input files were used, EDA5ds.mk, for the drip shield surface, and EDA5.mk for the waste package surface. The initial contents of the Mkhistor input file EDA5.mk are:

```
8,9,3          |number of files, columns, and columns to print
1,2,3          |print specified columns
NE_snf_mean_01_noBF_150_c_j4_27_03e_05_0_data  NEsf01noBF150cj42703e050 hst
NE_snf_mean_02_noBF_150_c_j4_27_03e_05_0_data  NEsf02noBF150cj42703e050 hst
NE_snf_mean_12_noBF_150_c_j4_27_03e_05_0_data  NEsf12noBF150cj42703e050 hst
NE_snf_mean_22_noBF_150_c_j4_27_03e_05_0_data  NEsf22noBF150cj42703e050 hst
NE_snf_mean_32_noBF_150_c_j4_27_03e_05_0_data  NEsf32noBF150cj42703e050 hst
```

NE_snf_mean_42_noBF_150_c_j4_27_03e_05_0_data	NESf42noBF150cj42703e050.hst
NE_snf_mean_52_noBF_150_c_j4_27_03e_05_0_data	NESf52noBF150cj42703e050.hst
NE_snf_mean_62_noBF_150_c_j4_27_03e_05_0_data	NESf62noBF150cj42703e050.hst

The first line of this Mkhhistory input file indicates that 8 thermal hydrologic history files (whose file names are listed in the first column of the Mkhhistory input file (starting on row 3)) are to be processed by Mkhhistory, these history files contain 9 columns of data, of which 3 will be extracted to the file name specified in the second column of the Mkhhistory input file. The second line of the Mkhhistory input file indicates that columns 1, 2, and 3 of the thermal hydrologic history files (whose file names are listed in the first column of the Mkhhistory input file (starting on row 3)) will be extracted to the file name specified in the second column of the Mkhhistory input file (i.e., data from NE_snf_mean_01_noBF_150_c_j4_27_03e_05_0_data is to be copied to NESf01noBF150cj42703e050.hst, etc.). The above are the contents of EDA5.mk before execution of Mkhhistory (several data segments are appended to this file during Mkhhistory program execution as discussed in Attachment I. The thermal hydrologic history files before and after processing by Mkhhistory and the EDA5.mk and EDA5ds.mk files after execution of Mkhhistory are included in the electronic media supporting this calculation (CRWMS M&O 1999a. *Supporting Media for RIP Input Tables From WAPDEG For LA Design Selection. Enhanced Design Alternative V*) (DTN MO9904MWDWAP73.001). Note that the contents of EDA5ds.mk cause Mkhhistory to extract the columns of thermal hydrologic data relevant to the drip shield surface and copy them to files with a * ds (for drip shield) file name suffix (which is then read by WAPDEG) in place of the previously discussed * hst file name suffix

Procedurally, the Mkhhistory program prompts the user for a list-file name (this is the Mkhhistory input file, i.e., EDA5.mk). The Mkhhistory program then prompts the user for the total number of waste packages to be considered. The user entered "0" to cause the default value of 1,000,000 waste packages to be used in order to retain the maximum possible six digits of accuracy for the fraction of waste packages represented by each thermal hydrologic history file.

5.2 WAPDEG INPUTS

WAPDEG version 3.09 requires several input files (*.inp, *.cdf, and *.hst files, see below) (DTN: MO9904MWDWAP73.001) and creates several output files (*.aux, *.bin, *.cam, *.crm, *.out, *.pat) (DTN: MO9904MWDWAP73.001). 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: MO9904MWDWAP73.001). The *.inp 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 (*.hst) or drip shields (*.ds, see the EDA5ds.mk file) (DTN: MO9904MWDWAP73.001).

- 2) Cumulative distribution functions (cdf) for the temperature threshold for the onset of corrosion. This threshold is used for the simulated outer barrier corrosion allowance material (CAM) of the drip shields and waste packages (file: A22TiTh.cdf) (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, p. 1/3 Response 1 and 3).
- 3) Cumulative distribution functions for the RH threshold for the onset of corrosion for the simulated CAM outer barrier of the drip shields and waste packages (file: A22TiRHth.cdf) (CRWMS M&O 1999c. *Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 1/3 Response 2 and 4).
- 4) Cumulative distribution functions for the titanium grade 7 drip shield general corrosion rates (see Attachment II) at 30, 60, and 120°C (files: gTi15050.cdf, gTi25050.cdf, and gTi35050.cdf) (DTN: MO9904MWDWAP73.001).
- 5) Cumulative distribution functions for general corrosion rates under dripping water conditions for the Alloy 22 corrosion resistant material (CRM) (files: gC*.cdf) (Bullard 1998) (DTN: MO9812MWDDSQ37.000).
- 6) Cumulative distribution functions for the CRM general corrosion rates with no dripping water at 25, 50, and 100°C (files: gnd*.cdf) (CRWMS M&O 1998e. *Cumulative Distribution Functions for No Drip Corrosion Resistant Material General Corrosion Model*, Section 6) (DTN: MO9810SPA00013.000).
- 7) The cumulative distribution function for the titanium grade 7 drip shield failures to use as drip start times for the waste packages underneath the failed drip shields (file: NE1a5s5EDA5-ds.cdf containing the first breach times from the WAPDEG simulation using the NE1a5s5EDA5-ds.inp input file). This cdf is used as a drip initiation time distribution in the WAPDEG simulation using the NE1a5s5EDA5-wp.inp input file.
- 8) 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.
- 9) A cumulative distribution function for the temperature threshold for the initiation of localized corrosion of the Alloy 22 waste package (file: A22LCTth.cdf) (CRWMS M&O 1999c. *QAP-3-12 Design Input Transmittal For License Application Design Selection Phase 2 Enhanced Design Alternatives Input on 1) Temperature and Relative Humidity Thresholds for Various Corrosion Modes of Alloy 22 And Ti-7 2) Cladding Degradation Due to Elevated Fuel Rod Temperatures Caused By the Use of Backfill or Higher Thermal Loading*, Item 1 p. 2/3 Response 6).

Three WAPDEG input files were used to generate the RIP input tables for the License Application Design Selection Analyses: Enhanced Design Alternative V. NE1a5s5EDA5-ds.inp (for the drip

shield under dripping conditions), NE1a5s5EDA5-wp.inp (for the waste package under dripping conditions only after drip shield failure), and NE0a5s6EDA5-wp.inp (for the waste package under no dripping conditions) These input files are included in the electronic media supporting this calculation (CRWMS M&O 1999a. *Supporting Media for RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative V*) (DTN MO9904MWDWAP73.001)

The first two characters of the input file name indicate that the Northeast (NE) region of the potential repository (using its thermal hydrologic history files) is being simulated. The next character in the input file name (0 or 1) indicates, respectively, that a no-drip case is being simulated or the waste packages are subject to dripping throughout the simulation. The next two characters (a5) indicate that the file is for the base case infiltration. The next characters (s5 or s6) refer to the different uncertainty/variability splits and percentile of the uncertainty distribution used for the median of the titanium grade 7 (drip shield) and Alloy 22 (waste package) general corrosion rate variability distributions. The classifications are as follows:

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

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

From the above table, it is apparent that the dripping input files (NE1a5s5EDA5-ds.inp and NE1a5s5EDA5-wp.inp) use a 50% uncertainty - 50% variability split and use the 50th percentile of the uncertainty distribution for the median of the general corrosion rate variability distributions. The non-dripping input file (NE0a5s6EDA5-wp.inp) uses a 75% uncertainty - 25% variability split and uses the 50th percentile of the uncertainty distribution for the median of the general corrosion rate variability distributions. The characters (EDA5) indicate that these input files are used in analyzing LA Design Selection Analyses: Enhanced Design Alternative V. For reference, below is shown the input file NE1a5s5EDA5-ds.inp used in the WAPDEG simulation of the dripping exposure condition

NE1a5s5EDA5-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
```

START OF PARAMETERS

```
3.09                                     |Version number of code
8                                       |Number of alternate histories
NEsf01noBP150cj42703e050 ds          |History file 1
    29819, 0, 0.                       |packs/history, T std, RH std
NEsf02noBP150cj42703e050 ds          |History file 2
    68202, 0, 0.                       |packs/history, T std, RH std
NEsf12noBP150cj42703e050 ds          |History file 3
    222362, 0., 0.                     |packs/history, T std, RH std
```

NEsf22noBF150cj42703e050.ds	History file 4
157514, 0., 0.	packs/history, T std, RH std
NEsf32noBF150cj42703e050.ds	History file 5
232108, 0., 0.	packs/history, T std, RH std
NEsf42noBF150cj42703e050.ds	History file 6
116876, 0., 0.	packs/history, T std, RH std
NEsf52noBF150cj42703e050.ds	History file 7
112854, 0., 0.	packs/history, T std, RH std
NEsf62noBF150cj42703e050.ds	History file 8
60261, 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, 965, 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 corrosion delay time
76.0	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
gT115050.cdf	Distribution parameter (s)
60.0	Temp appropriate for dist #2
File	Distribution type for #2
gT125050.cdf	Distribution parameter (mm/yr)
120.0	Temp appropriate for dist #3
File	Distribution type for #3
gT135050.cdf	Distribution parameter (mm/yr)
[Neutral Drip Features]	Required if any non-neutral drips can be seen
File	Dist for thermal protection temperature
A22T1Tth.cdf	Distribution parameter(s)
File	Dist type for CRM LC T init
A22LCTth.cdf	Distribution parameter
File	Dist type for humid-air initiation
A22T1RHth.cdf	Distribution parameter(s)
Fixed	Dist type for humid-air/aqueous transition
100.	Distribution parameter(s)
0 0, 0.0	Galvanic protect depth %, % patches protected
0.0	Spalling depth as a % of thickness
Fixed	Dist for multiple for CAM corrosion rate
1.0	Distribution parameter(s)
Fixed	Dist for multiple for CRM corrosion rate
1.0	Distribution parameter(s)
1.0	Pack variance share for multiples

Procedurally, the WAPDEG code was executed by typing the name of the executable (i.e. wap309) on the command line and entering the name of the WAPDEG input file (i.e., NE1a5s5EDA5-ds.inp).

The "raw" output from a WAPDEG simulation consists of six files: a *.out file, *.pat file, *.bin file, *.crm file, *.cam file, and *.aux file (where "*" is the input file name prefix). The content and format of these files are discussed in the WAPDEG version 3.09 Software Routine Report (CRWMS M&O 1998b, Section 4.1). These files are also included in the electronic media supporting this calculation (CRWMS M&O 1999a, *Supporting Media for RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative V*) (DTN: MO9904MWDWAP73.001). 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 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 V*) (DTN: MO9904MWDWAP73.001).

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 V*) (DTN: MO9904MWDWAP73.001). For brevity, only selected files are reproduced in hardcopy form within this section.

The primary outputs of Mkhistry are the *.hst files used as input to WAPDEG. For reference, the contents of NEEsf01noBF150cj42703e050.hst are:

1.000000	80.750000	0.512700
1.500000	85.510000	0.533860
2.000000	89.160000	0.549850
3.000000	94.010000	0.572400
4.000000	97.190000	0.589210
5.000000	99.610000	0.603300
6.000000	101.660000	0.614350

7.000000	103.350000	0.623680
8.000000	104.640000	0.632680
9.000000	105.870000	0.639680
10.000000	106.980000	0.639510
11.000000	107.820000	0.641390
12.000000	108.490000	0.644850
15.000000	109.980000	0.651920
20.000000	110.750000	0.660550
25.000000	110.570000	0.667820
26.000000	110.400000	0.670660
27.000000	110.210000	0.673940
30.000000	109.410000	0.688750
35.000000	108.540000	0.705020
40.000000	105.640000	0.733120
50.000000	103.610000	0.756790
51.000000	103.360000	0.758820
52.000000	103.130000	0.760880
55.000000	102.670000	0.766430
60.000000	101.480000	0.774850
65.000000	100.600000	0.781930
70.000000	99.770000	0.788610
75.000000	99.560000	0.794090
76.000000	134.750000	0.327950
77.000000	137.390000	0.291360
80.000000	140.780000	0.255840
90.000000	140.660000	0.261900
100.000000	137.200000	0.272780
101.000000	136.620000	0.276740
105.000000	135.180000	0.287540
110.000000	132.450000	0.309940
120.000000	128.590000	0.347240
130.000000	125.640000	0.379670
140.000000	123.690000	0.405110
160.000000	118.600000	0.480570
180.000000	117.360000	0.500430
200.000000	117.010000	0.506280
220.000000	113.480000	0.568380
250.000000	111.340000	0.609820
300.000000	108.010000	0.678220
350.000000	106.040000	0.722640
400.000000	104.560000	0.759800
450.000000	103.250000	0.802640
500.000000	102.240000	0.839230
550.000000	101.550000	0.863800
600.000000	100.970000	0.882170
700.000000	100.020000	0.901220
800.000000	98.220000	0.910210
900.000000	96.430000	0.916800
1000.000000	95.010000	0.922290
1100.000000	93.850000	0.926240
1200.000000	92.350000	0.930230
1300.000000	90.390000	0.934040
1400.000000	88.290000	0.937890
1500.000000	86.130000	0.941240
1600.000000	84.710000	0.943130
1800.000000	82.690000	0.947110
2000.000000	80.920000	0.951400
2200.000000	79.520000	0.952850
2500.000000	77.650000	0.955620
3000.000000	75.500000	0.958260
3500.000000	73.950000	0.958670

4000.000000	72.640000	0.960820
4500.000000	71.590000	0.961420
5000.000000	70.680000	0.963160
6000.000000	68.980000	0.964310
7000.000000	67.530000	0.963980
8000.000000	66.170000	0.964630
10000.000000	63.780000	0.965490
15000.000000	56.180000	0.970220
20000.000000	49.980000	0.971160
30000.000000	40.380000	0.977650
40000.000000	35.120000	0.981780
50000.000000	32.150000	0.984590
60000.000000	30.020000	0.987260
80000.000000	27.530000	0.990530
100000.000000	26.220000	0.992840
120000.000000	25.590000	0.993650
150000.000000	24.780000	0.995460
200000.000000	24.160000	0.996530
300000.000000	23.630000	0.997540
400000.000000	23.400000	0.998000
500000.000000	23.280000	0.998250
600000.000000	23.200000	0.998420
700000.000000	23.160000	0.998510
800000.000000	23.110000	0.998610
900000.000000	23.090000	0.998670

The other outputs of Mkhistry are appended to the EDA5.mk file and consist of the history file input segment (i.e., all the text in the input file lines from "8 [Number of alternate histories" to "60261, 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 V*).

For reference the RIP input table NE1a5s5EDA5-wp.rp (DTN: MO9904MWDWAP73.001) is shown below.

```

! From wapdeg file: NE1a5s5EDA5-wp
! From wapdeg version: 3.09
! Postprocessor: post308
! NE1a5s5EDA5-wp.inp
!
! snf, always drip, 10%, No Backfill, lta nominal i alpha mean
! Uncertainty/Variability=50/50 drip, 50th Quantile
! Alloy 22 2 cm WP
!
! START OF PARAMETERS
2
3 83
1 2 3
0.0000
9439.6088
14057.1011
37689.7598
88558.2556
125948.1709
138883.6419

```

147917.3740
158559.3529
168852.3835
173787.7610
179895.0395
186216.9409
191649.2816
194984.4600
199535.0472
204173.7945
207733.8143
212572.5565
216271.8524
218776.1624
221309.4710
225168.2723
229086.7653
233081.1733
237137.3706
239883.2919
244065.9505
248313.3105
251188.6432
254097.2706
257039.5783
260015.9563
264549.6526
269153.4804
273846.5006
278612.1169
281838.2931
285101.8268
288403.1503
293431.8120
298538.2619
301995.1720
305492.1113
309029.5433
312607.9367
318058.6385
323593.6569
327340.6949
331131.1215
334965.4392
338844.1561
346752.1703
354813.3892
358921.9346
367298.5281
380206.1942
389045.1450
395828.6230
405048.6561
414483.4513
424138.0111
431519.0768
439043.1398
446683.5922
454472.0670
462381.0214
470443.2001

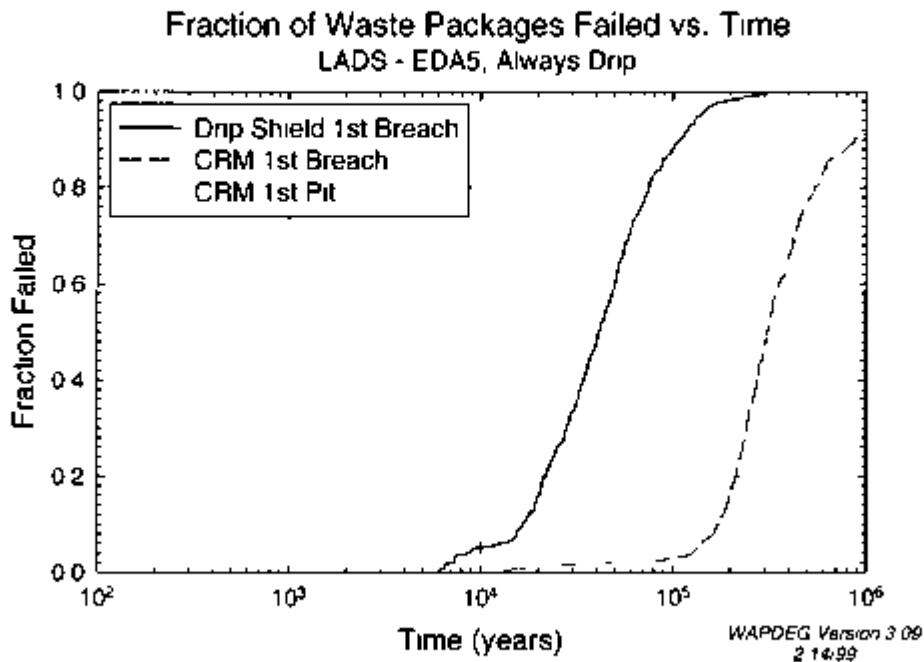
484193.7598
 501209.3776
 521838.3319
 540141.0639
 565697.0904
 592252.8994
 602559.5861
 616622.2449
 634610.4153
 680357.8931
 750093.0178
 813046.0101
 866036.0633
 939155.3300
 1000000.0000

0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0063	12.8466	0.0000
0.0174	11.2807	0.0000
0.0267	8.1860	0.0945
0.0397	5.8505	0.3817
0.0535	4.4879	0.6591
0.0667	3.7355	0.7864
0.0760	3.3942	0.9925
0.0899	3.2691	1.1549
0.1017	5.5181	1.2036
0.1144	2.5300	1.3256
0.1240	2.5120	1.5763
0.1363	2.5301	1.7781
0.1491	2.6489	1.7771
0.1587	3.5950	1.8834
0.1718	2.1391	2.0081
0.1844	3.9053	2.1408
0.1940	1.8865	2.3510
0.2059	2.1491	2.4283
0.2216	2.9444	2.4931
0.2351	1.3294	2.5313
0.2413	1.3317	2.6782
0.2521	1.3287	2.6970
0.2615	1.3385	2.8629
0.2748	1.3919	2.9840
0.2882	1.4401	3.0276
0.3040	2.0726	3.1876
0.3203	1.1163	3.2084
0.3311	1.1176	3.2697
0.3416	1.1784	3.3010
0.3501	1.3353	3.3917
0.3549	1.7680	3.5290
0.3639	1.4627	3.5897
0.3762	0.8639	3.6483
0.3921	0.8576	3.7299
0.4119	0.8436	3.7689
0.4254	0.8346	3.7908
0.4338	0.8413	3.8781
0.4379	0.8620	3.9619
0.4437	0.9153	4.0844
0.4583	1.0202	4.1025
0.4693	1.2465	4.1870
0.4795	2.4871	4.2702
0.4967	0.7399	4.2982
0.5037	0.7644	4.3829

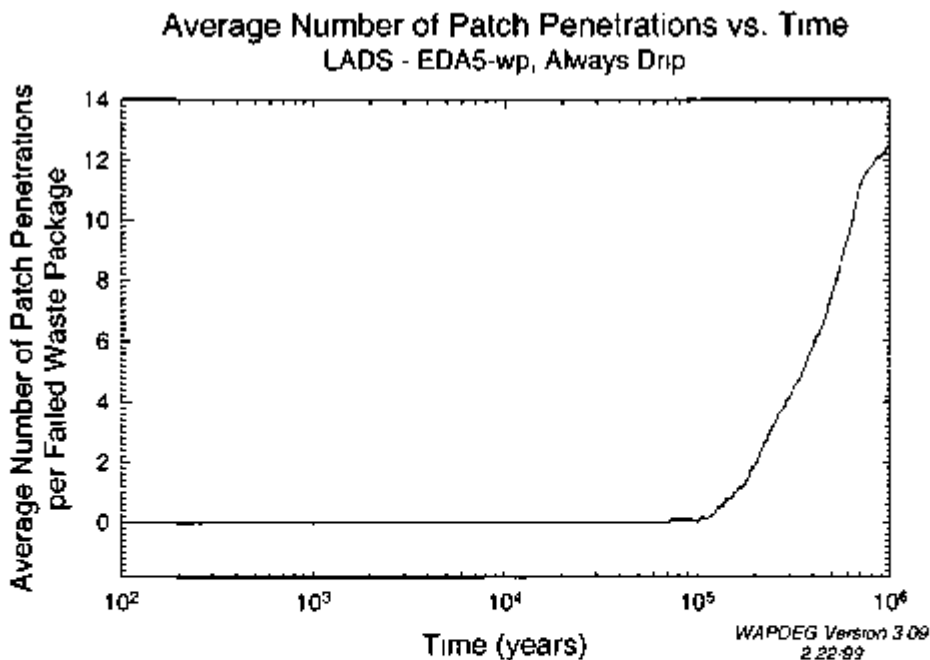
0.5175	0.7752	4.5115
0.5331	0.8347	4.5720
0.5417	0.9553	4.5827
0.5525	1.5776	4.6376
0.5617	1.0727	4.7090
0.5711	0.6391	4.7407
0.5813	0.6480	4.9113
0.5934	0.6572	5.0721
0.6041	0.6622	5.1482
0.6124	0.6953	5.3229
0.6236	0.7776	5.5818
0.6397	0.8520	5.7099
0.6506	1.0333	5.7731
0.6613	1.2507	5.9708
0.6731	1.3532	6.1246
0.6904	1.0651	6.2241
0.7007	0.9170	6.3403
0.7091	1.1888	6.4518
0.7249	2.5830	6.5143
0.7330	1.1503	6.6814
0.7422	1.3642	6.8040
0.7512	1.6411	6.9607
0.7587	1.2503	7.2842
0.7711	1.2606	7.6023
0.7823	0.5894	7.9709
0.7965	0.8563	8.2778
0.8068	1.0954	8.7986
0.8233	0.5981	9.2549
0.8331	0.6602	9.3892
0.8408	0.9167	9.6485
0.8542	1.3783	9.9883
0.8614	0.5974	10.8400
0.8727	0.5649	11.5560
0.8855	0.6120	11.8566
0.8940	0.6775	12.0796
0.9060	0.7712	12.2876
0.9125	0.9726	12.4575

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

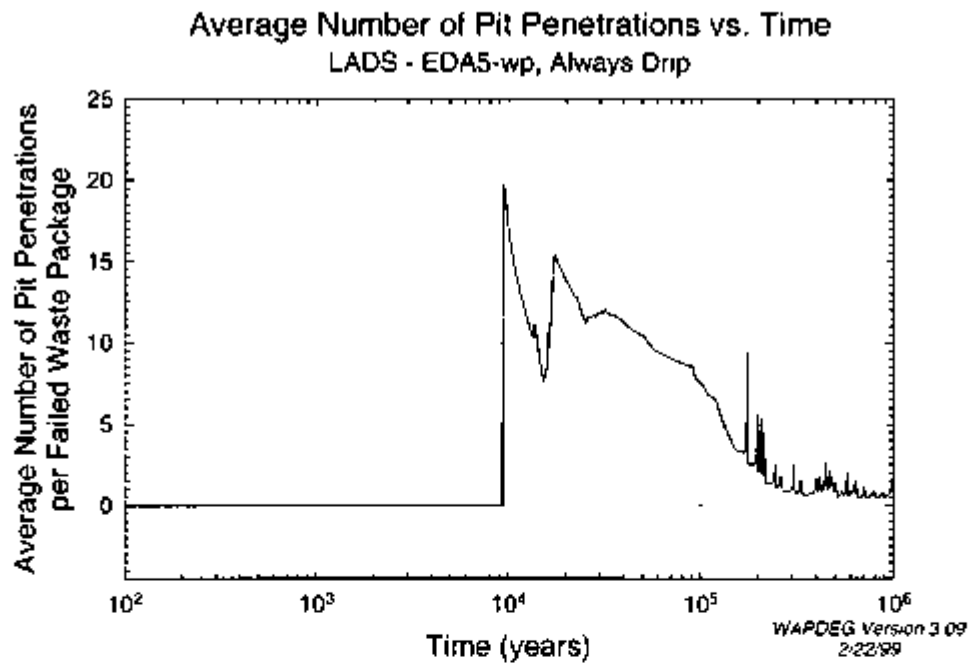
Presented below is a graph (derived from the NE1a5s5EDA5-ds.dat (for the drip shields) and NE1a5s5EDA5-wp.dat (for the waste packages) files) of the first breach (pit or patch) curves for the drip shields and waste packages. Also included is the first pit curve for the waste packages. There is no localized corrosion of the drip shields. Hence the first breach curve of the drip shields is equivalent to their first patch curve.



Presented below is a graph of the average number of patch penetrations per failed waste package (derived from the NE1a5s5EDA5-wp.asc file)



Presented below is a graph of the average number of pit penetrations per failed waste package (derived from the NE1a5s5EDA5-wp.asc file)



The first breach curve for the waste package and the average number of pit and patch penetrations per failed waste package curves are also represented in the RIP input table, NE1a5s5EDA5-wp.rip.

7. REFERENCES

1. Bullard, B. E. 1998. *Alloy 22 Dripping General Corrosion Rate Cumulative Distribution Functions*. Las Vegas, Nevada: CRWMS M&O. DTN: MO9812MWDDSQ37.000.
2. Buscheck, T.A. 1999. *LADS Phase II Multiscale TH Calculation for EDA V*. Livermore, California: Lawrence Livermore National Laboratory. DTN: LL990301804242.083.
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4. CRWMS M&O 1999b. *Design Input Transmittal For Waste Stream Information for LADS, Phase 2, EDAs*. Input Tracking No. PA-WP-99142.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990315.0047.
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8. CRWMS M&O 1999f. *Design Input Request For Performance Assessment (PA) For Enhanced Design Alternative (EDA), Option V*. Input Tracking No. SSR-PA-99117.Ra. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990226.0323.
9. 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.
10. 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.

11. 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.
12. 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.
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15. McCright, R. D. 1998. *Engineered Materials Characterization Report. Volume 3. Revision 1.1 Corrosion Data and Modeling: Update for Viability Assessment*. UCRL-ID-119564. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980806.0177.

8. ATTACHMENTS

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

ATTACHMENT I - MKHISTORY

CONTENTS

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

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 1998b, *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 1998b, *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 1998b, *Software Routine Report for WAPDEG (Version 3.09)*, p. 28).
- 2) prints, to both the screen and an output file, the fractions of the total number of waste packages to which each history is to be applied as well as the products of these fractions with the total number of waste packages, i.e., the number of waste packages to which each history is to be applied.
- 3) creates a columnar file of time, temperature, and relative humidity data for each history file processed for use in graphing the data.

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 1999a, *Supporting Media for RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative V*, \Attachment-1 directory) (DTN: MO9904MWDWAP73.001).

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
# of bin 0 of 9
temperature bin 2 of 2
zone 6 of 6 Center Center (CC)

12 9? PA property set
line load
sand pack(11)
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 = 26330.50 (m^2)

time(years) temp(C)      RH      air      SlUGJID      GW T      GW RH
0 0 18.04                1.000000    0.985620    0.908230    18.039000    0.998080
1 0 16.35                0.978930    0.985570    0.987270    13.580002    0.945950
1 3 17.97                0.954500    0.985570    0.983260    13.610005    0.850510
2 0 17.22                0.972290    0.985570    0.972670    14.699005    0.617240
2 3 18.60                0.972870    0.985570    0.907560    15.7150002    0.365880
3 0 19.84                0.097367    0.985570    0.745310    16.990005    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	0.354503
2 000000	179 220000	0.272293
2 500000	188 600000	0.172873
3 000000	198 940000	0.097367

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

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

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

```

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

```

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

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

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

```

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

```

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

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

```

h001e01      y001e02      b001e03      h002e01      h002e02      f002e03
1 000000      165 350000      0 378930      1 000000      170 040000      0 390000
1 500000      170 970000      0 354510      1 500000      176 780000      0 347130
2 000000      179 220000      0 372290      2 000000      186 340000      0 245050
2 500000      168 600000      0 170870      2 500000      196 470000      0 134700
3 000000      158 940000      0 097360      3 000000      206 950000      0 079440

```

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

3. DESCRIPTION OF TEST CASE

Because Mkhhistory is a very simple program that performs few calculations, relatively simple testing is performed to verify the program execution and results. The testing approach involves comparing the results of executing Mkhhistory with the list-file `mktest.mk` and comparing the results with hand calculations and visual inspection. Execution of the list-file `mktest.mk` and verification of its output by comparison with the files on the accompanying electronic media (CRWMS M&O 1999a, *Supporting Media for RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative V*, \Attachment-Hand directory) (DTN: MO9904MWDWAP73.001) are considered sufficient installation and checkout steps for successful first use of Mkhhistory on a new platform, operating system or new user's location.

3.1 TEST CASE INPUT

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

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

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

4.1 IDENTIFICATION OF LIMITATIONS ON SOFTWARE ROUTINE OR VALIDITY

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

5. REFERENCE LIST OF ALL DOCUMENTATION RELEVANT TO THE QUALIFICATION

CRWMS M&O 1999a. *Supporting Media for RIP Input Tables From WAPDEG For LA Design Selection: Enhanced Design Alternative V*. 210-73r0.exc. Windows self-extracting archive. Las Vegas, Nevada: CRWMS M&O. ACC MOL.19990201.0092. DTN: MO9904MWDWAP73.001.

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.

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), totalfrac
      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
      totalfrac = 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(:), hstyfl(i))
            OPEN (datafid, FILE = datafl(:), 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
                    2005 read(datafid, 2005) frac(i)
                        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
                nrow(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
c     IMPLICIT NONE
c     character line*(*), datafl*(*), hstyfl*(*)
c     integer linesize
c
c Local variables
c
c     integer i, starthst, endhst, startdat, enddat
c
c Find the positions in line where the file names are.
c
c     i = 1
c     do while (line(i:i) .eq. ' ')
c         i = i + 1
c     end do
c     startdat = i
c     do while (line(i:i) .ne. ' ')
c         i = i + 1
c     end do
c     enddat = i - 1
c     do while (line(i: i) .eq. ' ')
c         i = i + 1
c     end do
c     starthst = i
c     do while ((line(i: i) .ne. ' ') .and. (i .le. linesize))
c         i = i + 1
c     end do
c     endhst = i - 1
c     datafl = line(startdat:enddat)
c     hstyfl = line(starthst:endhst)
c     RETURN
c     END      !SUBROUTINE getfilenames
c
c *****
c

```


Attachment II - TITANIUM GRADE 7 GENERAL CORROSION RATES

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

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

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

$$s := 1.7146$$

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

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

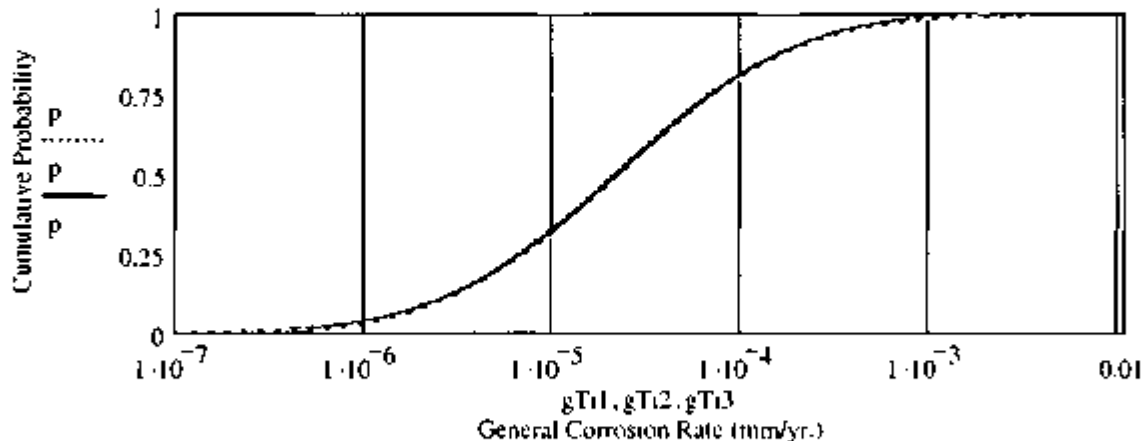
$$p := \frac{\text{cnorm}(z) - \text{cnorm}(-3)}{\text{cnorm}(3) - \text{cnorm}(-3)}$$

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

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

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

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



Range of values:

$$\min(gT11) = 1.2192 \cdot 10^{-7}$$

$$\text{median}(gT12) = 2.1644 \cdot 10^{-5}$$

$$\max(gT13) = 3.9167 \cdot 10^{-3}$$

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.

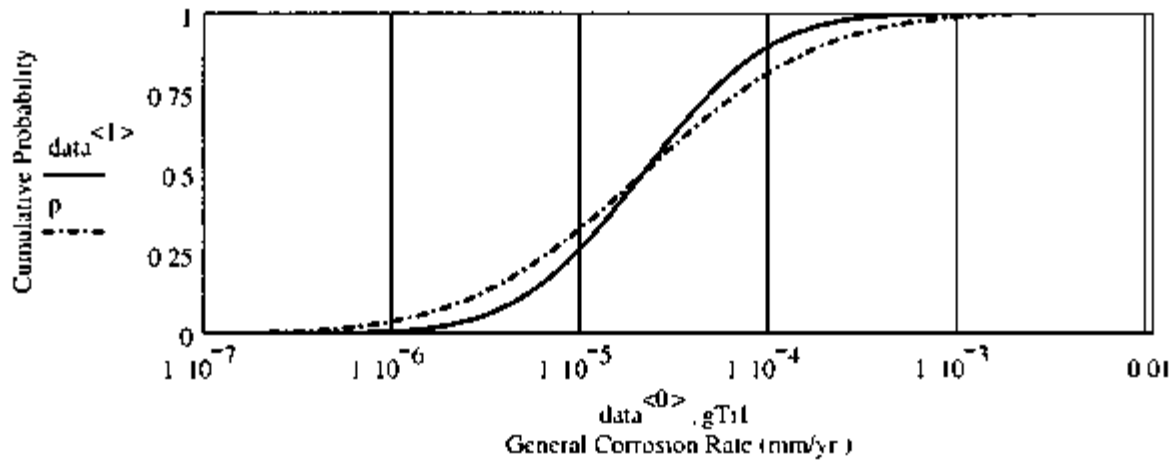
```

slnvar(x, p, wtu, qu) :=
  wtv ← 1 - wtu
  zu ← √wtu · qnorm(qu, 0, 1)
  for i ∈ 0..length(x) - 1
    zi ←
      -∞ if pi = 0
      ∞ if pi = 1
      qnorm pi, 0, 1 otherwise
    ln xi ← ln xi
    zvi ←
      -∞ if pi = 0
      ∞ if pi = 1
      | zu + zi √wtv otherwise
  for i ∈ (0..length(x) - 1)
    xvi ← expi linterp z, ln x, zvi
  augment(xv, p)
  
```

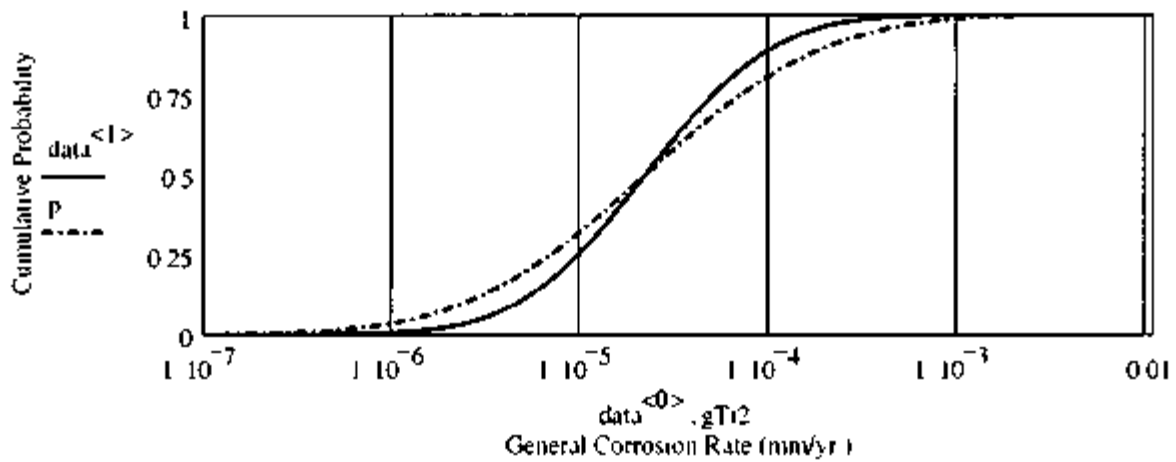
- `wtv` is the fraction of the variance that represents variability
- `zu` is the standard normal score value that corresponds with the given quantile.
- Values of `z` and `ln x` make up the lookup table.
- The probability values zero and one are mapped specifically to remove the appearances of infinity, 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 = "gT115050 cdf"  
data = slnvar(gT11,p,0.50,0.50)  
WRITEPRN(filnam) = (rows(data) cols(data) )  
APPENDPRN(filnam) = data
```



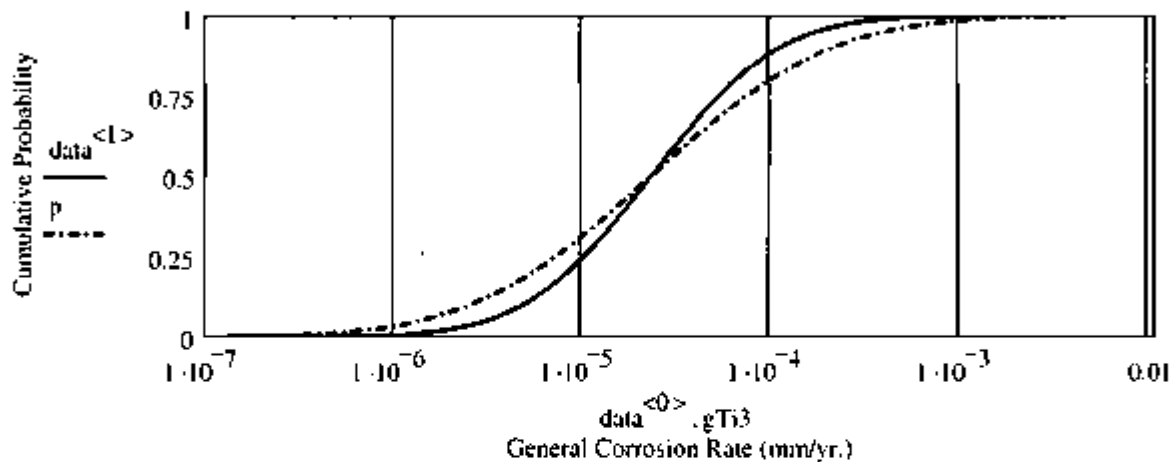
```
filnam = "gT125050 cdf"  
data = slnvar(gT12,p,0.50,0.50)  
WRITEPRN(filnam) = (rows(data) cols(data) )  
APPENDPRN(filnam) = data
```



```

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

```



References

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