OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT ANALYSIS/MODEL COVER SHEET *Complete Only Applicable Items*	1. QA: QA Page: 1 of: 104

2. ☒ **Analysis** — Check all that apply

Type of Analysis:
- ☐ Engineering
- ☒ Performance Assessment
- ☐ Scientific

Intended Use of Analysis:
- ☐ Input to Calculation
- ☒ Input to another Analysis or Model
- ☒ Input to Technical Document
- ☒ Input to other Technical Products

Describe use:

Input to TSPA-SR analysis for waste package and drip shield degradation.

3. ☒ **Model** — Check all that apply

Type of Model:
- ☐ Conceptual Model
- ☒ Abstraction Model
- ☐ Mathematical Model
- ☐ System Model
- ☐ Process Model

Intended Use of Model:
- ☐ Input to Calculation
- ☒ Input to another Model or Analysis
- ☐ Input to Technical Document
- ☒ Input to other Technical Products

Describe use:

Input to TSPA-SR analysis for waste package and drip shield degradation.

4. Title:
WAPDEG Analysis of Waste Package and Drip Shield Degradation

5. Document Identifier (including Rev. No. and Change No., if applicable):
ANL-EBS-PA-000001 REV 00 ICN 01

6. Total Attachments:
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10. Lead/Supervisor	Kevin G. Mon	Kevin Mon	11/9/00
11. Responsible Manager	Robert J. MacKinnon	[illegible] for R. MacKinnon	Nov 9 2000

12. Remarks:

Kevin Mon is responsible for the entire document.
Bryan Bullard and Ahmed Monib made significant contributions to Section 6.

For TSPA-SR.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET
Complete Only Applicable Items

2. Analysis or Model Title:

WAPDEG Analysis of Waste Package and Drip Shield Degradation

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

ANL-EBS-PA-000001 REV 00 ICN 01

4. Revision/Change No.	5. Description of Revision/Change
00	Initial Issue
00 ICN 01	Interim Change to incorporate changes due to the removal of backfill and new/revised upstream inputs Names of Alloy 22 outer barrier lids changed to extended closure lid and flat closure lid. Discusssion added for recommended versus used uncertainty models Section 6.3.

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1. PURPOSE

As directed by a written development plan (CRWMS M&O 1999a), an analysis of the degradation of the drip shield and waste package in the engineered barrier system (EBS) of the Yucca Mountain repository is to be conducted. The purpose of this analysis is to assist the Performance Assessment Department (PAD) and its Engineered Barrier Performance Section in analyzing waste package and drip shield corrosion degradation as a function of exposure time under exposure conditions anticipated in the repository. This analysis will allow PAD to provide a more detailed and complete waste package and drip shield degradation abstraction and to answer the key technical issues (KTI) raised in the Nuclear Regulatory Commission (NRC) Issue Resolution Status Report (IRSR) for the Container Lifetime and Source Term (CLST) Revision 2 (NRC 1999). Comments by the TSPA Peer Review Panel (Budnitz, et al. 1999) were considered. Because the comments were for the Viability Assessment design, none were applicable to the current analysis.

The abstracted models documented in this technical product are potentially important to the evaluation of principle factors for the post-closure safety case, particularly those related to performance of the drip shield and waste package barriers. Therefore, these abstraction models have primary (Level 1) importance. The WAste Package DEGradation (WAPDEG) model is the integrated model used for the analysis (CRWMS M&O 2000a). The abstractions of the process models for the corrosion degradation processes considered in this analysis and the exposure condition parameters for the waste packages and drip shields in the repository were incorporated into the WAPDEG Model. The output from the WAPDEG analysis is a set of profiles for the failure (i.e., initial breach) and subsequent number of penetration openings in the waste package and drip shield as a function of time. In the total system performance assessment (TSPA) analysis, these analysis results are used as input for waste form degradation analysis and radionuclide release analysis from failed waste packages. The WAPDEG Model is used directly in the TSPA for waste package degradation analysis. The analyses presented in this report are for the current potential repository design (CRWMS M&O 2000q). In this design, a drip shield is placed over the waste package and no backfill is emplaced over the drip shield (CRWMS M&O 2000q, Section 2.5 and Figure 2-25).

Two WAPDEG models are discussed in this document: the Current WAPDEG model and the Updated WAPDEG Model. The Updated WAPDEG Model incorporates changes in some models and model parameters due to recently updated inputs (CRWMS M&O 2000h, CRWMS M&O 2000i, and CRWMS M&O 2000u). The changes to models and model parameters are, for the most part, limited to the Stress Corrosion Cracking Abstraction Model and the Manufacturing Defects Abstraction Model.

2. QUALITY ASSURANCE

The Quality Assurance (QA) program applies to the development of this waste package and drip shield degradation analysis documentation. The Performance Assessment Department responsible manager has evaluated the technical document development activity in accordance with QAP-2-0, *Conduct of Activities*. The QAP-2-0 activity evaluation, *Conduct of Performance*

Assessment (CRWMS M&O 1999b), has determined that the preparation and review of this technical document is subject to *Quality Assurance Requirements and Description* (QARD) DOE/RW-0333P (DOE 2000) requirements. Preparation of this analysis did not require the classification of items in accordance with QAP-2-3, *Classification of Permanent Items.* This activity is not a field activity. Therefore, an evaluation in accordance with NLP-2-0, *Determination of Importance Evaluations* was not required. The methods used to control the electronic management of data as required by AP-SV.1Q, *Control of the Electronic Management of Information,* were not specified in the Development Plan, *WAPDEG Analysis of Waste Package and Drip Shield Degradation* (CRWMS M&O 1999a). With regard to the development of this AMR, the control of electronic management of data was evaluated in accordance with YAP-SV.1Q, *Control of the Electronic Management of Data.* The evaluation (CRWMS M&O 2000x) determined that current work processes and procedures are adequate for the control of electronic management of data for this activity. Though YAP-SV.1Q has been replaced by AP-SV.1Q, this evaluation remains in effect.

3. COMPUTER SOFTWARE AND MODEL USAGE

3.1 COMPUTER SOFTWARE

3.1.1 Excel 97 SR-2

Excel 97 SR-2 is a commercially available software used in this analysis. This software, in accordance with AP-SI.1Q, *Software Management*, is appropriate for this application as it offers all of the mathematical and graphical functionality necessary to perform and document the numerical manipulations used in this calculation. Excel 97 SR-2 was executed on a DELL PowerEdge 2200 Workstation equipped with two Pentium II 266 MHz processors (CRWMS M&O tag 112371, located in the Performance Assessment Department, Summerlin Offices, Las Vegas, Nevada) in the Windows NT 4.0 operating system.

3.1.2 WAPDEG 4.0

The WAPDEG software was developed, in accordance with AP-SI.1Q, *Software Management*, to implement the models documented in this analysis. The WAPDEG software is fully qualified and is used in this analyses and models report in accordance with AP-SI.1Q, *Software Management*. The following information is used to identify the WAPDEG software:

Software Name: WAPDEG

Software Version: 4.0

Software Tracking Number: 10000-4.0-00

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, located in the Performance Assessment Department, Summerlin Offices, Las Vegas, Nevada) in the Windows NT 4.0 operating system.

WAPDEG version 4.0 is, in accordance with AP-SI.1Q, *Software Management*, an appropriate tool for this application, because it was specifically designed to calculate drip shield and waste package failure profiles in a manner consistent with the information requirements of the total system performance assessment model. The software was used within its range of validation.

The WAPDEG 4.0 software is used in both the Current and Updated WAPDEG models.

3.1.3 GVP V1.02

Software routine Gaussian Variance Partitioning (GVP) was also developed, in accordance with AP-SI.1Q, *Software Management*, to implement the abstraction results of the variance sharing of stochastic model parameters. This software is appropriate for this application as it was developed to implement the results of the analyses. The simulations using GVP V1.02 were executed on a DELL PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371, located in the Performance Assessment Department, Summerlin Offices, Las Vegas, Nevada) in the Windows NT 4.0 operating system. This software routine was used within its range of validation in accordance with AP-SI.1Q. Details of the software routine verification are presented in a separate Software Routine Report (SRR) (CRWMS M&O 2000r). The GVP software routine is compiled as a windows Dynamic Link Library (DLL) and called by other programs. This routine was developed using Microsoft Developer Studio 97 Visual FORTRAN 5.0, Standard Edition. The GVP software routine is identified as follows:

Name and Version Number: GVP V1.02

SRR Document Identification Number: 10341-SRR-1.02-00

SRR Media Number (if applicable): 10341-PC-1.02-00

This software was obtained from the Software Configuration Manager in accordance with appropriate procedures. The GVP V1.02 software routine is used in both the Current and Updated WAPDEG Models.

3.1.4 MFD V1.01

Software routine ManuFacturing Defects (MFD) was developed, in accordance with AP-SI.1Q, *Software Management*, to implement the abstraction results of the probability of the occurrence and size of manufacturing defects in the closure-lid welds of the Alloy 22 waste package outer barrier. This software routine is appropriate for this application as it was developed to implement the results of the analyses. The simulations using MFD V1.01 were executed on a DELL PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371, located in the Performance Assessment Department, Summerlin Offices, Las Vegas, Nevada) in the Windows NT 4.0 operating system. This software routine was used within its range of validation in accordance with AP-SI.1Q. Details of the software routine verification are presented in a separate Software Routine Report (SRR) (CRWMS M&O 2000s). The MFD software routine is compiled as a windows Dynamic Link Library (DLL) and called by other programs. This routine was developed using Microsoft Developer Studio 97 Visual FORTRAN 5.0, Standard Edition. The MFD software routine is identified as follows:

Name and Version Number: MFD V1.01

SRR Document Identification Number: 10342-SRR-1.01-00

SRR Media Number (if applicable): 10342-PC-1.01-00

This software was obtained from the Software Configuration Manager in accordance with appropriate procedures. This software routine is used to implement the manufacturing defect model used in the Current WAPDEG Model only and is based on a previous version, REV 01, of the *Analysis of Mechanisms for Early Waste Package Failure* AMR (CRWMS M&O 2000o) and its abstraction (CRWMS M&O 2000g).

3.1.5 CWD V1.0

Software routine Closure Weld Defects (CWD) was developed, in accordance with AP-SI.1Q, *Software Management*, to implement the abstraction results of the probability of the occurrence and size of manufacturing defects in the closure-lid welds of the Alloy 22 waste package outer barrier. This software routine is appropriate for this application as it was developed to implement the results of the analyses. The simulations using CWD V1.0 were executed on a DELL PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371, located in the Performance Assessment Department, Summerlin Offices, Las Vegas, Nevada) in the Windows NT 4.0 operating system. This software routine was used within its range of validation in accordance with AP-SI.1Q. Details of the software routine verification are presented in a separate Software Routine Report (SRR) (CRWMS M&O 2000t). The CWD software routine is compiled as a windows Dynamic Link Library (DLL) and called by other programs. This routine was developed using Microsoft Developer Studio 97 Visual FORTRAN 5.0, Standard Edition. The CWD software routine is identified as follows:

Name and Version Number: CWD V1.0

SRR Document Identification Number: 10363-SRR-1.0-00

SRR Media Number (if applicable): 10363-PC-1.0-00

This software was obtained from the Software Configuration Manager in accordance with appropriate procedures. This software routine is used to implement the manufacturing defect model used in the Updated WAPDEG Model only and is based on the current version, REV 02, of the *Analysis of Mechanisms for Early Waste Package Failure* AMR (CRWMS M&O 2000u) and its abstraction (CRWMS M&O 2000i, Section 6.2).

3.1.6 SCCD V2.01

Software routine Stress Corrosion Cracking Dissolution (SCCD) was developed, in accordance with AP-SI.1Q, *Software Management*, to implement the abstraction results of the stress and stress intensity factor profiles in the closure-lid welds of the Alloy 22 waste package outer barrier. This software routine is appropriate for this application as it was developed to implement the results of the analyses. The simulations using SCCD V2.01 were executed on a DELL

PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371, located in the Performance Assessment Department, Summerlin Offices, Las Vegas, Nevada) in the Windows NT 4.0 operating system. This software routine was used within its range of validation in accordance with AP-SI.1Q. Details of the software routine verification are presented in a separate Software Routine Report (SRR) (CRWMS M&O 2000v). The SCCD software routine is compiled as a windows Dynamic Link Library (DLL) and called by other programs. This routine was developed using Microsoft Developer Studio 97 Visual FORTRAN 5.0, Standard Edition. The SCCD software routine is identified as follows:

Name and Version Number: SCCD V2.01

SRR Document Identification Number: 10343-SRR-2.01-00

SRR Media Number (if applicable): 10343-PC-2.01-00

This software was obtained from the Software Configuration Manager in accordance with appropriate procedures. The SCCD V2.01 software routine is used in both the Current and Updated WAPDEG Models.

3.1.7 PREWAP 1.0

Software routine PREWAP was also developed, in accordance with AP-SI.1Q, *Software Management*, to extract the data for the time-history of temperature and relative humidity of drip shields and waste packages, and pH of water contacting the drip shields and waste packages from various source tables. The extracted data are prepared as an output table in a format that is used as input to the WAPDEG code. The PREWAP routine is a stand alone executable that does not operate as a DLL under (TSPA-SR) software. This allows the WAPDEG input to be prepared independent of (TSPA-SR) software reducing run time for TSPA SR realizations. This software routine is appropriate for this application as it was developed to implement the results of the analyses. The simulations using PREWAP 1.0 were executed on a DELL PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371, located in the Performance Assessment Department, Summerlin Offices, Las Vegas, Nevada) in the Windows NT 4.0 operating system. This software routine was used within its range of validation in accordance with AP-SI.1Q. The PREWAP software routine interpolates thermophysical properties (i.e., pH and chloride ion concentration) as a function of repository exposure conditions (such as temperature and relative humidity). The thermophysical property input tables used for the PREWAP software do not cover the entire space of repository exposure conditions over which they are used. The PREWAP software routine uses bounding values when this situation is encountered. The use of bounding values has no impact on the results of this AMR because no models used in this analysis are chemistry dependent, with the exception of the localized corrosion initiation model used for the Alloy 22 waste package outer barrier (see Sections 4.1.5 and 6.4.10), which uses exposure pH. However, the localized corrosion initiation model used for the Alloy 22 waste package outer barrier does not allow for localized corrosion initiation at any pH (based on the $\pm 4\sigma$ confidence interval, see Figure 1). Therefore, the use of bounding values in the PREWAP software routine has no impact on the results of this AMR. Details of the software routine verification are presented in Attachment I. This routine was developed using Microsoft Developer Studio 97 Visual FORTRAN 6.0, Professional Edition. The PREWAP software routine is identified as follows:

Name and Version Number: PREWAP version 1.0

SRR Document Identification Number: N/A

SRR Media Number (if applicable): N/A

The PREWAP 1.0 software routine is used to prepare input for both the Current and Updated WAPDEG Models.

3.1.8 GoldSim 6.04.007

The GoldSim software (Golder Associates 2000) is used to implement the total system performance assessment model. The software was used to run the WAPDEG Model and implement other component models that are documented in this analysis. The GoldSim software was used to pass input to the WAPDEG software. The simulations using GoldSim 6.04.007 were executed on a DELL PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371, located in the Performance Assessment Department, Summerlin Offices, Las Vegas, Nevada) in the Windows NT 4.0 operating system. This software routine was used within its range of validation in accordance with AP-SI.1Q. The following information is used to identify the GoldSim software:

Software Name: GoldSim

Software Version: 6.04.007

Software Tracking Number: 10344-6.04.007-00

This software was obtained from the Software Configuration Manager in accordance with AP-SI.1Q, *Software Management*. The GoldSim software was executed on a DELL PowerEdge 2200 Workstation equipped with Dual (2) Pentium II 266 MHz processors (CRWMS M&O tag 112371, located in the Performance Assessment Department, Summerlin Offices, Las Vegas, Nevada) in the Windows NT 4.0 operating system.

GoldSim version 6.04.007 is an appropriate tool for this application, because it has the capabilities to interface with external software routines and was specifically configured to call WAPDEG 4.0. The GoldSim code was used within the range of values for which it was validated.

The GoldSim software is used in both the Current and Updated WAPDEG Models.

3.2 MODELS USED

The WAPDEG Model is documented in this report. The WAPDEG Model is composed of the WAPDEG code (see Section 3.1.2) and a number of sub-models (abstractions of process level models), which are implemented within the WAPDEG code. In this Section, the submodels which are documented in other Analyses and Models Reports are discussed.

3.2.1 Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model

This model is discussed in Sections 4.1.5 and 6.4.10. The localized corrosion initiation model used for the Alloy 22 waste package outer barrier is developed, documented, and validated in the Analyses and Models Report entitled *Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier* (CRWMS M&O 2000d) (DTN: MO0003SPAPCC03.004).

This model is implemented within the WAPDEG software (see Section 3.1.2) and is appropriate for its intended use because it was specifically developed for modeling the criterion for localized corrosion initiation and rate of propagation on the Alloy 22 waste package outer barrier. The localized corrosion initiation portion of the Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model was used within its range of validation (see CRWMS M&O 2000d and Sections 4.1.5 and 6.4.10). However, as discussed in Section 3.1.7, the PREWAP subroutine does make use of bounding pH values in the preparation of the input for the Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model. The localized corrosion rate portion of the Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model is validated by the observation, in Section 5.4, that the localized corrosion rate data is a conservative representation of localized corrosion rate of Alloy 22. This observation provides confidence in the adequacy of the localized corrosion rate model and that it is appropriate for its intended use.

The Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model is used in both the Current and Updated WAPDEG Models.

3.2.2 Manufacturing Defect Abstraction Model

This model is discussed in Sections 4.1.7 and 6.4.11. All of the data and parameters used in this model are documented in the AMR entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i) and are tracked by DTN: MO0010SPASUP04.011.

For the Current WAPDEG Model, this model is implemented partly within the WAPDEG software (see Section 3.1.2) and partly within the MFD software routine (see Section 3.1.4) (CRWMS M&O 2000s). In the Updated WAPDEG model, the Manufacturing Defect Abstraction Model is implemented partly within the WAPDEG software and partly within the CWD software routine (see Section 3.1.5) (CRWMS M&O 2000t). The Manufacturing Defect Abstraction Model is developed, documented, and validated in the Analyses and Models Report entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i). Further discussion related to model validation is presented in Section 6.4.11. The Manufacturing Defect Abstraction Model was used within its range of validation. The Manufacturing Defect Abstraction Model is appropriate for its intended use, because it was specifically developed for modeling the occurrence of manufacturing defects in the Alloy 22 waste package outer barrier extended and flat closure lid weld regions.

The Manufacturing Defect Abstraction Model is used in both the Current and Updated WAPDEG Models.

3.2.3 Stress and Stress Intensity Factor Profile Abstraction Model

This model is discussed in Sections 4.1.8 and 6.4.12. All of the data and parameters used in this model are documented in the AMR entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i) and are tracked by DTN: MO0010MWDSUP04.010.

This model is implemented within the SCCD software routine (CRWMS M&O 2000v). The Stress and Stress Intensity Factor Profile Abstraction Model is validated in the Analyses and Models Report entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i). Further discussion related to model validation is presented in Section 6.4.12. The Stress and Stress Intensity Factor Profile Abstraction Model was used within its range of validation. The Stress and Stress Intensity Factor Profile Abstraction Model is appropriate for its intended use, because it was specifically developed for modeling the stress and stress intensity factor profiles in the Alloy 22 waste package extended and flat closure lid weld regions.

The Stress and Stress Intensity Factor Profile Abstraction Model is used in both the Current and Updated WAPDEG Models.

3.2.4 Slip Dissolution Abstraction Model

This model is discussed in Sections 4.1.9 and 6.4.13. All of the data and parameters used in this model are documented in the AMR entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i) and are tracked by DTN: MO0010MWDSUP04.010.

This model is implemented partly within the WAPDEG software (see Section 3.1.2) and partly within the SCCD software routine (see Section 3.1.6) (CRWMS M&O 2000v). The Slip Dissolution Abstraction Model is validated in the Analyses and Models Report entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i). Further discussion related to model validation is presented in Section 6.4.13. The Slip Dissolution Abstraction Model was used within its range of validation. The Slip Dissolution Abstraction Model is appropriate for its intended use, because it was specifically developed for modeling the slip dissolution stress corrosion cracking process in the Alloy 22 waste package outer barrier extended and flat closure lid weld regions.

The Slip Dissolution Abstraction Model is used in both the Current and Updated WAPDEG Models.

4. INPUTS

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

4.1 DATA AND PARAMETERS

4.1.1 Waste Package and Drip Shield Design Input

Waste package and drip shield dimensions were obtained and are presented in Table 1.

Table 1. Waste Package and Drip Shield Dimensions.

Parameter Name	Parameter Value	Source
Waste Package Outer Barrier (Shell) Outer Diameter (OD)	1564 mm	CRWMS M&O 2000p Attachment I Page 1 of 2
Waste Package Inner Barrier Length	4775 mm	CRWMS M&O 2000p Attachment I Page 1 of 2
Waste Package Outer Barrier Thickness	20 mm	CRWMS M&O 2000p Attachment I Page 2 of 2
Drip Shield Height	2521 mm	CRWMS M&O 2000w Attachment II Page II-1
Drip Shield Width	2512 mm	CRWMS M&O 2000w Attachment II Page II-1
Drip Shield Thickness	15 mm	CRWMS M&O 2000w Attachment II Page II-1

These inputs are used to calculate the total surface areas of the waste package barriers or drip shield. These surface areas are discussed further in Section 5.1. The technical product output information listed in Table 1 were obtained from controlled and confirmed sources and thus do not require data tracking numbers.

4.1.2 Relative Humidity Threshold Abstraction Model

The critical relative humidity (RH) threshold for the initiation of corrosion degradation (general corrosion, localized corrosion and stress corrosion cracking processes) is a function of exposure temperature. The relationship between the critical threshold RH and exposure temperature is based on the assumption (Section 5.2) of the presence of a sodium nitrate ($NaNO_3$) salt film on the waste package and drip shield surface and the deliquescence point of the salt as documented in the Analyses and Models Report entitled *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier* (CRWMS M&O 2000b, Section 6.4.1 and Table 8) (also see Data Tracking Number (DTN): LL991212305924.108). The RH threshold used is contained in a file named WDRHcrit.fil which is listed in Section 6.4.8.1. This data is considered accepted data.

4.1.3 Drip Shield General Corrosion Abstraction Model

Details of the general corrosion rate distribution used for the Titanium Grade 7 drip shield (WDgTi7Sr00.cdf) are given in a calculation entitled *Calculation of General Corrosion Rate of*

Drip Shield and Waste Package Outer Barrier to Support WAPDEG Analysis (CRWMS M&O 2000c) and is tracked with DTN: MO0010SPASIL02.002. This data is qualified. In the calculation, experimentally measured general corrosion rates of Titanium Grade 7 (CRWMS M&O 2000f, Section 6.5.2, DTN: LL990610605924.079) are sorted in ascending order and assigned cumulative probability values. The general corrosion rates were then corrected for the effects of silica deposition (CRWMS M&O 2000e, Section 6.5.5) resulting in the general corrosion rate distribution (WDgTi7SR00.cdf) used in the model. Also see Section 6.4.5 for discussion of implementation.

4.1.4 Waste Package Outer Barrier General Corrosion Abstraction Model

Details of the primary general corrosion rate distribution used for the Alloy 22 waste package outer barrier (WDgA22SR00.cdf) are given in a calculation entitled *Calculation of General Corrosion Rate of Drip Shield and Waste Package Outer Barrier to Support WAPDEG Analysis* (CRWMS M&O 2000c) and is tracked with DTN: MO0010SPASIL02.002. This data is qualified. In that calculation, experimentally measured general corrosion rates of Alloy 22 (CRWMS M&O 2000e, Section 6.5.2, DTN: LL990610605924.079, LL000112205924.112) are sorted in ascending order and assigned cumulative probability values. The general corrosion rates were then corrected for the effects of silica deposition (CRWMS M&O 2000e, Section 6.5.5) resulting in the general corrosion rate distribution (WDgA22SR00.cdf) used in the model. Also see Section 6.4.6 for discussion of implementation.

4.1.5 Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model

The localized corrosion initiation model used for the Alloy 22 waste package outer barrier and associated model parameters are discussed in the Analysis Model Report entitled *Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier* (CRWMS M&O 2000d, Section 6.3.1). In summary, the localized corrosion initiation threshold is based on potentiodynamic polarization data for Alloy 22 measured in several repository-relevant solution compositions. The data consisted of measurements of the critical potential for localized corrosion initiation, *Ecrit1*, and the corrosion potential, *Ecorr*, at various temperatures, chloride concentrations and *pH* values. The potential difference $\Delta E = (Ecrit1 - Ecorr)$ (in mV) was fit to a function of *pH* (the dependence of the potential difference on temperature and chloride concentration was negligible)

$$\Delta E = c_0 + c_1 \cdot pH + c_2 \cdot pH^2 + \varepsilon \qquad \text{(Eq. 1)}$$

where c_o, c_1, and c_2 are constants determined from fitting to Equation 1 to the collected potential difference data. ε (referred to as the "error" variance or "residual" variance) is a term representing data variance not explained by the fitting procedure and has a normal distribution with a mean of zero. Linear regression gives the following estimates for the parameters in Equation 3: $c_o = 1160$, $c_1 = -193$ and $c_2 = 12.0$. The covariance matrix (s) and correlation matrix (C) resulting from the fitting procedure were determined to be:

$$s=\begin{bmatrix} 3530 & -1040 & 64.4 \\ -1040 & 364 & -24.4 \\ 64.4 & -24.4 & 1.69 \end{bmatrix} \qquad C=\begin{bmatrix} 1 & -0.915 & 0.835 \\ -0.915 & 1 & -0.982 \\ 0.835 & -0.982 & 1 \end{bmatrix} \qquad \text{(Eq. 2)}$$

and the variance of ε determined from the linear regression fitting procedure is *4670.*

Figure 1 shows a plot of how the median potential difference (ΔE) given by Equation 1 varies with *pH*. Also shown are the $\pm 3\sigma$ and $\pm 4\sigma$ confidence intervals. These inputs are tracked by DTN: MO0003SPAPCC03.004 and are qualified.

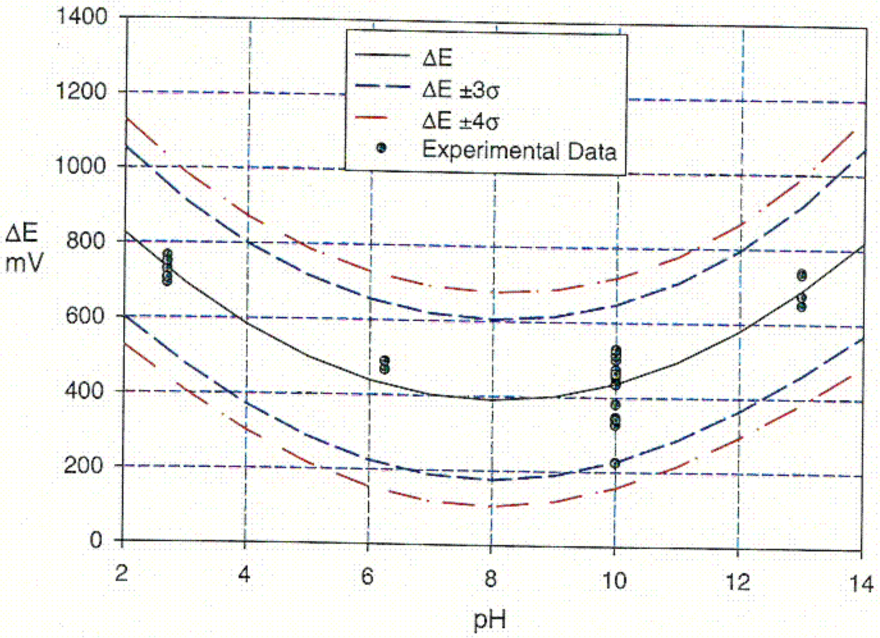

Figure 1. Plot of *ΔE* vs. *pH* for Alloy 22 from Equation 1 and 2 showing the $\pm 3\sigma$ and $\pm 4\sigma$ confidence intervals and the experimental data from which the model was derived.

The distribution of localized corrosion rates presented in Table 22 of the AMR entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.6.6) will be used for localized corrosion modeling of the Alloy 22 waste package outer barrier. These rates are reproduced in Table 2 (with rates converted from µm/yr to mm/yr). The localized corrosion rates are assumed to be loguniformly distributed (see Section 5.4).

Table 2. Distribution of Localized Corrosion Rates for Alloy 22 (DTN: LL991213705924.109).

Percentile (%)	Localized Corrosion Rate (mm/yr)
0th	12.7E-3
50th	127E-3
100th	1270E-3

C01

These data are tracked by DTN: LL991213705924.109 these data are considered to be conservative bounding values to the Alloy 22 localized corrosion rates (see Section 5.4) and thus are considered verified.

4.1.6 Drip Shield Localized Corrosion Initiation Threshold and Rate Abstraction Models

The localized corrosion initiation model used for the Titanium Grade 7 drip shield and model parameters are discussed in the Analyses and Models Report entitled *Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier* (CRWMS M&O 2000d, Section 6.4.1). In summary, the localized corrosion initiation threshold is based on potentiodynamic polarization data for Titanium Grade 7 measured in several repository-relevant solution compositions. The data consisted of measurements of the critical potential for localized corrosion initiation, *Ecrit1*, and the corrosion potential, *Ecorr*, at various temperatures, chloride concentrations and *pH* values. The potential difference $\Delta E = (Ecrit1 - Ecorr)$ (in mV) was fit to a function of *pH* (the dependence of the potential difference on temperature and chloride concentration was negligible).

$$\Delta E = f_0 + f_1 \cdot pH + \varepsilon \qquad \text{(Eq. 3)}$$

where f_0, and f_1 are constants determined from fitting to Equation 3 to the collected potential difference data. ε (referred to as the "error" variance or "residual" variance) is a term representing data variance not explained by the fitting procedure and has a normal distribution with a mean of zero. Linear regression gives the following estimates for the parameters in Equation 3: $f_0 = 1670$ and $f_1 = -52.2$. The covariance matrix (s) and correlation matrix (C) resulting from the fitting procedure were determined to be:

$$s = \begin{bmatrix} 2040 & -230 \\ -230 & 31.9 \end{bmatrix} \quad C = \begin{bmatrix} 1 & -0.904 \\ -0.904 & 1 \end{bmatrix} \qquad \text{(Eq. 4)}$$

and the variance of ε determined from the linear regression fitting procedure is *1080*.

Figure 2 shows a plot of how the median potential difference (ΔE) given by Equation 3 varies with *pH*. Also shown are the $\pm 3\sigma$ and $\pm 4\sigma$ confidence intervals. These inputs are tracked by DTN: MO0003SPAPCC03.004 and are qualified.

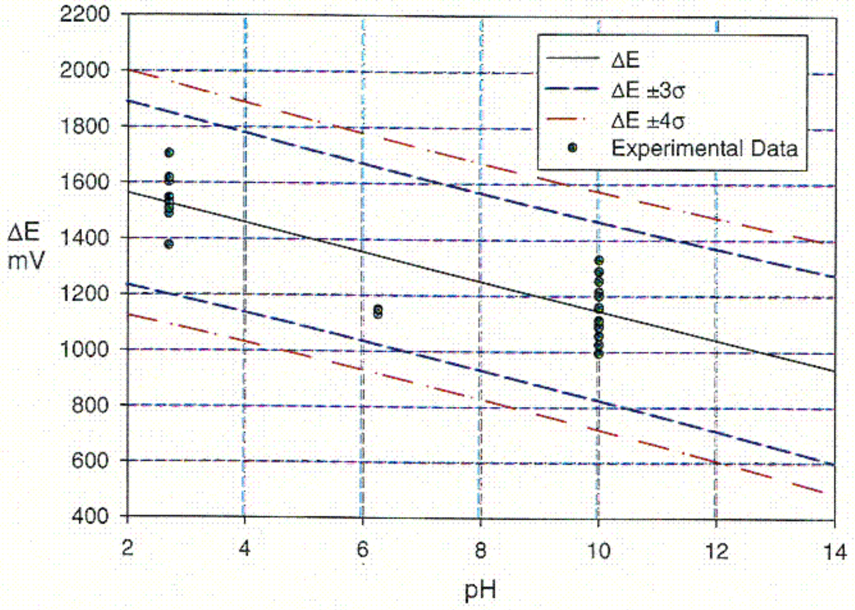

Figure 2. Plot of *ΔE* vs. *pH* for Titanium Grade 7 from Equation 3 and 4 showing the ±3σ and ±4σ confidence intervals and the experimental data from which the model was derived.

The distribution of localized corrosion rates presented in Table 16 of the AMR entitled *General Corrosion and Localized Corrosion of the Drip Shield* (CRWMS M&O 2000f, Section 6.7) will be used for localized corrosion modeling of the Titanium Grade 7 drip shield. These rates are reproduced in Table 3 (with rates converted from μm/yr to mm/yr).

Table 3. Distribution of Localized Corrosion Rates for Titanium Grade 7.

Percentile (%)	Localized Corrosion Rate (mm/yr)
0th	490E-3
100th	1120E-3

The localized corrosion rates are uniformly (or rectangularly) distributed between the bounds specified in Table 3 (CRWMS M&O 2000f, Section 6.7, paragraph 4). These data are tracked by DTN: LL981212005924.062, these data are considered to be conservative bounding values to the Titanium Grade 7 localized corrosion rates (see Section 5.3) and thus are considered verified.

4.1.7 Manufacturing Defect Abstraction Model

Table 4 lists the inputs to the Current WAPDEG Model manufacturing defects abstraction analysis for the Alloy 22 waste package outer barrier (or outer shell) closure-lid welds. In this analysis, the waste package outer shell extended closure lid shall be referred to simply as the extended closure lid and the waste package outer shell flat closure lid shall be referred to as the flat closure lid.

C02

Table 4. Manufacturing Defect Abstraction Model Data and Parameters Used in the Current WAPDEG Model and Their Sources

Parameter Name	Parameter Value	Source
Lid Thickness	25 mm Alloy 22 for extended closure lid 10 mm Alloy 22 for flat closure lid	CRWMS M&O 2000p Attachment I Page 2 of 2
Lid Radius	0.76 m for both lids	CRWMS M&O 2000g Section 5
b, Location Parameter for Probability of Non-Detection	Uniform over the range (1.6, 5.0) mm	CRWMS M&O 2000g DTN: MO0001SPASUP03.001
v, the scale parameter of the non-detection probability	Uniform over the range (1, 3)	CRWMS M&O 2000g DTN: MO0001SPASUP03.001
ψ, the fraction of flaws considered	Uniform over the range (0.3481, 0.3632)	CRWMS M&O 2000i, Section 6.2.1 DTN: MO0010SPASUP04.011

Table 5 lists the inputs to the Updated WAPDEG Model manufacturing defects abstraction analysis for the Alloy 22 waste package outer barrier closure-lid welds.

Table 5. Manufacturing Defect Abstraction Model Data and Parameters used in the Updated WAPDEG Model and Their Sources

Parameter Name	Parameter Value	Source
Lid Thickness	25 mm Alloy 22 for extended closure lid 10 mm Alloy 22 for flat closure lid	CRWMS M&O 2000p Attachment I Page 2 of 2
Lid Radius	770.5 mm for extended closure lid 763.5 mm for flat closure lid	CRWMS M&O 2000p Attachment I Page 1 of 2
b, Location Parameter for Probability of Non-Detection	Uniform over the range (2.5, 5.0) mm	CRWMS M&O 2000i, Section 6.2.1 DTN: MO0010SPASUP04.011
v, the scale parameter of the non-detection probability	Uniform over the range (1, 3)	CRWMS M&O 2000i, Section 6.2.1 DTN: MO0010SPASUP04.011
ψ, the fraction of considered flaws	Uniform over the range (0.3481, 0.3632)	CRWMS M&O 2000i, Section 6.2.1 DTN: MO0010SPASUP04.011
F_{OS}, fraction of outer surface-breaking flaws	Uniform over the range (0.0013, 0.0049)	CRWMS M&O 2000i, Section 6.2.1 DTN: MO0010SPASUP04.011

The technical product output information listed in Table 4 and Table 5 (lid thicknesses and radii) were obtained from controlled and confirmed sources and thus do not require data tracking numbers. The DTNs quoted in Table 4 and Table 5 (DTN: MO0001SPASUP03.001 and MO0010SPASUP04.011) are technical product output information developed using qualified methods per AP-3.10Q and obtained from controlled and confirmed sources. Any changes to this document that may occur, as a result of completing the confirmation activities, will be reflected in subsequent revisions. The status of the input information quality may be confirmed by review of the Document Input Reference System database.

4.1.8 Stress and Stress Intensity Factor Profile Abstraction Model (Waste Package Closure-Lid Welds)

Data and parameters that are input to this analysis include stress and stress intensity factor profiles (stress or stress intensity factor versus depth) and model parameters appropriate for both the extended closure and flat closure lids of the waste package outer barrier. Table 6 summarizes these data, their sources, data tracking numbers (DTNs), and Table numbers.

Table 6. Stress and Stress Intensity Factor Profile Data and Parameters and Their Sources

Parameter Name	Parameter Value	Source
Stress Intensity Factor Profiles	Table 7	CRWMS M&O 2000i DTN: MO0010MWDSUP04.010
Stress Profile Coefficients	Table 8, Table 9	CRWMS M&O 2000i DTN: MO0010MWDSUP04.010
Yield Strength	Table 10	CRWMS M&O 2000i DTN: MO0010MWDSUP04.010
Fraction of Yield Strength	Table 10	CRWMS M&O 2000i DTN: MO0010MWDSUP04.010

This data is qualified.

Table 7. Stress Intensity Factor (K_I) Vs. Depth Tables for the Extended And Flat Closure-Lids of Waste Package Outer Barrier.

Extended Closure Lid		Flat Closure Lid	
KI ($MPa \cdot m^{1/2}$)	**Depth (mm)**	**KI ($MPa \cdot m^{1/2}$)**	**Depth (mm)**
-8.096912553	0.3988	-7.201806034	0.3277
-11.08864448	0.8001	-10.05117186	0.6579
-13.12743778	1.1989	-12.14661052	0.9855
-14.62395207	1.6002	-13.83718048	1.3132
-15.74125563	1.9990	-15.26051182	1.6408
-16.56494834	2.4003	-16.48813922	1.971
-17.16634511	2.7991	-17.60873931	2.2987
-17.5702798	3.2004	-18.62418012	2.6264
-17.79521296	3.5992	-19.34568044	2.954
-17.85960516	3.9980	-18.27353932	3.2842
-17.77785124	4.3993	-17.05876838	3.6119
-17.56148906	4.7981	-15.73543176	3.9395
-17.22755067	5.1994	-14.40693057	4.2697
-16.78515648	5.5982	-13.09502192	4.5974
-16.23441637	5.9995	-11.74410433	4.9251
-15.58159374	6.3983	-10.37129779	5.2527
-14.83251247	6.7970	-8.992063026	5.5829
-13.99233711	7.1984	-7.619959749	5.9106
-13.06249616	7.5971	-6.28349195	6.2382
-12.03771518	7.9985	-5.021547684	6.5659
-10.93137807	8.3972	-3.791766552	6.8961
-9.747286832	8.7986	-2.602642611	7.2238
-8.489320377	9.1973	-1.461856773	7.5514
-7.161148843	9.5987	-0.376262524	7.8791
-5.7664094	9.9974	0.6479086	8.2093
-4.327309665	10.3962	1.602739435	8.5369
-2.830795383	10.7975	2.489890331	8.8646
-1.280437794	11.1963	3.304704392	9.1948
0.320255595	11.5976	4.043027992	9.5225
1.967753102	11.9964	4.701256926	9.8501
3.658542826	12.3977	5.276226526	10.1778
5.415098304	12.7965	5.809253288	10.508
7.218783158	13.1978	6.267459831	10.8356
9.05768593	13.5966	6.633989902	11.1633
10.92825736	13.9954	6.907239191	11.491
12.82690422	14.3967	7.086141819	11.8212
14.74987947	14.7955	7.170016506	12.1488
16.73175271	15.1968	7.171796631	12.4765
18.7698867	15.5956	7.082153019	12.8067
20.82285508	15.9969	6.8851964	13.1343
22.88648224	16.3957	6.581695963	13.462
24.95692222	16.7945	6.173014275	13.7897
27.03021919	17.1958	5.661052333	14.1199
29.13461342	17.5946	5.214086954	14.4475
31.33328838	17.9959	5.185517036	14.7752
33.52559005	18.3947	5.092620849	15.1028
35.70701317	18.7960	4.940639873	15.433
37.87294261	19.1948	4.735255128	15.7607
40.01865333	19.5961	4.482741007	16.0884
42.13953021	19.9949	4.18995429	16.4186

Stress (σ_s in MPa) as a function of depth (x in mm) is given by a third order polynomial equation of the form (CRWMS M&O 2000h, Section 6.2.2.2):

$$\sigma_s(x) = A_0 + A_1 \cdot x + A_2 \cdot x^2 + A_3 \cdot x^3 \qquad \text{(Eq. 5)}$$

where the values of the coefficients (A_i's) used in the Current WAPDEG Model are given in Table 8.

Table 8. Stress Coefficients Used in the Current WAPDEG Model for the Extended and Flat Closure Lids of Waste Package Outer Barrier in Metric Units (i.e., Stress in MPa).

Coefficient	Extended Closure Lid	Flat Closure Lid
A_0	-356.26778	-437.720543
A_1	37.180767	176.967239
A_2	1.436391	-15.606072
A_3	-0.065282	0.367099

The values of the coefficients (A_i's) used in the Updated WAPDEG Model are given in Table 9

Table 9. Stress Coefficients Used in the Updated WAPDEG Model for the Extended and Flat Closure Lids of Waste Package Outer Barrier in Metric Units (i.e., Stress in MPa).

Coefficient	Extended Closure Lid	Flat Closure Lid
A_0	-356.30449	-437.720543
A_1	37.188256	176.967239
A_2	1.435966	-15.606072
A_3	-0.065277	0.367099

Note that the Current and Updated WAPDEG Model stress coefficients differ only for the extended closure lid.

The provided hoop stress state was determined to vary with angle (θ) around the circumference of the Alloy 22 waste package extended and flat closure-lid welds ($\theta = 0$ point arbitrarily chosen) according to the following functional form (CRWMS M&O 2000h, Section 6.2.2.5 and CRWMS M&O 2000i, Section 6.3.1):

$$\sigma_t(x,\theta) = \sigma_s(x) - (17.236892) \cdot (1 - \cos(\theta)) \qquad \text{(Eq. 6)}$$

Note that σ_s (defined in Equation 5) uses the stress coefficients (A_i) defined in Table 8 or Table 9 with x in units of mm. Based on the angular stress variation in Equation 6, the stress intensity factor variation with angle is given by (CRWMS M&O 2000h, Section 6.2.2.5 and CRWMS M&O 2000i, Section 6.3.1):

$$K_t(x,\theta) = K_s(x) \cdot \left(\frac{\sigma_t(Thck,\theta)}{\sigma_t(Thck,0)} \right) \qquad \text{(Eq. 7)}$$

where *Thck* is the lid thickness and $K_s(x)$ is given by the values in Table 7.

The uncertainty in the stress state and stress intensity factor is introduced through a scaling factor, $sz(z)$. The functional form of the scaling factor (CRWMS M&O 2000i, Section 6.3.1) is shown in Equation 8.

$$sz(z) = \left(\frac{z \cdot YS \cdot F}{3} \right) \quad \text{(Eq. 8)}$$

YS is the yield strength, F is the yield strength scaling factor (a constant), and z is the magnitude of the uncertainty variation from the mean profile (sampled from a distribution). The yield strength scaling factor, F, defines the maximum uncertainty variation possible (the bounds). The yield strength, uncertainty scaling factors, and distribution for z used for the two lids are given in Table 10.

Table 10. Yield Strength and Fraction of Yield Strength for the Extended and Flat Closure Lids of Waste Package Outer Barrier.

Parameter	Value
Yield Strength (*YS*)	322.3 MPa
Yield Strength Scaling Factor (*F*)	0.05 - Optimum 0.10 - Realistic 0.30 - Conservative
Uncertainty variation, *z*	Triangular between ±3 with a mode of 0

Note that three different values of the yield strength scaling factor, F, are considered in this analysis (CRWMS M&O 2000h, Section 5 Assumption 3 and Section 6.2.2). The stress uncertainty range of ±5% (yield strength scaling factor of 0.05) is used to represent the optimum case that is achievable through stringent control of such processes as welding, stress mitigation, material variability, and other fabrication steps. The stress uncertainty range of ±10% (yield strength scaling factor of 0.10) is used to represent the realistic case that is achievable through appropriate levels of process controls. The stress uncertainty range of ±30% (yield strength scaling factor of 0.30) is used to represent the worst-case that might result from inadequate control of the processes (CRWMS M&O 2000h, Section 6.2.2).

The stress relation, accounting for uncertainty, is given by

$$\sigma(x,\theta,z) = \sigma_t(x,\theta) + sz(z) \quad \text{(Eq. 9)}$$

and the stress intensity factor relation is given by

$$K(x,\theta,z) = K_s(x)\frac{\sigma_t(Thck,\theta)}{\sigma_t(Thck,0)} + 0.058534 \cdot sz(z) \cdot \sqrt{\pi \cdot x} \quad \text{(Eq. 10)}$$

This formulation corresponds to Uncertainty Model 2 in the upstream abstraction Analyses and Models Report entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i, Section 6.3.1).

The elicited radial crack path for the extended closure lid (driven by the hoop stress) is in a direction normal to the outer surface (CRWMS M&O 2000h), thus, the crack length corresponds to the crack depth for the extended closure lid. However, the elicited crack path for the flat closure lid is at an angle to the normal of the lid surface (CRWMS M&O 2000h, p. I-60 and I-61), and the depth of the crack with respect to the surface is determined by projecting the crack length onto the lid surface normal. The angle of projection (about 37.5 degrees) was estimated from the length of the hoop stress plane and the thickness of the flat closure lid (see CRWMS M&O 2000h, Figure AI-1). Thus the *sine* of the angle (0.60887312121) multiplied by the crack length results in the crack depth with respect to the flat closure lid surface (i.e., in a direction normal to the flat closure lid outer surface).

All of the data and parameters discussed in this section were documented in the AMR entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i) and are tracked by DTN: MO0010MWDSUP04.010.

4.1.9 Slip Dissolution Abstraction Model

The Slip Dissolution Model for stress corrosion cracking requires a threshold stress, an incipient crack density, and crack growth rate model parameters. These data and their sources for the Current WAPDEG Model are listed in Table 11.

Table 11. Slip Dissolution Model Parameters Used in Current WAPDEG Model and Their Sources

Parameter Name	Parameter Value	Source
Threshold Stress	Uniform over the range (0.2, 0.3) fraction of the Yield Strength	CRWMS M&O 2000i DTN: MO0010MWDSUP04.010
Incipient crack size	0.05 mm	CRWMS M&O 2000i DTN: MO0010MWDSUP04.010
n, repassivation slope	Uniform over the range (0.75, 0.84)	CRWMS M&O 2000i DTN: MO0010MWDSUP04.010
$\overline{A}$, crack growth preexponent	Equation 12	CRWMS M&O 2000i

The Slip Dissolution Model data used in the Updated WAPDEG Model and their sources are listed in Table 12.

Table 12. Slip Dissolution Model Parameters Used in Updated WAPDEG Model and Their Sources

Parameter Name	Parameter Value	Source
Threshold Stress	Uniform over the range (0.1, 0.4) fraction of the Yield Strength	CRWMS M&O 2000i DTN: MO0010MWDSUP04.010
Incipient crack size	0.05 mm	CRWMS M&O 2000i DTN: MO0010MWDSUP04.010
n, repassivation slope	Uniform over the range (0.843, 0.92)	CRWMS M&O 2000i DTN: MO0010MWDSUP04.010
$\overline{A}$, crack growth preexponent	Equation 12	CRWMS M&O 2000i

The threshold stress is defined as the minimum stress at which cracks start growing at a rate determined by Equation 11. As suggested in the upstream process model analysis (CRWMS M&O 2000h, Section 6.5.2), the range of variation of the threshold stress is due to uncertainty only. Furthermore, the uncertainty range is given by a uniform distribution. Thus, the resulting uncertainty range for the threshold stress is uniformly distributed between 64.46 and 96.60 MPa in the Current WAPDEG model and between 32.23 and 128.92 for the Updated WAPDEG Model. In the Stress Corrosion Cracking (SCC) analysis of Alloy 22 waste package outer barrier extended and flat closure-lid welds with WAPDEG, for each realization (or each run), the threshold stress is sampled from the range with a uniform distribution, and the sampled threshold stress is used for all the closure-lid weld patches of the waste packages under consideration.

In the SCC process, the crack initiation is associated with microscopic crack formation at localized corrosion or mechanical defect sites that are associated with pitting, intergranular attack, scratches, weld defects, or design notches. The crack growth rate increases as the microscopic cracks coalesce, and approaches a steady-state value when a crack can be detected (CRWMS M&O 2000h, Section 6.4.1). The analysis assumes that the above crack depth range represents the minimum crack depth for which the slip dissolution model can be applied. Those cracks are referred to as "incipient" cracks. An exponential distribution with a maximum size of 50 μm and a median size of 20 μm was suggested for the incipient crack size distribution. Because the effect of differing incipient crack sizes (within the suggested range) on crack penetration time is much smaller than the other model parameters (i.e., n and K_I in Equation 11), the maximum crack size (50 μm or 0.05 mm) is used for all the incipient cracks considered in the SCC analysis, a conservative assumption (see Section 5.7).

Once crack growth initiates the crack(s) grow at a velocity given by (CRWMS M&O 2000h, Section 6.4.4 and CRWMS M&O 2000i Section 6.4.2):

$$V_t = \bar{A}(K_I)^{\bar{n}} \qquad \text{(Eq. 11)}$$

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

$$\bar{A} = 7.8x10^{-2}\, n^{3.6}\left(4.1x10^{-14}\right)^{n} 3.1558149x10^{7} \qquad \text{(Eq. 12)}$$

$$\bar{n} = 4n \qquad \text{(Eq. 13)}$$

Note that *3.1558149E+7* is a conversion factor between seconds and years.

In the Current WAPDEG Model, the model parameter n is represented by a uniform distribution with an upper bound of 0.84 and a lower bound of 0.75, and thus $\bar{n}$ would be represented by a uniform distribution with an upper bound of 3.36 and a lower bound of 3. In the Updated WAPDEG Model, the model parameter n is represented by a uniform distribution with an upper bound of 0.92 and a lower bound of 0.843, and thus $\bar{n}$ would be represented by a uniform distribution with an upper bound of 3.68 and a lower bound of 3.372.

All of the data and parameters discussed in this section were documented in the AMR entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer*

Barrier and Hydrogen Induced Corrosion of Drip Shield (CRWMS M&O 2000i) and are tracked by DTN: MO0010MWDSUP04.010. This data is qualified.

4.1.10 Waste Package Outer Barrier Microbial Induced Corrosion Abstraction Model

The Waste Package Outer Barrier Microbial Induced Corrosion (MIC) Model requires a threshold relative humidity for microbial activity and a corrosion rate multiplier to model the affect of microbial activity. The MIC corrosion enhancement factor is applied to the "effective" penetration rate (e.g., general and localized corrosion rate). In the current analysis, the enhancement factor is applied only to the general corrosion because localized corrosion does not occur. These data and their sources are listed in Table 13.

Table 13. Waste Package Outer Barrier Microbial Induced Corrosion Model Parameters and Their Sources

Parameter Name	Parameter Value	Source
Threshold RH	0.9	CRWMS M&O 2000e Section 6.10
General Corrosion Multiplier Distribution	Uniform over the range (1, 2)	CRWMS M&O 2000e Section 6.8

The technical product output information listed in Table 13 were developed using qualified methods per AP-3.10Q and obtained from controlled and confirmed sources. According to the upstream analysis entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.10 paragraph 1), general corrosion rates should be enhanced to model the effect of MIC above 90% relative humidity. Both the Current and Updated WAPDEG Models conservatively use the RH threshold for the initiation of corrosion degradation (Sections 4.1.2, 5.8, and 6.4.8.1) as well as for the initiation of MIC. This conservatism was necessary due to input limitations of the WAPDEG code. The upstream analysis recommends the general corrosion rate of the waste package outer barrier be enhanced by a factor between 1 and 2 (i.e., no enhancement up to the general corrosion rate being doubled) (CRWMS M&O 2000e, Section 6.8 paragraph 1). Thus, the general corrosion rate enhancement factor will be sampled from a uniform distribution with an upper bound of 2 and a lower bound of 1. The same upstream analysis recommends that, while bacteria preferentially colonize weldments, heat affected zones, and charged regions, it should be assumed that the general corrosion rate enhancement factor is uniformly distributed with respect to areal distribution (i.e., MIC enhanced corrosion could occur anywhere on the waste package surface) (CRWMS M&O 2000e, Section 6.8 paragraph 5).

4.1.11 Waste Package Outer Barrier Aging and Phase Instability Abstraction Model

The Waste Package Outer Barrier Aging and Phase Instability Model requires a corrosion rate multiplier to model the effect of aging and phase instability. The aging corrosion enhancement factor is applied to the "effective" penetration rate (e.g., general and localized corrosion rate). In the current analysis, the enhancement factor is applied only to the general corrosion because localized corrosion does not occur. These data and their sources are listed in Table 14.

According to the upstream analysis entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.7.3 paragraph 2), general corrosion rates will be enhanced to model the effect of aging and phase stability. The upstream analysis recommends the general corrosion rate of the waste package outer barrier be enhanced by a factor between 1 and 2.5 (i.e., no enhancement up to the general corrosion rate being multiplied by 2.5) (CRWMS M&O 2000e, Section 6.7.3 paragraph 2). Thus, the general corrosion rate enhancement factor will be sampled from a uniform distribution with an upper bound of 2.5 and a lower bound of 1. This enhancement factor is applied only to the closure weld region of the waste package outer barrier as discussed in Section 5.9.

Table 14. Waste Package Outer Barrier Aging and Phase Instability Model Parameters and Their Sources

Parameter Name	Parameter Value	Source
General Corrosion Multiplier Distribution	Uniform over the range (1, 2.5)	CRWMS M&O 2000e Section 6.7.3

The technical product output information listed in Table 14 were developed using qualified methods per AP-3.10Q and obtained from controlled and confirmed sources.

4.1.12 Waste Package and Drip Shield Exposure Conditions

The waste package and drip shield exposure conditions (relative humidity (RH), temperature, dripping water exposure period(s) and dripping water chemistry) are input to the WAPDEG DLL (see Section 6.4.16). The preparation and documentation of these data are included in the upstream analyses that serve as inputs to this analysis (CRWMS M&O 2000k, 2000l, and 2000m) (DTN: SN0007T0872799.014, MO0002SPALOO46.010, MO9911SPACDP37.001). This technical product input information requires confirmation as discussed in Section 7. See Attachment I for further discussion of these inputs and their preparation.

4.2 CRITERIA

This section provides a summary of the NRC review and acceptance criteria outlined in the Issue Resolution Status Report (IRSR) that applies to the Container Life and Source Term Key Technical Issues (KTIs) (NRC 1999). The following six subissues are identified in the IRSR (NRC 1999, Section 2.2).

(1) The effects of corrosion processes on the lifetime of the containers (NRC 1999, Section 2.2).

(2) The effects of phase instability of materials and initial defects on the mechanical failure and lifetime of the containers (NRC 1999, Section 2.2).

(3) The rate at which radionuclides in spent nuclear fuel (SNF) are released from the Engineered Barrier System (EBS) through the oxidation and dissolution of spent fuel (NRC 1999, Section 2.2).

(4) The rate at which radionuclides in high-level waste (HLW) glass are leached and released from the EBS (NRC 1999, Section 2.2).

(5) The effect of in-package criticality on waste package (WP) and EBS performance (NRC 1999, Section 2.2).

(6) The effects of alternate EBS design features on container lifetime and radionuclide release from the EBS (NRC 1999, Section 2.2).

Of these subissues, only subissues (1) and (2) are relevant to this analysis.

4.2.1 Acceptance Criteria Applicable To All Six Subissues

(1) The collection and documentation of data, as well as development and documentation of analyses, methods, models, and codes, are accomplished under approved quality assurance and control procedures and standards (NRC 1999, Section 4.0).

(2) Expert elicitation's, when used, are conducted and documented in accordance with the guidance provided in NUREG-1563 (Kotra, et. al., 1996) or other acceptable approaches (NRC 1999, Section 4.0).

(3) Sufficient data (field, laboratory, and natural analog) are obtained to adequately define relevant parameters for the models used to evaluate performance aspects of the subissues (NRC 1999, Section 4.0).

(4) Sensitivity and uncertainty analyses (including consideration of alternative conceptual models) are used to determine whether additional data would be needed to better define ranges of input parameters (NRC 1999, Section 4.0).

(5) Parameter values, assumed ranges, test data, probability distributions, and bounding assumptions used in the models are technically defensible and can reasonably account for known uncertainties (NRC 1999, Section 4.0).

(6) Mathematical model limitations and uncertainties in modeling are defined and documented (NRC 1999, Section 4.0).

(7) Primary and alternative modeling approaches consistent with available data and current scientific understanding are investigated and their results and limitations considered in evaluating the subissue (NRC 1999, Section 4.0).

(8) Model outputs are validated through comparisons with outputs of detailed process models, empirical observations, or both (NRC 1999, Section 4.0).

(9) The structure and organization of process and abstracted models adequately incorporate important design features, physical phenomena, and coupled processes (NRC 1999, Section 4.0).

4.2.2 Acceptance Criteria For Subissue 1

(1) Identify and consider likely modes of corrosion for container materials, including dry-air oxidation, humid-air corrosion, and aqueous corrosion processes, such as general corrosion, localized corrosion, microbial-induced corrosion (MIC), stress corrosion cracking (SCC), and hydrogen embrittlement, as well as the effect of galvanic coupling (NRC 1999, Section 4.1.1).

(2) Identify the broad range of environmental conditions within the WP emplacement drifts that may promote the corrosion processes listed previously, taking into account the possibility of irregular wet and dry cycles that may enhance the rate of container degradation (NRC 1999, Section 4.1.1).

(3) Demonstrate that the numerical corrosion models used are adequate representations, taking into consideration associated uncertainties, of the expected long-term behaviors and are not likely to underestimate the actual degradation of the containers as a result of corrosion in the repository environment (NRC 1999, Section 4.1.1).

(4) Consider the compatibility of container materials, the range of material conditions, and the variability in container fabrication processes, including welding, in assessing the performance expected in the container's intended waste isolation function (NRC 1999, Section 4.1.1).

(5) Justify the use of data collected in corrosion tests not specifically designed or performed for the Yucca Mountain repository program for the environmental conditions expected to prevail at the Yucca Mountain site (NRC 1999, Section 4.1.1).

(6) Conduct a consistent, sufficient, and suitable corrosion-testing program at the time of the LA submittal. In addition, DOE shall identify specific plans for further testing to reduce any significant area(s) of uncertainty as part of the performance confirmation program (NRC 1999, Section 4.1.1).

(7) Establish a defensible program of corrosion monitoring and testing of the engineered subsystems components during the performance confirmation period to assure they are functioning as intended and anticipated (NRC 1999, Section 4.1.1).

4.2.3 Acceptance Criteria for Subissue 2

(1) Identify and consider the relevant mechanical failure processes that may affect the performance of the proposed container materials (NRC 1999, Section 4.2.1).

(2) Identify and consider the effect of material stability on mechanical failure processes for the various container materials as a result of prolonged exposure to the expected range of temperatures and stresses, including the effects of chemical composition, microstructure, thermal treatments, and fabrication processes (NRC 1999, Section 4.2.1).

(3) Demonstrate that the numerical models used for container materials stability and mechanical failures are effective representations, taking into consideration associated uncertainties, of the expected materials behavior and are not likely to underestimate the actual rate of failure in the repository environment (NRC 1999, Section 4.2.1).

(4) Consider the compatibility of container materials and the variability in container manufacturing processes, including welding, in its WP failure analyses and in the evaluation of radionuclide release (NRC 1999, Section 4.2.1).

(5) Identify the most appropriate methods for nondestructive examination of fabricated containers to detect and evaluate fabrication defects in general and, particularly, in seam and closure welds (NRC 1999, Section 4.2.1).

(6) Justify the use of material test results not specifically designed or performed for the Yucca Mountain repository program for environmental conditions (i.e., temperature, stress, and time) expected to prevail at the proposed Yucca Mountain repository (NRC 1999, Section 4.2.1).

(7) Conduct a consistent, sufficient, and suitable materials testing program at the time of the License Application submittal. In addition, DOE has identified specific plans for further testing to reduce any significant area(s) of uncertainty as part of the performance confirmation program (NRC 1999, Section 4.2.1).

(8) Establish a defensible program of monitoring and mechanical testing of the engineered subsystems components, during the performance confirmation period, to assure they are functioning as intended and anticipated, in the presence of thermal and stress perturbations (NRC 1999, Section 4.2.1).

4.3 CODES AND STANDARDS

The acceptance criteria listed above are consistent with the methodology described in the ASTM Standard Practice C-1174 for prediction of the long-term behavior of EBS components in a geologic repository (ASTM C 1174-97 1998).

5. ASSUMPTIONS

None of the following assumptions require any further confirmation in addition to the bases provided below prior to the use of the parameters developed in this document.

5.1 WASTE PACKAGE AND DRIP SHIELD DESIGN INPUT

The following assumptions are made for Titanium Grade 7 drip shield corrosion degradation modeling relevant to design inputs:

- The drip shield (DS) is assumed to be composed of three parts; two vertical parallelepipeds (the drip shield side plates) and one horizontal parallelepiped (the drip shield top) each 15 mm thick. The surface area of the drip shield is therefore

$$DS\ Surface\ Area = 2 \cdot (2521 \cdot 4775) + (2512 \cdot 4775) = 3.607 \cdot 10^7\ mm^2 \qquad \text{(Eq. 14)}$$

  This assumption is used in the WAPDEG input file contained in the WAPDEG_Inputs element shown in Figure 6 (see Section 6.4.1). This assumption has no effect on the results of this analysis. The WAPDEG code outputs the number of pit, crack, and patch penetrations versus time. The patch and drip shield surface areas are used only to determine the number of patches per drip shield to be simulated.

- The variability in drip shield degradation is adequately characterized by modeling 400 waste package/drip shield pairs with 500 patches per drip shield. This assumption results in a drip shield patch area of 7.214E+04 mm^2. This assumption is based on analyses documented in Section 6.4.3. This assumption is used in the WAPDEG input file contained in the WAPDEG_Inputs element shown in Figure 6 (Section 6.4.1). While this assumption is generally non-conservative relative to the use of a larger number of patches per drip shield (more stochastic samples considered), it is shown in Figure 7 of Section 6.4.3, that results obtained using 500 patches per drip shield are virtually indistinguishable from those for a larger number of patches.

The following assumptions are made for Alloy 22 waste package outer barrier corrosion degradation modeling relevant to design inputs:

- The waste package is assumed to be the 21-PWR Waste Package identified in the *Design Analysis for UCF Waste Packages* (CRWMS M&O 2000p). The surface area of the waste package is therefore

$$WP\ Surface\ Area = 2 \cdot \pi \cdot \left(\tfrac{1564}{2} \cdot 4775\right) = 2.346 \cdot 10^7\ mm^2 \qquad \text{(Eq. 15)}$$

  This assumption is used in the WAPDEG input file contained in the WAPDEG_Inputs element shown in Figure 6 (Section 6.4.1). This assumption has no effect on the results of this analysis. The WAPDEG code outputs the number of pit, crack, and patch penetrations versus time. The patch and waste package surface areas are used only to determine the number of patches per waste package to be simulated.

- The variability in waste package outer barrier degradation is adequately characterized by modeling 400 waste package/drip shield pairs with 1,000 patches per waste package. This assumption results in a waste package patch area of 2.346E+04 mm^2. Based on the discussion of the similar drip shield modeling assumption above, in which it was found that WAPDEG results obtained using 500 patches per drip shield are virtually indistinguishable from those for a larger number of drip shield patches, it is concluded that the use of 1,000 patches for the waste package, almost twice that used for the drip shield, is a reasonable number to use. As shown in Figure 7, the mean profile for waste package failures versus time for the case using 1,000 patches per waste package is about the same as that of the case using 1,500 patches per waste package. This assumption is used in the WAPDEG input file contained in the WAPDEG_Inputs element shown in Figure 6 (Section 6.4.1).

- The weld filler metal used for the Alloy 22 waste package outer barrier closure lid welds is assumed to be Alloy 22. This assumption is consistent with CRWMS M&O 2000n, Section 6.3 in which it is stated that "Filler metal material shall be selected to be compatible with the base material." This assumption is used throughout this document in the WAPDEG degradation models through the use of model parameters appropriate for Alloy 22 in the weld regions.

The following assumptions are made for the 316NG stainless steel waste package inner barrier degradation modeling:

- The stainless-steel waste-package inner layer, which is to provide structural support to the waste package, was not included in the analysis. Although it would provide a certain level of performance for waste containment and potentially act as a barrier to radionuclide transport after waste package breach, the potential performance credit of the stainless-steel layer was not included in the nominal TSPA-SR analysis. This assumption is used throughout the analysis. This assumption is conservative.

These assumptions are used in the formulation of both the Current and Updated WAPDEG Models.

5.2 RELATIVE HUMIDITY THRESHOLD

- The relationship between the critical threshold RH and exposure temperature is based on the assumption of the presence of a sodium nitrate ($NaNO_3$) salt film on the waste package and drip shield surface (see Section 4.1.2). The sodium nitrate salt film is assumed to be present in the absence or presence of dripping water. This assumption is conservative. This assumption is used throughout the analysis.

This assumption is used in both the Current and Updated WAPDEG Models.

5.3 LOCALIZED CORROSION OF DRIP SHIELD

- It is assumed that localized corrosion (LC) is not possible on the Titanium Grade 7 drip shield under all expected repository conditions. This assumption is based on results and conclusions of upstream analyses (CRWMS M&O 2000d, Section 7.1) which were reproduced in Figure 2. Localized corrosion is considered to initiate when the corrosion potential, *Ecorr*, exceeds the critical potential, *Ecrit* (i.e., $\Delta E < 0$). From Figure 2, this can not happen even if exposure *pH* exceeds 14 based on the -4σ confidence interval shown. This assumption is consistent with the available data. This assumption is used throughout the analysis.

- It is assumed that the localized corrosion rate distribution used for Titanium Grade 7 (presented in Section 4.1.6 and Table 3) does not require further verification. This distribution is based on data that are a conservative representation of localized corrosion rate of Titanium Grade 7 under repository conditions. The basis of this assumption is that the lower bound of the localized corrosion rate distribution presented in Table 3 is based on a localized corrosion rate measured in a 19% HCl + 4% $FeCl_3$ + 4% $MgCl_2$ solution at 82°C and the upper bound is based on a localized corrosion rate measured in boiling 3:1 Aqua Regia solution (CRWMS M&O 2000f, Table 16). Hence the use of this data to model Titanium Grade 7 localized corrosion in the proposed repository is conservative. Furthermore, as stated in the previous assumption, localized corrosion of the drip shield will never initiate under expected repository exposure conditions. Therefore, this assumption has no impact on the results of this analysis. This assumption is used in Section 4.1.6.

These assumptions are used in the formulation of both the Current and Updated WAPDEG Models.

5.4 LOCALIZED CORROSION OF WASTE PACKAGE OUTER BARRIER

- Localized corrosion of Alloy 22 is considered to initiate when *Ecorr* exceeds *Ecrit* (i.e., $\Delta E < 0$). From Figure 1, this can not happen based on the -4σ confidence interval shown. While it could be assumed that localized corrosion (LC) is not possible on the Alloy 22 waste package outer barrier for the same reasons as the Titanium Grade 7 drip shield, that assumption was not made. Instead, localized corrosion models and initiation criteria from upstream analysis (CRWMS M&O 2000d) were implemented into the WAPDEG_Inputs element (see Figure 6), even though, based on conclusions of the upstream analyses (CRWMS M&O 2000d, CRWMS M&O 2000e), localized corrosion of the Alloy 22 waste package outer barrier can never occur under repository relevant exposure conditions (see Figure 1). Inclusion of localized corrosion models and initiation criteria for the Alloy 22 outer barrier allows for easier implementation of sensitivity studies should the need arise. This assumption is used throughout the analysis. This assumption has no impact on the results of this analysis.

- In this analysis, localized corrosion of the waste package outer barrier is assumed to initiate only under dripping conditions. This is because of the necessary presence of aggressive ions (such as chloride) in order to initiate and sustain pit and crevice growth, and because the only mechanism for these ions to gain ingress to the drift is through drips. This assumption has no impact on the results of this analysis given the previous paragraph. This assumption is used throughout this analysis.

- It is assumed that dripping water resulting from condensation on the underside of the drip shields (if it occurs) does not lead to initiation of localized corrosion. The basis of this assumption is that the condensed water does not have the aggressive aqueous chemistry associated with dripping water from other sources. This assumption is used in the WAPDEG Model in that localized corrosion of the Alloy 22 waste package outer barrier is not allowed to initiate in the absence of dripping water contact (i.e., the waste package is assumed to undergo humid-air corrosion only while the dripshield remains unbreached). This assumption is used throughout the analysis.

- The localized corrosion rates for Alloy 22 (Table 2) are assumed to be loguniformly distributed. The basis for this assumption is that the values in Table 2 span three orders of magnitude and the percentiles provided are consistent with a loguniform distribution. This assumption is used in the localized corrosion for the Alloy 22 waste package outer barrier and closure lids. This assumption is used throughout the analysis. This assumption has no impact on the results of this analysis.

- It is assumed that the localized corrosion rate distribution used for Alloy 22 (presented in Section 4.1.5 and Table 2) does not require further verification. This distribution is based on data that are a conservative representation of localized corrosion rates of Alloy 22 under repository conditions. The basis of this assumption is that the upstream analysis (CRWMS M&O 2000e, Section 6.6.6) from which the data was obtained indicates that "This distribution reasonably bounds those extreme penetration rates found in the literature . . ." Hence the use of this data to model Alloy 22 localized corrosion in the proposed repository is conservative. This assumption is used in Section 4.1.5.

These assumptions are used in the formulation of both the Current and Updated WAPDEG Models.

5.5 MANUFACTURING DEFECTS IN CLOSURE-LID WELDS

The major assumptions used to develop the abstraction for the probability of the occurrence and size of manufacturing defects in the Alloy 22 waste package outer barrier closure-lid welds are given below. Details of the assumptions employed are described in the companion calculation (CRWMS M&O 2000g).

- Pre-existing surface-breaking defects and the defects embedded in the outer ¼ of the weld thicknesses are considered as potential sites for crack growth by stress corrosion cracking. There is uncertainty associated with this assumption because, as general corrosion propagates, some of the existing surface-breaking defect flaws may disappear and some of the embedded defects may become surface-breaking defects. This evolution of the surface-breaking defects was not considered in detail leading to some uncertainty. Use of this assumption is conservative as the WAPDEG model does not allow existing surface-breaking defects to be removed due to general corrosion processes (see Section 5.7) during the simulation leading to a greater number of defects capable of propagation. Defects in the remaining ¾ of the weld thickness are not considered capable of propagation as the sum of the surface-breaking defects and the defects embedded in the outer ¼ of the weld thicknesses is a reasonably bounding conservative measure of the total defect density capable of propagation. This assumption is used in the analysis of manufacturing defects in Alloy 22 waste package outer barrier closure-lid welds in both the Current and Updated WAPDEG Models (Sections 6.4 and 6.5).

- Only the closure-lid welds of the waste package develop residual stresses high enough to cause stress corrosion cracking. Other fabrication welds used in waste package fabrication are fully annealed prior to waste emplacement, and thus do not develop residual stress high enough for stress corrosion cracking to occur (CRWMS M&O 2000h, Section 5, Assumption 1). This assumption is consistent with available data. This assumption is used in both the Current and Updated WAPDEG Models by restricting Stress Corrosion Cracking processes to occur only on that fraction of waste package patches that are considered closure weld patches (Sections 6.4 and 6.5).

- Defects are assumed to be spatially randomly distributed as represented by a Poisson process (CRWMS M&O 2000g). This assumption is consistent with available data. This assumption is used in the analysis of manufacturing defects in the Alloy 22 waste package outer barrier closure-lid welds in both the Current and Updated WAPDEG Models (Sections 6.4 and 6.5).

- The mean flaw density (Poisson distribution parameter) of the closure-lid weld, 0.6839 flaws/meter, is assumed to be as given in CRWMS M&O (2000u, Section 6.2.1). This is a reasonable value based on the literature reviewed in CRWMS M&O 2000u. This assumption is neither conservative nor nonconservative. This assumption is used in the analysis of manufacturing defects in the Alloy 22 waste package outer barrier closure-lid welds in both the Current and Updated WAPDEG Models (Sections 6.4 and 6.5).

- The fraction of flaws considered is assumed to be uniformly distributed between 34.81% and 36.32%. The basis of this assumption is that the three values quoted (34.81%, 36.17%, and 36.32%) in (CRWMS M&O 2000i, Table 6) are not sufficient to determine a single representative average value. The use of the uniform distribution is a reasonable representation of the uncertainty in expressing this value. This assumption is consistent with available data and analyses (CRWMS M&O 2000u and CRWMS M&O 2000g). This assumption is used in the analysis of manufacturing defects in the Alloy 22 waste package outer barrier closure-lid welds in both the Current and Updated WAPDEG Models (Sections 6.4 and 6.5).

- The fraction of outer surface-breaking flaws (used only in the Updated WAPDEG Model) is assumed to be uniformly distributed between 0.13% and 0.49%. The basis of this assumption is that the three values quoted (0.13%, 0.40% and 0.49%) in (CRWMS M&O 2000i, Table 6) are not sufficient to determine a single representative average value. The use of the uniform distribution is a reasonable representation of the uncertainty in expressing this value. This assumption is consistent with available data and analyses (CRWMS M&O 2000u and CRWMS M&O 2000g). This assumption is used in the analysis of manufacturing defects in the Alloy 22 waste package outer barrier closure-lid welds in the Updated WAPDEG Model (Sections 6.4 and 6.5).

- Pre-inspection flaw sizes are assumed to be lognormally distributed, with distribution parameters (dependent on the weld thickness) as given in CRWMS M&O (2000i, Section 6.2.1). This assumption is consistent with available data and analyses. This assumption is used in the analysis of manufacturing defects in the Alloy 22 waste package outer barrier closure-lid welds in both the Current and Updated WAPDEG Models (Sections 6.4 and 6.5).

- The probability of non-detection (PND) is given as a function of flaw size as discussed in CRWMS M&O 2000o, Section 6.2.1. The model is dependent on the following parameters: the detection threshold (p), the location parameter (b), and the scale parameter (v). The b and v parameters are taken to be uncertain with a uniform distribution (see Section 4.1.7). The ranges for these distributions are listed in Table 4 and Table 5. This is a reasonable assumption, as these values are based on similar industrial manufacturing practices as reviewed in the upstream analysis (CRWMS M&O 2000o and CRWMS M&O 2000u). This assumption is used in the analysis of manufacturing defects in the Alloy 22 waste package outer barrier closure-lid welds in both the Current and Updated WAPDEG Models (Sections 6.4 and 6.5).

- It is assumed that all flaws detected are repaired to specified acceptance criteria or removed in such a manner that they are eliminated from consideration for further failure analysis. This assumption is consistent with upstream analysis (CRWMS M&O 2000u, Section 5.3). This assumption is used in the analysis of manufacturing defects the Alloy 22 waste package outer barrier closure-lid welds in both the Current and Updated WAPDEG Models (Sections 6.4 and 6.5).

5.6 STRESS AND STRESS INTENSITY FACTOR PROFILES IN CLOSURE-LID WELDS

The following assumptions were used to develop abstractions for stress and stress intensity factor profiles in the Alloy 22 waste package outer barrier closure lid welds (extended and flat closure lids). Details of the assumptions employed and the abstraction analyses are given in the companion AMR (CRWMS M&O 2000i).

- It is assumed that all fabrication welds of the waste package, except the welds for the waste package closure lids, are not subject to SCC. The basis of this assumption is that all welds, except the welds for the waste package closure lids, are fully annealed before the waste packages are loaded with waste (CRWMS M&O 2000n, Section 8.1.7). Localized stress-relief treatments (induction annealing of the extended closure lid welds and laser peening of the flat closure lid welds) will be applied to the closure lid welds (CRWMS M&O 2000p, Section 6.4). These treatments will result in the formation of compressive surface stresses in the Alloy 22 waste package outer barrier closure lid weld regions to a depth of at least 1.5 to 6 mm (CRWMS M&O 2000i, Section 6.3.1). For a smooth surface without the presence of manufacturing defects, SCC will not initiate until these compressive regions are removed by general corrosion processes. The localized stress-relief treatments will not result in appreciable heating of the spent fuel elements within the waste package. This assumption is consistent with one used in the upstream analysis (CRWMS M&O 2000h, Section 5). This assumption is used in both the Current and Updated WAPDEG Models in that SCC processes are only allowed to occur on those patches with closure lid welds on them. This assumption is used throughout the analysis.

- The hoop stress (and the corresponding stress intensity factor for radial cracks) is the prevailing stress in the closure-lid welds that fail the waste packages by SCC, if it occurs. Thus, the abstraction is limited to the profiles for the hoop stress and corresponding stress intensity factor for radial cracks. This assumption is conservative. The hoop stress profiles supplied are more severe than the radial or longitudinal stress profiles (CRWMS M&O 2000h, Attachment I). This assumption is used in both the Current and Updated WAPDEG Models in the stress profiles used in the Slip Dissolution Abstraction Model. This assumption is used throughout the analysis.

- The hoop stress and corresponding stress intensity factor profiles in the Alloy 22 waste package outer barrier flat closure lid welds from the process-level analysis are for a plane that is inclined at an angle of about 37.5° with the outer surface of the Alloy 22 waste package outer barrier flat closure lid (CRWMS M&O 2000h). Because the SCC analysis in the integrated waste package degradation model (WAPDEG) assumes that cracks propagate in the direction of the normal to the lid surface, the profiles from the process-level analysis were projected to the plane normal to the outer surface of the lid. It is assumed the SCC analysis with the "simple" projection of the profiles represents the hoop stress and stress intensity factor profiles for the inclined plane. This assumption is consistent with the upstream analysis. This assumption is used in both the Current and Updated WAPDEG Models in the Stress and Stress Intensity Factor Profile Abstraction Model inputs (see Section 6.4.12.1).

- The hoop stress and corresponding stress intensity factor profiles, as a function of depth in the Alloy 22 waste package outer barrier closure-lid welds from the process-level analyses, represent the mean profiles. The uncertainties in the hoop stress and corresponding stress intensity factor profiles are represented with triangular distributions around the mean profiles. This assumption is consistent with upstream analysis (CRWMS M&O 2000h, Section 6.2.2.5). This assumption is used in both the Current and Updated WAPDEG Models in the Stress and Stress Intensity Factor Profile Abstraction Model inputs (see Section 6.4.12.1).

- The hoop stress and stress intensity factor profiles vary along the circumference of the Alloy 22 waste package outer barrier closure-lid welds, and those represent the variability in the profiles for a given waste package. It is assumed that the same degree of the profile variability is applied equally to all the waste packages in the repository, and there is no variability in the profiles among waste packages. This assumption is consistent with upstream analysis (CRWMS M&O 2000h, Section 6.2.2.5). This assumption is used in both the Current and Updated WAPDEG Models in the Stress and Stress Intensity Factor Profile Abstraction Model inputs (see Section 6.4.12.1).

- As a crack propagates in the Alloy 22 waste package outer barrier closure lid welds or the welds are corroded, stresses in the welds may re-distribute such a way that the SCC initiation and crack growth are mitigated (CRWMS M&O 2000h). Such a stress re-distribution or relaxation is not considered in the abstraction. This is a conservative approach. This assumption is used in both the Current and Updated WAPDEG Models in Stress and Stress Intensity Factor Profile Abstraction Model (see Section 6.4.12.1).

5.7 SLIP DISSOLUTION MODEL

The following assumptions were used to develop the abstractions for the slip dissolution model for the SCC crack initiation and growth. Details of the assumptions employed and the abstraction analyses are described in the companion abstraction AMR (CRWMS M&O 2000i).

- Induction-heating solution annealing is used to mitigate residual stress in the Alloy 22 waste package outer barrier extended closure-lid welds, and laser peening is used in the Alloy 22 waste package outer barrier flat closure-lid welds. The manufacturing defect analyses (CRWMS M&O 2000o and CRWMS M&O 2000u) and their abstractions (CRWMS M&O 2000g and CRWMS M&O 2000i) are assumed applicable to the Alloy 22 waste package outer barrier closure-lid welds after the stress mitigation processes. This assumption is consistent with upstream analysis (CRWMS M&O 2000i). This assumption is conservative in that the effect of annealing is generally to blunt defect asperities and lessen the severity of stress states around defects. This assumption is used in the Slip Dissolution Abstraction Model (see Section 6.4.13).

- It is assumed that the analyses for incipient cracks reported in (CRWMS M&O 2000h) are applicable to the Alloy 22 waste package outer barrier closure-lid welds after the stress mitigation process. This assumption is consistent with upstream analysis. This assumption is used in the Slip Dissolution Abstraction Model (see Section 6.4.13).

- An exponential distribution with a maximum size of 0.05 mm and a median size of 0.02 mm was suggested for the incipient crack size distribution (CRWMS M&O 2000h, Section 6.5.2). In this analysis, the maximum crack size (0.05 mm) is used for all the incipient cracks considered in the SCC analysis. This is a conservative assumption. This assumption is used in the Slip Dissolution Abstraction Model (see Sections 4.1.9 and 6.4.13).

- It is assumed that the drip shield is not subject to stress corrosion cracking (SCC). This assumption is based on conclusions of upstream analyses (CRWMS M&O 2000h, Section 5). This assumption is used in the WAPDEG Model in that no SCC model input is supplied to the WAPDEG Model and thus, no SCC of the drip shield is allowed to occur. This assumption is used throughout the analysis.

- It is assumed that SCC of the of the Alloy 22 waste package outer barrier closure lid welds can initiate as long as the relative humidity threshold is satisfied (i.e., it is conservatively assumed that a critical environment can be formed in the presence of any stable water film), the stress state at the crack depth exceeds the stress threshold, and the stress intensity factor is positive. The basis of this assumption is that in order for stress corrosion cracking (SCC) to occur, the following three factors must be present: metallurgical susceptibility (Alloy 22 is susceptible), critical environment, and a static (or sustained) tensile stress (CRWMS M&O 2000h, Section 6.1). This assumption is used in the Slip Dissolution Abstraction Model (see Section 6.4.13).

- It is assumed that manufacturing defects and incipient cracks extend by general corrosion processes at the crack tip, i.e., the defects and cracks maintain their depth relative to the general corrosion front. The assumption is conservative as pre-existing manufacturing defects that are included in the analysis are not removed due to general corrosion processes. This assumption is used in the Slip Dissolution Abstraction Model (see Section 6.4.13).

5.8 EFFECT OF MICROBIOLOGICALLY INFLUENCED CORROSION (MIC)

The following assumptions were used for the effect of microbiologically influenced corrosion (MIC) of the drip shield (Titanium Grade 7) and waste package outer barrier (Alloy 22).

- The drip shield is assumed not subject to microbiologically influenced corrosion (MIC). The basis of this assumption is given in CRWMS M&O (2000f, Sections 5.8 and 6.9) in which it is stated that the effect of microbial growth on the corrosion potential is not significant and the initiation of crevice corrosion under bio-films formed on titanium has never been observed. This assumption is used in both the Current and Updated WAPDEG Models in that no MIC model input is supplied to the WAPDEG Model and thus, no MIC of the drip shield is allowed to occur. This assumption is used throughout the analysis.

- The waste package outer barrier is conservatively assumed to be subject to MIC upon satisfaction of the RH threshold for the initiation of corrosion degradation (Section 4.1.2 and Section 6.4.8.1). In the Analyses and Models Report entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.10) it is stated that corrosion rates will be enhanced to account for MIC above 90% RH. The basis of this assumption is that it is conservative since all RH threshold values for the initiation of corrosion degradation are less than 90% (see the listing of WDRHCrit.fil in Section 6.4.8.1). Furthermore, This assumption is used in both the Current and Updated WAPDEG Models in the MIC Abstraction Model input parameters (see Section 6.4.14.1).

- It is assumed that the effect of MIC on corrosion degradation of the waste package outer barrier is represented by a general corrosion enhancement factor (localized corrosion does not occur). The enhancement factor is assumed to have uniform distribution between one and two. The basis of this assumption is described in CRWMS M&O (2000e, Section 6.8) in which it is stated that the general corrosion rate enhancement factor is uniformly distributed between one and two. This assumption is used in both the Current and Updated WAPDEG Models in the MIC Abstraction Model input parameters (see Section 6.4.14.1).

- It is assumed that the MIC general corrosion enhancement factor for the waste package outer barrier varies among waste packages and among patches for a given waste package. The basis of this assumption is given in CRWMS M&O (2000e, Section 6.8). This assumption is used in both the Current and Updated WAPDEG Models in the MIC Abstraction Model input parameters (see Section 6.4.14.1).

5.9 EFFECT OF AGING AND PHASE INSTABILITY

The following assumptions were used for the effect of aging and phase instability on corrosion degradation of the drip shield (Titanium Grade 7) and waste package outer barrier (Alloy 22).

- The drip shield is assumed immune to long-term aging and phase instability under the thermal conditions expected in the repository. The basis of this assumption is given in CRWMS M&O (2000f, Section 5.9) in which it is stated that the effects of phase instability on degradation of Titanium Grade 7 are expected to be insignificant. While Titanium Grade 7 does contain small additions of Palladium (Pd), Titanium-Palladium intermettallic compounds have not been reported to form in Titanium Grade 7 under normal heat treatments. This assumption is used in both the Current and Updated WAPDEG Models in that no Aging and Phase Instability Abstraction Model input is supplied for the Titanium Grade 7 drip shield, thus there is no effect of aging and phase instability on the drip shield degradation characteristics. This assumption is used throughout the analysis.

- It is assumed that the waste package outer barrier and all fabrication welds of waste package (not including the welds for the closure lids) are fully annealed before the waste packages are loaded with waste and are not subject to the effects of aging and phase stability. This assumption is based on an assumption used in an upstream analysis (CRWMS M&O 2000e, Section 5, Assumption 9) in which it is stated that aging and phase stability will not effect corrosion performance of Alloy 22 *base metal*. Fully annealed material is considered to perform like base metal. This assumption is used in both the Current and Updated WAPDEG Models in that the effects of aging and phase stability are only applied to the Alloy 22 waste package outer barrier closure lid weld regions. This assumption is used throughout the analysis.

- The Alloy 22 waste package outer barrier closure welds can be subject to long-term thermal aging and phase instability under the repository thermal conditions. It is assumed that the thermal aging effect on corrosion degradation of the Alloy 22 waste package outer barrier closure welds is represented by a general corrosion enhancement factor (localized corrosion does not occur). The enhancement factor is assumed to have uniform distribution between the limits of 1 and 2.5. The basis of this assumption is described in CRWMS M&O (2000e, Sections 5.9 and 6.7) in which it is stated that the general corrosion rate enhancement factor due to the effects of aging and phase stability is assumed to have uniform distribution between the limits of 1 and 2.5. This assumption is used in the Aging and Phase Instability Abstraction Model input (see Section 6.4.15.1).

- It is assumed that the general corrosion enhancement factor (localized corrosion does not occur) for the thermal aging of the waste package outer barrier varies among waste packages and among patches for a given waste package. The basis of this assumption is given in CRWMS M&O (2000e, Section 6.7) in which it is stated that the distribution (uniform distribution between the limits of 1 and 2.5) is one-half uncertainty and one-half variability. This is implemented in both the Current and Updated WAPDEG Models in the Aging and Phase Instability Abstraction Model input (see Section 6.4.15.1) by assigning an uncertain share of variance of this distribution to waste-package-to-waste-package variance and patch-to-patch variance through the use of the variance partitioning procedures within the WAPDEG code (see Section 6.4.17).

5.10 EFFECT OF RADIOLYSIS

- Both the drip shield (Titanium Grade 7) and waste package outer barrier (Alloy 22) are assumed not to be subject to radiolysis-enhanced corrosion under the expected repository conditions. The basis of this assumption is described in the companion AMRs: Sections 5.7 and 6.8 of CRWMS M&O 2000f for the drip shield and Sections 5.7 and 6.4.4 of CRWMS M&O 2000e for the waste package outer barrier. To summarize, the shift in corrosion potential due to gamma radiolysis will be less than 200 mV and this shift in corrosion potential is insufficient to cause localized corrosion initiation (also see Figure 1 and Figure 2). This assumption is consistent with the upstream analysis. This assumption is used in the WAPDEG Model in that no effect of radiolysis is included in the model. This assumption is used throughout the analysis.

5.11 HYDROGEN INDUCED CRACKING (HIC) OF DRIP SHIELD

- It is assumed that the Titanium Grade 7 drip shield is not subject to hydrogen induced cracking (HIC) under repository exposure conditions. The basis of this assumption is described in CRWMS M&O 2000i in which it is concluded that even if HIC did occur on the drip shield (due to general corrosion or galvanic couple formation) resulting in through-wall cracks, the crack openings will be plugged by corrosion products and/or other mineral precipitates (CRWMS M&O 2000j, Section 6.2.4) leading to very little water transport through the drip shield. Therefore HIC is of little consequence to drip shield performance. For these reasons, no additional analysis of HIC of the drip shield was conducted. This assumption is used in both the Current and Updated WAPDEG Models in that no HIC Model input is provided for the drip shield. This assumption is used throughout the analysis.

6. ANALYSIS/MODEL

This section provides descriptions for the approach to and the conceptual model for the waste package and drip shield degradation analysis using both the Current and Updated WAPDEG Models. The implementation of the abstraction models of the process-level models for the corrosion degradation processes considered is described. Then the WAPDEG analysis results are discussed in terms of a set of profiles for the waste package and drip shield failure and penetration openings as a function of time. The results of all analyses documented in this Analyses and Models Report (AMR) are tracked by DTN: MO0010MWDWAP01.009.

6.1 APPROACH TO WASTE PACKAGE AND DRIP SHIELD DEGRADATION ANALYSIS

The TSPA-SR subsystem model for evaluating degradation of the waste package and drip shield is the WAste Package DEGradation (WAPDEG) model (CRWMS M&O 2000a). The WAPDEG Model is based on a stochastic simulation approach and provides a description of waste package and drip shield degradation, which occurs as a function of time and repository location for specific design and thermo-chemical-hydrologic exposure conditions. [For a convenience of discussion in this section, the drip shield is considered to be an integral part of the waste package, and no separate discussion is given for the drip shield.] The purposes of the stochastic approach and WAPDEG Model are three fold:

- Provide realistic representation of waste package degradation processes in the repository (rather than taking an excessively conservative approach that is routinely chosen to simplify the analysis);
- Capture the effects of variation and uncertainty both in exposure conditions and degradation processes over a geologic time scale; and
- Perform analysis within reasonable computational resources and time.

Abstractions of the process-level models for implementation in the WAPDEG Model were developed in such a way that important features of the process-level models are captured as explicitly as possible, and that the degradation processes and their characteristics are properly represented in the waste package degradation analysis.

The TSPA-SR waste package degradation analysis simulates the behavior of a few hundred waste packages (see Sections 5.1 and 6.4). Effects of spatial and temporal variations in the exposure conditions over the repository were modeled by explicitly incorporating relevant exposure condition histories into the waste package degradation analysis. The exposure condition parameters that were considered varying over the repository are relative humidity and temperature at the waste package surface, seepage into the emplacement drift, and the chemistry of the seepage water. In addition, potentially variable corrosion processes within a single waste package were represented by dividing the waste package surface into "patches" and populating stochastically the corrosion model parameter values and/or corrosion rates over the patches. The model parameter values and corrosion rates were sampled from their variance, which is dictated by the range of the expected local exposure conditions. The "patches" approach is an attempt to explicitly represent the variability in corrosion rates within a single waste package at a given time.

The TSPA-SR analysis has incorporated more explicit representation (than previous TSPA analyses) of the uncertainty and variability in waste package degradation (waste package failure and penetration number profiles). For the corrosion models and parameters for which data and analyses are available, their uncertainty and variability were quantified and implemented into the WAPDEG analysis. For other models and parameters for which the uncertainty and variability is not quantifiable, the variance in their value was assumed (see Section 6.4.17), or the entire variance was used as uncertainty. The sources and/or processes that may contribute to *uncertain* variability in corrosion processes may include local (or micro-scale) chemistry of solution contacting waste package, temporally and spatially varying long-term post-closure exposure conditions (such as water dripping), manufacturing of waste package, variation of the materials properties (especially microstructure-scale), etc.

In the TSPA-SR analysis, waste package degradation was analyzed with multiple realizations of WAPDEG for the uncertainty analysis of the uncertain corrosion parameters—each WAPDEG realization corresponding to a complete WAPDEG run for a given number of waste packages. Accordingly, each of the WAPDEG analysis outputs discussed above (i.e., waste package failure time, crack penetration number, pit penetration number, and patch penetration number) are reported as a group of "degradation profile curves" that represent the potential range of the output parameters. For example, the waste-package failure time profiles are reported with a group of "curves" for the cumulative probability of waste package failures as a function of time.

6.2 CONCEPTUAL MODEL FOR WAPDEG ANALYSIS OF WASTE PACKAGE AND DRIP SHIELD

In the TSPA-SR analysis, WAPDEG models various types of corrosion mechanisms that may occur on a waste package and drip shield as a function of the exposure time and conditions. [For convenience of discussion in this Section, the drip shield is considered to be an integral part of the waste package. Except where it is necessary, no separate discussion is given for the drip shield.] In the nominal case analysis of TSPA-SR, the waste package outer barrier (WPOB) and drip shield were included in the waste package degradation analysis. The stainless-steel waste-package inner layer, which is to provide structural support to the waste package, was not included in the analysis. Although it would provide a certain level of performance for waste containment and potentially act as a barrier to radionuclide transport after waste package breach, the potential performance credit of the stainless-steel layer was ignored in the nominal TSPA-SR analysis.

In this analysis, a humid-air corrosion condition is defined as an exposure condition for which the RH at the waste package surface is equal to or greater than the threshold RH in the absence of drips. An aqueous corrosion condition requires the presence of dripping water. Corrosion and other degradation processes and their models and parameters that have been incorporated into the TSPA-SR waste package degradation analysis are described below.

- Threshold relative humidity (RH) for corrosion initiation. The threshold RH is based on the deliquescence point of $NaNO_3$ salt and is a function of exposure temperature (see Sections 4.1.2 and 5.2). The same threshold RH is used for both the dripping and non-dripping cases. It is assumed (Section 5.2) that a stable water layer on the surface that can support electrochemical reactions of corrosion forms if the RH is equal to or greater than the threshold RH.

- Humid-air and aqueous general corrosion rate of waste package outer barrier. The same general corrosion rate is used for both aqueous and humid-air general corrosion.

- Humid-air and aqueous general corrosion rate of drip shield. The same general corrosion rate is used for both aqueous and humid-air general corrosion.

- Localized corrosion (pitting and crevice corrosion) initiation threshold for the waste package outer barrier, which is based on the corrosion potential (E_{corr}) and threshold corrosion potential (E_{th}) as a function of the contacting solution pH. If $E_{corr} \geq E_{th}$, localized corrosion initiates. Localized corrosion also requires the presence of dripping water (see Section 5.4). Localized corrosion ceases if the exposure condition changes such that E_{corr} becomes less than E_{th}.

- Localized corrosion (pitting and crevice corrosion) penetration rate for waste package outer barrier.

- Localized corrosion (pitting and crevice corrosion) of the drip shield is assumed not to occur (see Section 5.3).

- The hoop stress and corresponding radial-crack stress intensity factor versus depth in the Alloy 22 outer barrier extended and flat closure lid welds of the waste package.

- The Slip Dissolution Model for Stress Corrosion Cracking (SCC).

- Probability of occurrence and size of manufacturing defects in Alloy 22 waste package outer barrier closure-lid welds and its effect on SCC.

- Threshold RH for the initiation of microbiologically influenced corrosion (MIC) of waste package outer barrier and the enhancement factor (uniform distribution between 1 and 2) for general corrosion rate due to MIC. The drip shield is assumed (Section 5.8) not to be subject to MIC.

- The enhancement factor (uniform distribution between 1 and 2.5) to the general corrosion rate for long-term aging and phase instability of Alloy 22 waste package outer barrier closure welds. The drip shield is assumed (Section 5.9) not to be subject to thermal aging.

- Radiation enhanced corrosion of waste package outer barrier and drip shield. It was assumed (Section 5.10) that the waste package and drip shield are not subject to radiation enhanced corrosion under the repository conditions.

- Because both the upper and under sides of the drip shield are exposed to the exposure conditions in the emplacement drift, both sides are subject to corrosion if the initiation threshold is met.

- When the waste package fails, the waste package degradation analysis also considers corrosion degradation of the waste package on its inner surface (inside-out corrosion). The inside-out corrosion analysis includes general corrosion and localized corrosion of the Alloy 22 waste-package outer barrier. The inside-out corrosion would cause penetrations by general and localized corrosion in addition to those by outside-in corrosion only. The inside-out general corrosion initiates at the time of the waste package failure. Like the outside-in localized corrosion, initiation of the inside-out localized corrosion is based on the corrosion potential and threshold corrosion potential, which are a function of the pH of water inside the breached waste package. The in-package water chemistry is determined from analysis of degradation of the waste form and other internal materials (such as basket materials) provided to the WAPDEG Model through the waste package and drip shield exposure conditions (see Section 4.1.12 and Section 2.2.3 of Attachment I).

The drip shield was assumed not to be subject to SCC because it will be fully annealed before it is placed in the emplacement drift. Likewise, all the fabrication welds in the waste container, except the welds for the Alloy 22 waste package outer barrier closure lids, were assumed fully annealed and thus not subject to SCC. Therefore, only the Alloy 22 waste package outer barrier closure-lid welds were considered in the SCC analysis. It was assumed that SCC is operative on the Alloy 22 waste package outer barrier closure-lid welds if the RH of the waste package surface is greater than the threshold RH. In addition, two alternative SCC models, the slip dissolution model and the threshold stress intensity factor model, were considered.

As discussed in detail in Section 6.2.2 of CRWMS M&O 2000h, a dual closure-lid design for the Alloy 22 waste package outer barrier (or outer shell) has been proposed to mitigate potential premature failure of waste packages by SCC. The two closure lids are referred to as the extended closure lid and flat closure lid in this report. The extended closure lid is 25-mm thick and the flat closure lid is 10-mm thick. There is a physical separation between the two lids. Thus, any SCC cracks initiated in the extended closure-lid stop after penetrating it, and then the flat closure-lid welds are subject to the SCC crack initiation and growth. See CRWMS M&O 2000p for details of the design. A schematic of the dual closure-lid design is shown in Figure 3.

In order to implement the SCC processes in the dual closure-lids in an explicit way and capture the intended purpose of the dual lid design features in the waste package degradation analysis, the following modeling approach has been implemented within the WAPDEG Model.

- The waste package outer barrier is modeled as two layers, with their thicknesses being consistent with that of the two closure lids: the "pseudo"-outer layer is 25-mm thick, and the "pseudo"-inner layer is 10-mm thick. The actual design thickness of the outer barrier is 20-mm (see Section 4.1.1). Figure 4 shows a schematic of the waste package configuration in the WAPDEG analysis to implement the SCC of the dual closure-lid welds.

- As illustrated in Figure 4, the general corrosion rate distribution that is applied to the "pseudo"-outer layer (25-mm thick) was constructed by increasing the original Alloy 22 general corrosion rate (see Section 4.1.4) by a factor of 2.5. Because the general corrosion rate is time-independent, this is equivalent to analyzing a 10-mm thick layer. Likewise, the localized corrosion penetration rate for the "pseudo"-outer layer was constructed by increasing the original penetration rate (Section 4.1.5) by a factor of 2.5. The Alloy 22 localized penetration rate is also time-independent. The original general and localized corrosion rate was applied to the outer layer closure-lid patches.

- The original general corrosion rate distribution (Section 4.1.4) and localized corrosion penetration rate (Section 4.1.5) were used for the "pseudo"-inner layer (10 mm thick) without modification. The same original general and localized corrosion rate was applied to the inner closure-lid patches.

- As discussed above, inside-out corrosion of the waste package, after an initial breach, is also included in the TSPA-SR waste package degradation analysis. The inside-out corrosion contributes to penetrations by general and localized corrosion in addition to those by the outside-in corrosion only. The number of penetration openings (or the number of penetration openings as a function of time) in the inner layer is used for the radionuclide release rate from the failed waste packages. For the purpose of the inside-out corrosion analysis, the "pseudo"-inner layer (10 mm thick) is treated as the actual outer barrier (20 mm thick). Thus, in the WAPDEG implementation, because the thickness of the "pseudo"-inner layer is defined as 10-mm, the general corrosion rate for the inside-out corrosion was constructed by decreasing the original Alloy 22 rate by a factor of 2. Likewise, the localized corrosion penetration rate for the inside-out corrosion was reduced by a factor of 2. This is equivalent to analyzing the inside-out corrosion of a 20-mm thick outer barrier. The same general and localized corrosion rate was used for inside-out corrosion of the inner closure-lid patches.

The exposure conditions that were included in the TSPA-SR waste-package degradation analyses are temperature and relative humidity at the waste package and drip shield surface, in-drift dripping water contact, and pH of the water contacting the waste package and drip shield. The temperature and relative humidity histories at the waste package and drip shield surface are provided from the thermal-hydrologic model abstraction (CRWMS M&O 2000k). The evolution of the water chemistry contacting the waste package and drip shield surfaces are provided in the *In-Drift Precipitates/Salts Analysis* (CRWMS M&O 2000l). The evolution of the exposure conditions inside the waste package is provided in the *In-Package Chemistry Abstraction for TSPA-LA* (CRWMS M&O 2000m).

In the analysis, the waste package surface RH is tested against the threshold RH (RH_{th}) for corrosion initiation of the drip shield (DS) and waste package outer barrier (WPOB). When the surface RH becomes greater than the threshold RH, the waste package and drip shield could undergo different corrosion degradation modes depending on whether they are dripped on or not.

For waste packages that are not dripped on, the waste package outer barrier (and drip shield) undergoes humid-air corrosion. Under humid-air conditions, the waste package outer barrier (and drip shield) undergoes general corrosion all the time and fails eventually by gradual thinning. As discussed in Sections 4.1.3 and 4.1.4, the general corrosion rates of the waste package outer barrier (and drip shield) are very low.

For waste packages and drip shields that are dripped on, the wetted areas (by drips) of the drip shield or waste package is assumed to undergo aqueous corrosion if the RH at the surface is greater than the threshold RH. If the RH at the waste package or drip shield surface is less than the threshold RH, the dripping water will evaporate resulting in exposure conditions more resembling those of humid-air than aqueous corrosion. It is also assumed that dripping water resulting from condensation on the underside of the drip shields (if it occurs) does not lead to the aggressive aqueous corrosion conditions associated with dripping water from other sources (i.e., the waste package is assumed to undergo humid-air corrosion only while the dripshield remains unbreached) (see Section 5.4). General corrosion occurs all the time under aqueous corrosion conditions. Initiation of localized (pitting and crevice) corrosion is dependent on the local exposure environment on the wetted patches. In this analysis, localized corrosion of the waste package outer barrier is assumed to initiate only under dripping conditions (i.e., through a breached drip shield, see Section 5.4). Localized corrosion for a waste package outer barrier patch is assumed (Section 5.4) to initiate if the corrosion potential (E_{corr}) is greater than or equal to the threshold corrosion potential (E_{th}). After initiated, localized corrosion continues while $E_{corr} \geq E_{th}$. If E_{corr} becomes less than E_{th}, localized corrosion stops. As discussed previously (see Section 5.7), SCC of the waste package closure-lid welds was assumed operative as long as the RH is greater than the threshold RH, regardless of whether it is dripped on or not.

The WAPDEG analysis provides an assessment of corrosion degradation of waste packages for three types of penetration modes: crack penetration by SCC, (in the Alloy 22 waste package outer barrier closure lid weld regions only) pit penetration by pitting and crevice corrosion, and large (or patch) opening by general corrosion. The analysis provides, as output, the cumulative probability of waste package failure by one of the three penetration modes as a function of time, and the number of penetrations for each of the penetration modes as a function of time. The waste package failure time and penetration number profiles are used as input to other analyses such as waste form degradation and radionuclide release rate from failed waste packages.

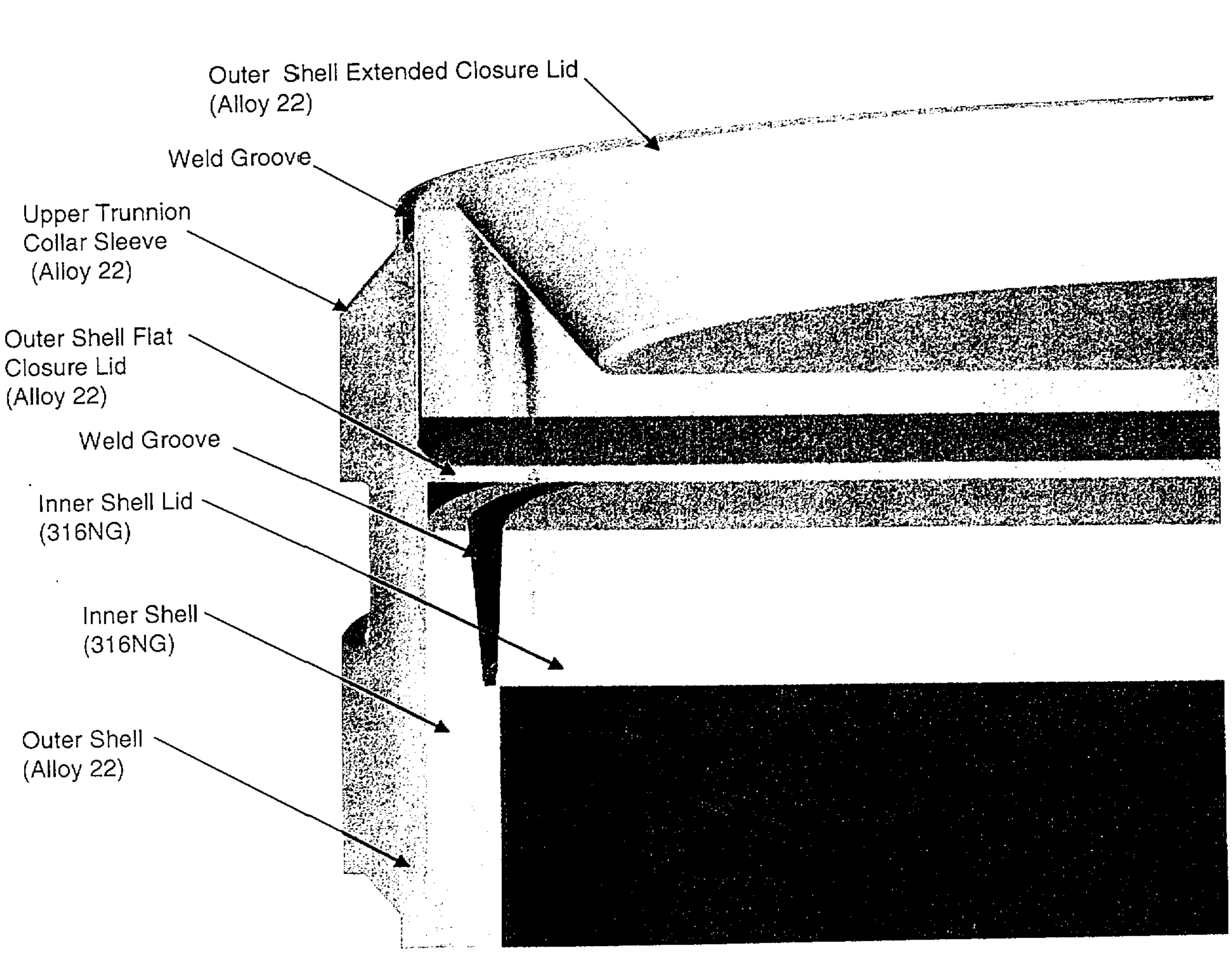

Figure 3. Schematic of the Dual Closure Lids of Waste Package Outer Barrier. Note that the Alloy 22 Waste Package Outer Barrier is Referred to as the Outer Shell in this Figure.

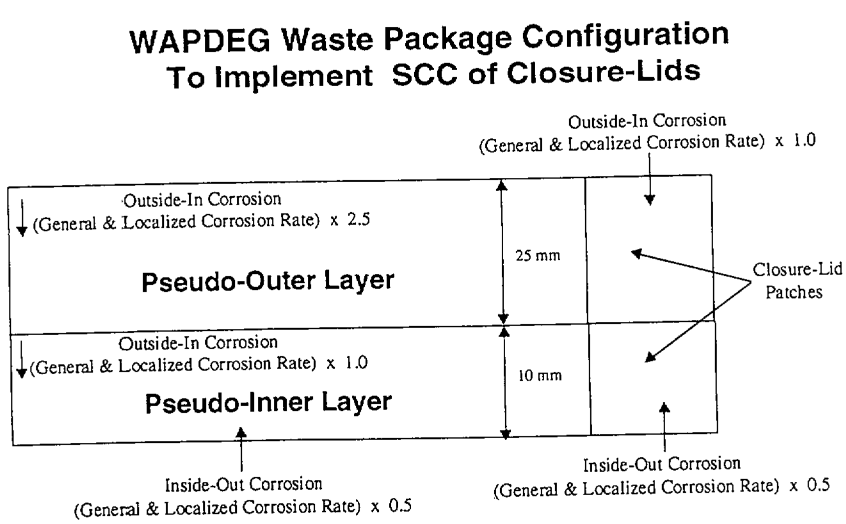

Figure 4. Schematic of Waste Package Configuration in WAPDEG Analysis to Implement SCC of Dual Closure-Lids of Waste Package Outer Barrier

6.3 RECOMMENDED VERSUS IMPLEMENTED UNCERTAINTY TREATMENTS

The purpose of this section is to summarize the uncertainty treatments of corrosion models and/or parameters recommended in their respective process-level Analyses and Models Reports (AMRs) and that alternative interpretations were applied for their implementation in the WAPDEG model. The relevant models, recommendations, and actual implementations are summarized in Table 15.

Table 15. Summary of Comparisons between Recommended and Used Uncertainty treatments for the WAPDEG Model

Model	AMR Recommends	WAPDEG Uses
Titanium Grade 7 General Corrosion	Variability given by triangular distribution with mode based on regression fit to measured data and bounds based on arbitrary lines.	Gaussian Variance Partitioning (CRWMS M&O 2000r) to decompose a distribution based on experimentally measured data points (CRWMS M&O 2000c, Section 6) into a variability distribution at a given uncertainty level.
Alloy 22 General Corrosion	Variability given by triangular distribution with an uncertain mode and bounds based on minimum and maximum general corrosion rates.	Gaussian Variance Partitioning (CRWMS M&O 2000r) to decompose a distribution based on experimentally measured data points (CRWMS M&O 2000c, Section 6) into a variability distribution at a given uncertainty level.
Alloy 22 Aging and Phase Instability	50% uncertainty and 50% variability	100% variability
Alloy 22 Microbially Induced Corrosion	50% uncertainty and 50% variability	100% variability

Note: The uncertainty treatment of the Stress Corrosion Cracking (SCC) model parameters are consistent between the process-level and abstraction AMRs.

6.3.1 General Corrosion Uncertainty Treatments

The Analyses and Models Report (AMR) entitled *General Corrosion and Localized Corrosion of the Drip Shield* (CRWMS M&O 2000f, Section 6.5.4) recommends a treatment of uncertainty in general corrosion rates (note that the general corrosion rates of Titanium Grade 16 were used to generate the distribution to be used for Titanium Grade 7) in Section 6.5.4. The section begins by stating " . . .the entire distribution is assumed to be due to uncertainty." The report then goes on to recommend the use of a triangular distribution for variability with a mode, x, based on a regression fit to the experimentally measured data. Figure 5, below, is a reproduction of Figure 22 in the *General Corrosion and Localized Corrosion of the Drip Shield* (CRWMS M&O 2000f, Section 6.5.4) AMR.

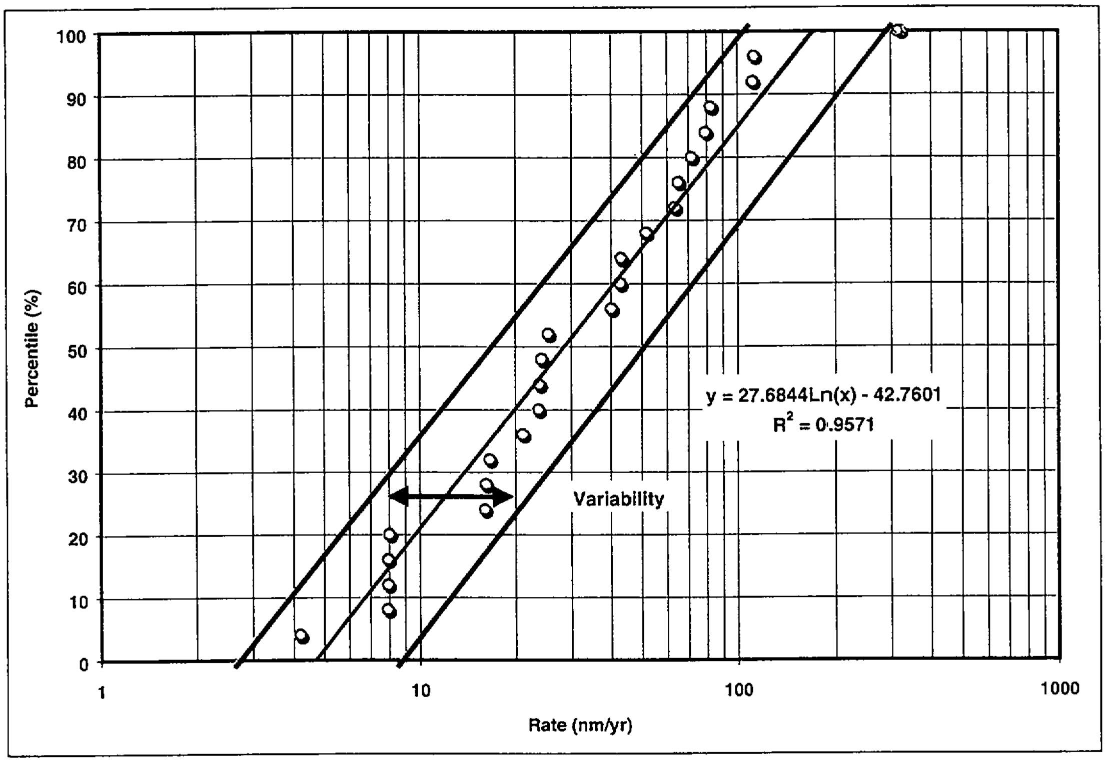

Figure 5. Distribution of Logarithm of General Corrosion Rates of Ti Grade 16: LTCTF 12-Month Weight Loss and Crevice Samples–No Negative Rates

The distribution function y is given in percent and is described by the following correlation (CRWMS M&O 2000f, Section 6.5.4):

$$y = 27.6844\ln(x) - 42.7601 \qquad R^2 = 0.9571 \qquad \text{(Eq. 16)}$$

where x is the general corrosion rate in nanometers per year. The bounding line on the left is the lower bounding value distribution for the triangular distribution for variability and the bounding line on the right is the upper bounding value distribution for the triangular distribution for variability. The equations for the bounding lines are not specified, nor is any technical bases for these choices evident. Although the mechanics of how to use this information is unspecified, for each realization of uncertainty, one would sample a value, call it y', from (what one would have to assume is) a uniform distribution between 0 and 100% and then solve for the mode, x', and the upper and lower bounding values to specify the triangular distribution to be used for variability. Note that the highest general corrosion rates observed would not be sampled unless the value of y', was close to one and that the highest general corrosion rate would never be sampled as it lies outside the bounding lines.

For Alloy 22, a significantly different approach to general corrosion rate uncertainty is proposed in the AMR entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.5.4). As for the drip shield analysis, the section begins by stating " . . .the entire distribution is assumed to be due to uncertainty." The report then goes on to recommend the use of a triangular distribution for variability with upper and lower bounds of zero and the maximum observed rate of 750 nm/yr (CRWMS M&O 2000e, Section 6.5.4) (note that these rates were not corrected for silica deposition) and a mode, c, determined by the relation,

$$c = \alpha \cdot (750 - 0) \qquad \text{(Eq. 17)}$$

where the uncertainty parameter alpha (α) is less than 0.5. Although the mechanics of how to use this information is unspecified, for each realization of uncertainty, one might sample a value of α from (what one would have to assume is) a uniform distribution between 0 and 0.5 and evaluate Equation 17 for the mode. Again, no technical bases for these elicitations is provided. Note that the median general corrosion rate would never exceed the median of the original distribution.

The WAPDEG model makes use of the Gaussian Variance Partitioning (GVP) technique, used in the previous Total System Performance Assessment (CRWMS M&O 1998, Section 5.7.2.2) and implemented in a fully qualified software routine (CRWMS M&O 2000r). For each realization of uncertainty, Gaussian Variance Partitioning separates the input general corrosion rate cumulative distribution function (CDF), containing both uncertainty and variability, into two separate distributions, one that characterizes variability and another that characterizes uncertainty. Each distribution has only a fraction of the input CDFs total variance (i.e., if the fraction of the total variance due to uncertainty is U, then the fraction due to variability is 1-U). The median value of the variability distribution is sampled from the uncertainty distribution. The fraction of the total variance due to uncertainty (U) is itself uncertain and is sampled from a uniform distribution between 0 and 1. The quantile at which to sample the median general corrosion rate is also uncertain and is sampled from a uniform distribution between 0 and 1. In this way the same sampling method is used for both waste package materials to sample the uncertain space of possible general corrosion rate variability distributions. Although there is also no technical bases for this approach to uncertainty modeling, it does reflect that

- the variances of the general corrosion rate distributions are potentially due to uncertainty and variability
- the fraction of variance due to uncertainty and variability is itself uncertain

These facts are readily apparent from the process-level AMRs and the general corrosion analyses presented in them as summarized above. Unlike the uncertainty models presented in the process-level AMRs, in the GVP technique, it is possible to sample the highest general corrosion rates in every realization (this may be highly improbable in some realizations) and the median corrosion rate of the variability distribution can exceed the median corrosion rate of the original distribution. Based on the information currently available for the uncertainty characterization of the general corrosion rate distribution, the GVP technique for the treatment of uncertainty is more reasonable than the approaches recommended in the process-level models.

6.3.2 Aging and Phase Instability Uncertainty Treatment

For Alloy 22, in the AMR entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.7.3), it is stated that the effects of aging and phase instability can be represented by an enhancement factor applied to the general corrosion rate. The corrosion enhancement factor range is based on a limited data set. The distribution for the general corrosion rate enhancement factor, uniform distribution between the limits of 1 and 2.5, is stated to be one-half uncertainty and one-half variability (CRWMS M&O 2000e, Section 6.7.3). No guidance is provided as to how this separation is to be accomplished nor is any technical bases for this elicitation provided. In the WAPDEG Model (Section 5.9), the aging and phase instability general corrosion rate enhancement factor distribution is considered to be 100% variability and its variance is partitioned between waste package to waste package variability and patch-to-patch variability. The treatment of this parameter is sufficient given the uncertainty treatment utilized in the WAPDEG model for the general corrosion rates (Section 6.3.1) and the fact that the effect of aging and phase instability is implemented as an enhancement factor to the general corrosion rate used. The assumption of 100% variability is more conservative in terms of the first failure time of waste package.

6.3.3 Microbially Induced Corrosion Uncertainty Treatment

For Alloy 22, in the AMR entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.8), it is stated that the effects of microbially induced corrosion can be represented by an enhancement factor applied to the general corrosion rate. The distribution for the general corrosion rate enhancement factor, uniform distribution between the limits of 1 and 2, is stated to be one-half uncertainty and one-half variability (CRWMS M&O 2000e, Section 6.8). No guidance is provided as to how this separation is to be accomplished nor is any technical bases for this elicitation provided. In the WAPDEG Model (Section 5.8), the microbially induced corrosion general corrosion rate enhancement factor distribution is considered to be 100% variability and its variance is partitioned between waste package to waste package variability and patch-to-patch variability. The treatment of this parameter is sufficient given the uncertainty treatment utilized in the WAPDEG model for the general corrosion rates (Section 6.3.1) and the fact that the effect of MIC is implemented as an enhancement factor to the general corrosion rate used. The assumption of 100% variability is more conservative in terms of the first failure time of waste package.

6.4 IMPLEMENTATION OF CORROSION MODELS AND SIMULATION PARAMETERS

In this analysis, the waste package degradation model is composed of two components; the WAPDEG dynamic-link library (WAPDEG DLL), which is responsible for modeling the variability in waste package degradation, and the implementation thereof in the GoldSim software (which calls the WAPDEG DLL and is responsible for treating the uncertainty in the parameters used by the WAPDEG DLL (CRWMS M&O 2000a)). Throughout this Section, reference will be made to various parts of the GoldSim (Golder Associates 2000) implementation as well as the various input files and parameters and parameter distributions used in waste package degradation modeling.

6.4.1 GoldSim Implementation Overview

A schematic of the GoldSim implementation, which calls the WAPDEG software, is shown in Figure 6.

WDSeed is a stochastic element characterized by a uniform distribution between 1 and 2^{31}-1 (the maximum positive 32-bit integer). WDSeed is used to generate a different integer for each GoldSim realization with which to seed the WAPDEG random number generator (note that the output of the WDSeed element is fed into the WAPDEG_Inputs element).

The number of waste packages per GoldSim realization (entered in the GoldSim data element labeled NumPak) was set at 400. Note that the output of the NumPak element is fed into the WAPDEG_Inputs element.

The four GoldSim containers (not to be confused with waste containers) GVP_External, MFD_External, SCCD_External, and Variance_Shares shall be discussed later in this document in relation to their specific functions.

The hist_Index data element contains the logical function if (Backfill_case == 1, 13, 23), i.e., based on the value of the external input variable (assigned elsewhere in the TSPA Model) Backfill_case, the value of hist_Index could be the number 13 (Backfill_case equal to 1) or the number 23 (Backfill_case not equal to 1). This represents the file index (line number in a file named WD4DLL.WAP, which will be discussed in the next section) of the thermal hydrologic and chemistry time history file. For all simulations discussed in this report, Backfill_case is equal to 0, thus the value of hist_Index is 23, i.e., a no backfill case is being simulated using the file WDHLW_nbf_high_bin2.ou. This value is passed to the WAPDEG_Inputs data element.

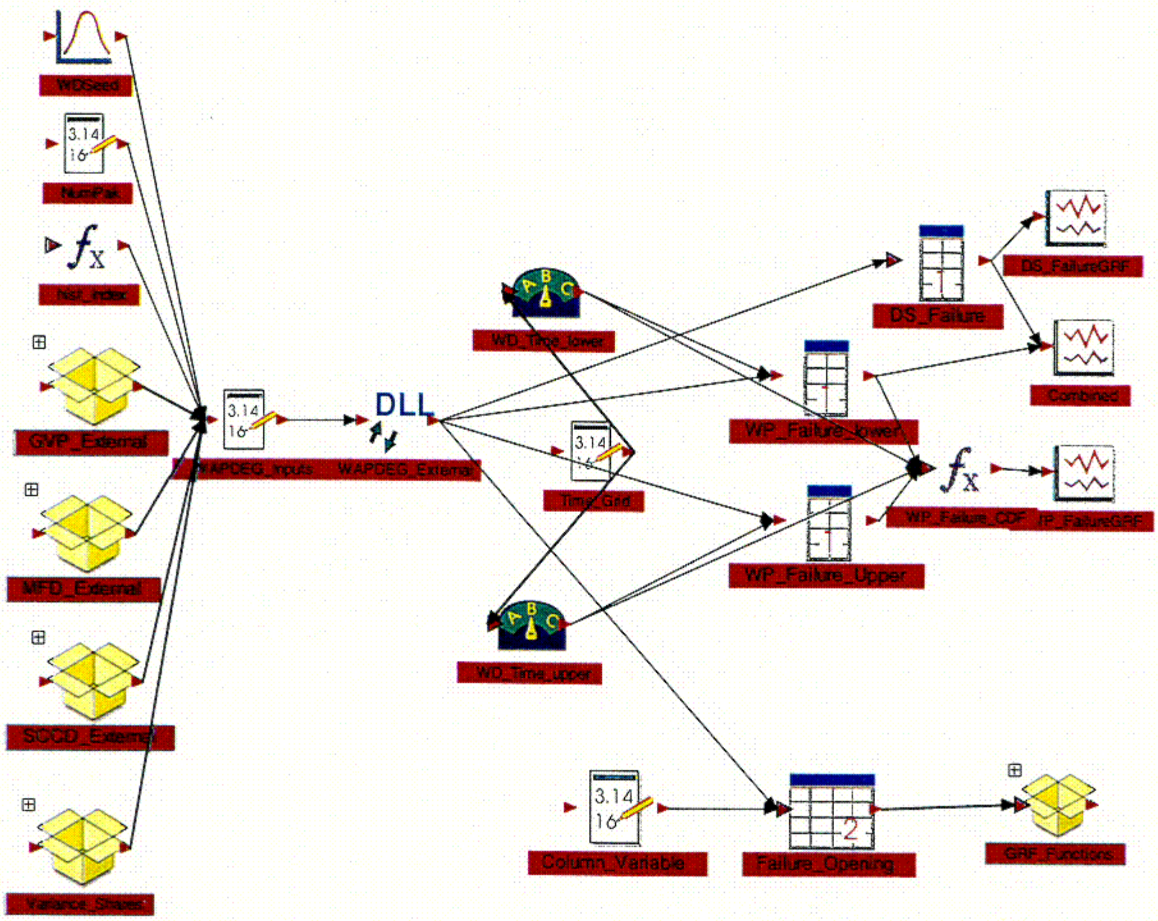

Figure 6. GoldSim implementation which calls the WAPDEG software.

The WAPDEG_External element calls the WAPDEG DLL and is discussed in the next section.

A first breach curve smoothing/correction algorithm was implemented in the waste package degradation module. This algorithm was necessitated by the fact that the waste package degradation module and the TSPA-SR Model evaluate the fraction of waste packages failed using different time steps. The waste package degradation module uses the time steps contained within the thermal hydrology file WDHLW_nbf_high_bin2.ou while the TSPA-SR Model uses 500-year time steps. A "Master Time Grid" was developed by recording each unique time listed in each of the 14 thermal hydrology time history files contained in the WDHLW_nbf_high_bin2.ou file. These 98 unique time points are stored in a GoldSim data element labeled Time_Grid within the waste package degradation module. The fraction of waste packages failed at each time listed in the Time_Grid element are determined. Linear interpolation is performed to determine the fraction of waste packages failed at times in between the times listed in the Time_Grid element.

At each TSPA-SR time step, ETime, the TSPA-SR Model time, is compared to the times listed in the Time_Grid data element. The upper and lower bounding times from the Time_Grid data element are determined such that ETime is between these bounds. This is accomplished through the GoldSim selectors WD_Time_lower and WD_Time_upper, i.e., WD_Time_lower is equal to

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the lower bounding time and WD_Time_upper is equal to the upper bounding time. The fraction of waste packages failed at WD_Time_lower is determined using the GoldSim 1-D table WP_Failure_lower and the fraction of waste packages failed at WD_Time_upper is determined using the GoldSim 1-D table WP_Failure_upper. The GoldSim function element WP_Failure_CDF performs linear interpolation to find the fraction of waste packages failed at Etime.

The other elements in the GoldSim implementation (DS_FailureGRF, Combined, WP_FailureGRF, GRF_Functions) are used only to produce graphs of the results stored in the DS_Failure, WP_Failure, and Failure_Opening elements.

6.4.2 WAPDEG-GoldSim Interface Overview

The WAPDEG DLL (called by GoldSim through the WAPDEG_External element) is passed 1100 real numbers (by GoldSim through the WAPDEG_Inputs element). Some of these inputs tell the WAPDEG DLL which degradation models to use, while others are values of degradation model parameters. Note that only real numbers are passed between GoldSim and the WAPDEG DLL. As it was desired for some degradation model parameters to be represented by distributions stored in text files, GoldSim and WAPDEG share a "file index" file, WD4DLL.WAP, the contents of which are shown below:

```
 Line   File Name
1  WDdA22x2p5.cdf
2  WDdA22SR00.cdf
3  WDdTi7Sr00.cdf
4  WDKISCCO.fil
5  WDStressO.fil
6  WDndTi7SR00.cdf
7  WDKISCCM.fil
8  WDStressM.fil
9  WDRHcrit.fil
10 WDdA22x0p5.cdf
11 WDMFDNDO.cdf
12 WDMFDSizeO.cdf
13 WDHLW_high_bin2.ou
14 WDKIinO.fil
15 WDKIinM.fil
16 WDMFDNDM.cdf
17 WDMFDSizeM.cdf
18 WDgA22x2p5.cdf
19 WDgA22SR00.cdf
20 WDgTi7Sr00.cdf
21 WDgA22x0p5.cdf
22 WDiA22x2p5.cdf
23 WDHLW_nbf_high_bin2.ou
```

The line numbers and the column headings are not part of the WD4DLL.WAP file, but are included for clarity. Using the WD4DLL.WAP file, GoldSim and WAPDEG can pass file indices (line numbers in the WD4DLL.WAP file) in place of actual file names. The 1100 real numbers and the contents of the files identified in the WD4DLL.WAP file are the only inputs to the WAPDEG DLL.

The DS_Failure, WP_Failure_CDF, and Failure_Opening elements receive the output from the WAPDEG DLL. The DS_Failure element receives a one dimensional table of drip shield first failure times. The WP_Failure_CDF element receives a one dimensional table of waste package first failure times. The format of both of these tables is similar; one column containing the drip shield or waste package first failure times in years (sorted in increasing order) and another column containing the cumulative fraction of waste packages of drip shields failed. The Failure_Opening element receives a two dimensional table containing 33 columns and 300 rows. The column contents are explained in Table 16.

Table 16. Column Contents of the Failure_Opening Element.

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

Waste package failure (for the purposes of averaging) is defined as any penetration (patch, pit, or crack) of the waste package layer 2 (the pseudo-inner layer in Figure 4). If there are penetrations of layer 1 (the pseudo-outer layer in Figure 4) of a waste package, but no waste container failures (penetrations of layer 2), the number of waste package failures is set to 0.

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

Given drip shield (DS) and waste package (WP) surface areas and patch sizes, WAPDEG determines the number of patches to be simulated. As discussed in Section 5.1, 500 drip shield patches were assumed to be sufficient to model the variability in drip shield degradation and 1000 waste package patches were assumed to be sufficient to model the variability in waste package degradation. To investigate the validity of these assumptions five sensitivity studies were simulated. One used 500 DS patches and 1000 WP patches, another 1000 DS patches and 1000 WP patches, another 500 DS patches and 500 WP patches, another 500 DS patches and 1500 WP patches, and another 250 DS patches and 1000 WP patches. Each simulation used 100 realizations of 400 DS/WP pairs. The results of these sensitivity studies are shown in Figure 7. In Figure 7, the mean DS and WP failure curves of the five sensitivity studies are shown. Many of the failure curves overlap each other. The use of 1000 DS patches with 1000 WP patches resulted in the earliest (although not dramatically so) DS failure curve. The waste package failure curves are almost identical for all of the five sensitivity studies. It was decided to use 500 DS patches and 1000 WP patches for the nominal case WAPDEG simulations primarily because this choice allowed for computational efficiency while still maintaining a large enough sample of drip shield/waste package patches to adequately capture the effects of variability in any sensitivity simulations conducted.

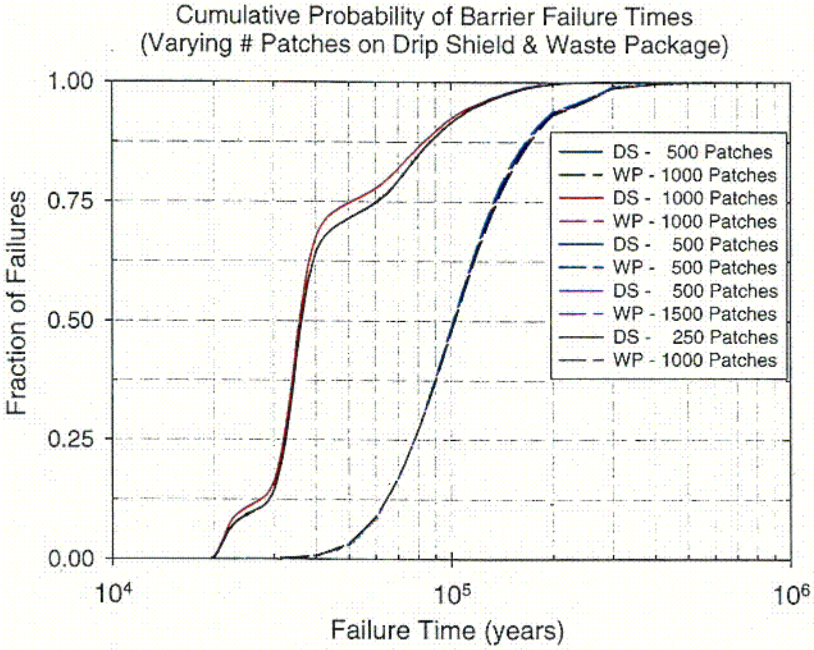

Figure 7. Fraction of drip shield and waste package failures versus time for mean of 100 simulations using 250, 500, or 1000 drip shield patches and 500, 1000, or 1500 waste package patches with 400 waste package/drip shield pairs per simulation

Also in Section 5.1, it was stated that 400 waste package/drip shield pairs were sufficient to model the variability in waste package outer barrier degradation. This conclusion was based on

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the results of sensitivity studies such as the one shown in Figure 8, in which the number of waste package/drip shield pairs was varied using values of 200, 400, and 800 pairs per simulation. 100 realizations using 500 DS patches and 1000 WP patches were simulated. The results of using 200 versus 400 or 800 waste package/drip shield pairs are very similar. The value of 400 pairs was decided upon to allow for computational efficiency while still maintaining a large enough sample of drip shield/waste package pairs to adequately capture the effects of variability in any sensitivity simulations conducted.

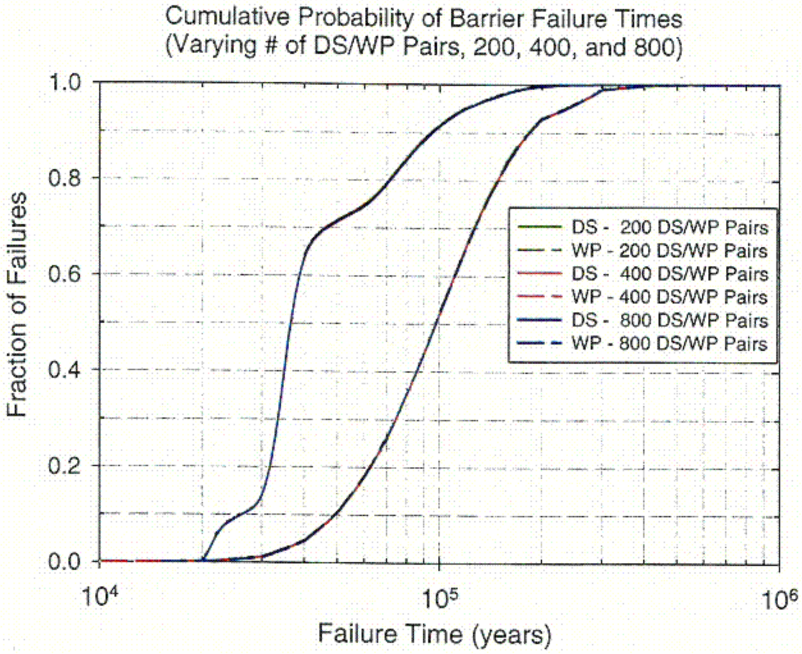

Figure 8. Fraction of drip shield and waste package failures versus time for simulations using 200, 400 and 800 waste package/drip shield pairs per simulation with 1000 waste package and 500 drip shield patches.

6.4.4 Waste Package Design Input

The waste package design consists of a 20-mm thick Alloy 22 outer barrier encompassing a 50-mm thick 316 NG stainless steel inner barrier (CRWMS M&O 2000n, Section 8.1). No performance credit is taken for the 316 NG stainless steel inner barrier, i.e., the inner barrier is not considered in waste package degradation modeling. The waste package outer barrier has one Alloy 22 lid on one end of the waste package outer barrier and two Alloy 22 closure lids (one 10-mm thick flat closure lid and one 25-mm thick extended closure lid) on the closure end of the waste package outer barrier. All welds used in waste package fabrication are assumed to be completely stress-annealed with the exception of the closure welds on the two closure lids (see Section 5.5 and 5.6). Thus only the Alloy 22 waste package outer barrier closure lids are subject to stress corrosion cracking. As discussed in Section 6.2, in order to best model the dual Alloy 22 lid design for the waste package outer barrier, the 20-mm Alloy 22 outer barrier is modeled as being composed of two layers; one 25-mm thick and one 10-mm thick. The model parameters

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(e.g. corrosion rates) are chosen in such a way that the 25-mm thick layer behaves like a 10-mm layer except for the region of that layer that comprises the closure-lid area. For example, the general corrosion rates applied to the 25 mm layer are 2.5 times greater than those for Alloy 22 except for the lid region for which general corrosion rates appropriate for Alloy 22 are used. In the WAPDEG code, waste package failure is defined to be the time of first penetration of the innermost barrier, i.e., the 10-mm inner layer.

6.4.5 Drip Shield General Corrosion Abstraction Model

6.4.5.1 Drip Shield General Corrosion Abstraction Model Implementation

The rate of general corrosion of the Titanium Grade 7 drip shield, over the range of thermal-mechanical-chemical repository-relevant exposure conditions, was determined to be insensitive to temperature, stress state, or water chemistry (CRWMS M&O 2000f). In the WAPDEG conceptual model, the water condition above the drip shield could potentially have humid-air conditions followed by dripping water conditions followed by humid-air conditions. The general corrosion rate distribution provided for the drip shield (WDgTi7SR00.cdf) applies to both humid-air and dripping water (aqueous) conditions. However, the variance of the general corrosion rate distribution is due to both uncertainty and variability, which differs for the two conditions. Therefore, two calls are made to the Gaussian Variance Partitioning (GVP) DLL (see Section 6.3.7); one with WDgTi7SR00.cdf as the input and WDdTiSR00.cdf as the output general corrosion rate distribution (used under dripping water conditions), and another with the same WDgTi7SR00.cdf as the input and WDndTiSR00.cdf as the output general corrosion rate distribution (used under humid-air conditions). Details of the GVP implementation are discussed in Section 6.3.7.

6.4.5.2 Drip Shield General Corrosion Abstraction Model Validation

The Drip Shield General Corrosion Abstraction Model (DSGCAM) is an abstraction model. The validation method used in this section is to review the model parameters for reasonableness, or consistency in explanation of all relevant data. This results in an appropriate level of confidence in the DSGCAM to consider it validated. As the DSGCAM is an abstraction model, the only data relevant to this validation exercise is the process-level model being abstracted. The general corrosion rate distribution used in the DSGCAM (WDgTi7SR00.cdf) was derived entirely in a calculation entitled *Calculation of General Corrosion Rate of Drip Shield and Waste Package Outer Barrier to Support WAPDEG Analysis* (CRWMS M&O 2000c) and is tracked with DTN: MO0010SPASIL02.002. This data is qualified. In that calculation, experimentally measured general corrosion rates of Titanium Grade 7 (CRWMS M&O 2000f, Section 6.5.2, DTN: LL990610605924.079) are sorted in ascending order and assigned cumulative probability values. The general corrosion rates were then corrected for the effects of silica deposition resulting in the general corrosion rate distribution (WDgTi7SR00.cdf) used in the model. The fact that the general corrosion rate distribution used in the DSGCAM is derived from qualified experimental data provided by the process-level model (CRWMS M&O 2000f, Section 6.5.2) (DTN: LL990610605924.079) is considered sufficient to validate the model inputs (i.e., the abstracted model is consistent with the process-level model). The DSGCAM is implemented within the WAPDEG software, which is fully qualified (see Section 3.1.2). Therefore, the DSGCAM inputs are validated and the model is implemented within qualified software. This results in an appropriate level of confidence in the DSGCAM to consider it validated.

As noted in Section 6.3.1, the uncertainty treatment applied to the DSGCAM in this analysis is not identical to the uncertainty treatment recommended in the process-level model. However, the uncertainty treatment used in this analysis is more reasonable than that recommended in the process-level model. Therefore, this disagreement has no effect on the validation status of this model.

6.4.6 Waste Package Outer Barrier General Corrosion Abstraction Model

6.4.6.1 Waste Package Outer Barrier General Corrosion Abstraction Model Implementation

The rate of general corrosion of the Alloy 22 waste package outer barrier, over the range of repository-relevant exposure conditions, was determined to be insensitive to temperature, stress state, or water chemistry (CRWMS M&O 2000e). In the WAPDEG conceptual model, the waste package outer barrier could potentially be contacted by humid-air, dripping, and in-package (inside-out corrosion) water conditions. The general corrosion rate distribution provided for the Alloy 22 waste package outer barrier (WDgA22Sr00.cdf) applies to all these water conditions. As mentioned in Sections 6.2 and 6.3.4, the Alloy 22 waste package outer barrier is modeled as two layers. This necessitated the creation of two additional input cumulative distribution functions (CDFs), both derived from WDgA22SR00.cdf; WDgA22x0p5.cdf in which the general corrosion rates from WDgA22SR00.cdf are multiplied by 0.5 (for inside-out corrosion of the pseudo inner layer) and the cumulative probabilities are left unchanged; and WDgA22x2p5.cdf in which the general corrosion rates are multiplied by 2.5 (for the outside-in corrosion of the pseudo-outer layer) and the cumulative probabilities are left unchanged. Again the variance of the general corrosion rate distributions is due to both uncertainty and variability. Therefore, four calls are made to the Gaussian Variance Partitioning (GVP) DLL; once with WDgA22x2p5.cdf as the input and WDdA22x2p5.cdf as the output general corrosion rate distribution (used under humid-air and dripping conditions for the waste package outer layer), once with WDgA22SR00.cdf as the input and WDdA22SR00.cdf as the output general corrosion rate distribution (used under humid-air and dripping conditions for the waste package inner layer), once with WDgA22x2p5.cdf as the input and WDiA22x2p5.cdf as the output general corrosion rate distribution (used under in package conditions for the waste package outer layer), and once with WDgA22x0p5.cdf as the input and WDdA22x0p5.cdf as the output general corrosion rate distribution (used under in package conditions for the waste package inner layer). As discussed in Section 6.4.2, waste package failure is defined as any penetration (patch, pit, or crack) of the waste package (pseudo) layer 2 (see Figure 4). Therefore, inside-out corrosion of waste package layer 1 (possible only after waste package breach) has no impact on the results of a given WAPDEG simulation. However, input must be provided to the WAPDEG code for all possible degradation mechanisms. Details of the GVP implementation are discussed in Section 6.4.7.

6.4.6.2 Waste Package Outer Barrier General Corrosion Abstraction Model Validation

The Waste Package Outer Barrier General Corrosion Abstraction Model (WPOBGCAM) is an abstraction model. The validation method used in this section is to review the model parameters for reasonableness, or consistency in explanation of all relevant data. This results in an appropriate level of confidence in the WPOBGCAM to consider it validated. As the WPOBGCAM is an abstraction model, the only data relevant to this validation exercise is the process-level model being abstracted. The general corrosion rate distribution used in the WPOBGCAM (WDgA22SR00.cdf) was derived entirely in a calculation entitled *Calculation of General Corrosion Rate of Drip Shield and Waste Package Outer Barrier to Support WAPDEG Analysis* (CRWMS M&O 2000c) and is tracked with DTN: MO0010SPASIL02.002. This data is qualified. In that calculation, experimentally measured general corrosion rates of Alloy 22 (CRWMS M&O 2000e, Section 6.5.2, DTN: LL990610605924.079, LL000112205924.112) are sorted in ascending order and assigned cumulative probability values. The general corrosion rates were then corrected for the effects of silica deposition resulting in the general corrosion rate distribution (WDgA22SR00.cdf) used in the model. The fact that the general corrosion rate distribution used in the WPOBGCAM is derived from qualified experimental data provided by the process-level model (CRWMS M&O 2000e, Section 6.5.2, DTN: LL990610605924.079, LL000112205924.112) is considered sufficient to validate the model inputs (i.e., the abstracted model is consistent with the process-level model). The WPOBGCAM is implemented within the WAPDEG software, which is fully qualified (see Section 3.1.2). Therefore, the WPOBGCAM inputs are validated and the model is implemented within qualified software. This results in an appropriate level of confidence in the WPOBGCAM to consider it validated.

As noted in Section 6.3.1, the uncertainty treatment applied to the WPOBGCAM in this analysis is not identical to the uncertainty treatment recommended in the process-level model. However, the uncertainty treatment used in this analysis is more reasonable than that recommended in the process-level model. Therefore, this disagreement has no effect on the validation status of this model.

6.4.7 Gaussian Variance Partitioning

Two containers in the GoldSim implementation have not been discussed; the GVP_External container and the Variance_Shares container. The function of these containers are similar. Gaussian Variance Partitioning (GVP) is a routine that decomposes a cumulative distribution function (CDF) containing both uncertainty and variability into two distributions that characterize each element separately. This is accomplished primarily by partitioning the variance of the original distribution between the two resulting distributions. Gaussian Variance Partitioning provides a better understanding of the sensitivity of TSPA models to the elements of uncertainty and variability. For further discussion of the GVP algorithm, refer to Section 6.3.1 and the *GVP Software Routine Report* (CRWMS M&O 2000r). As shown in Figure 9, the container GVP_External contains six containers.

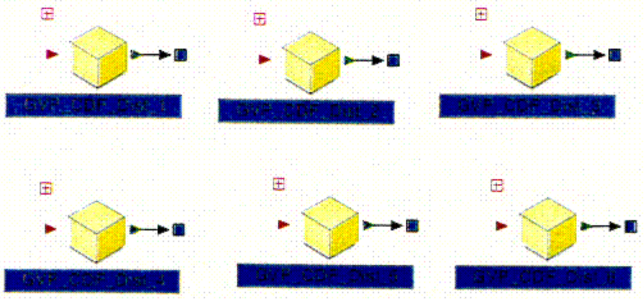

Figure 9. Contents of the GVP_External Container in the GoldSim implementation (see Figure 6).

Each of these contains the necessary inputs and parameters for a call to the GVP subroutine. For example, Figure 10 shows the contents of the GVP_CDF_Dist_1 container.

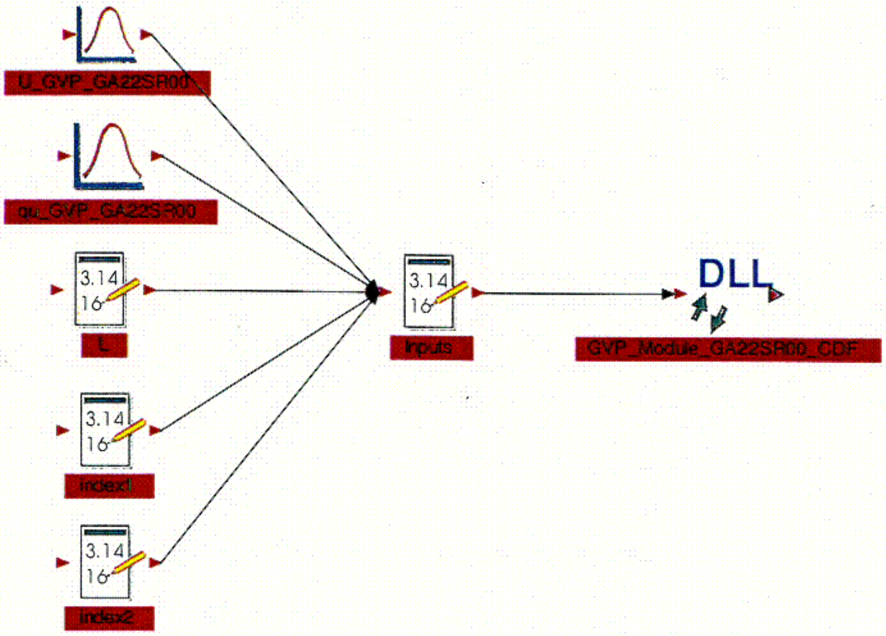

Figure 10. Contents of the GVP_CDF_Dist_1 Container in the GoldSim implementation (see Figure 6).

The stochastic element, U_GVP_GA22SR00, is the uncertain fraction of the original distribution's variance that is due to uncertainty and is sampled from a uniform distribution with bounds of zero and one. The uncertain probability, qu_GVP_GA22SR00, is used to sample the median of the variability distribution from the uncertainty distribution and is uniformly distributed between zero and one. L is a "flag" used to determine whether the natural logarithm should be taken of the input CDF values (column 1) before GVP operates (and antilogartithms afterward). If L is greater than zero, then logarithms are taken. For all six GVP calls, logarithms of the input values were not taken (L<0). Index1 is the file index (line number in the WD4DLL.wap file) of the input CDF and Index2 is the file index of the output CDF (the partitioned CDF output by the GVP subroutine). These inputs are stacked in a data element named Inputs before being passed to the GVP DLL through the GVP_Module_GA22SR00_CDF

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element. The other five calls to the GVP DLL are similar, differing only in the file indexes used and the name given to the GVP_Module element.

6.4.8 Relative Humidity Threshold Abstraction Model

6.4.8.1 Relative Humidity Threshold Abstraction Model Implementation

The relative humidity (RH) threshold (WDRHcrit.fil) variance is totally due to variability as no uncertainty treatment was presented in the upstream analysis that supplied this data (CRWMS M&O 2000b, Section 6.4.1 and Table 8) (also see DTN: LL991212305924.108). For a given WAPDEG realization, the RH threshold distribution is applied as an initiation criteria for all corrosion degradation modes on the drip shield and both of the waste package layers. If the RH read from the exposure file exceeds the threshold RH (which is a function of the temperature read from the exposure file), then corrosion degradation can initiate.

The relationship between the threshold RH and exposure temperature is given by a lookup table (WDRHcrit.fil), which is listed below:

```
!  WDRHCrit.fil
!
#  1     2
#    19
#    1.0
!  T (°C), RH (frac.)
5          0.7857
10         0.7753
15         0.7646
20         0.7536
25         0.7425
30         0.7314
35         0.7206
40         0.71
45         0.6999
50         0.6904
55         0.6815
60         0.6735
65         0.6664
70         0.6604
75         0.6556
80         0.6522
85         0.6503
90         0.65
120.6      0.501
```

The lines preceded by a "!" are comment lines. The first line preceded by a "#" indicates that there is 1 RH critical relationship with 2 columns. The next line preceded by a "#" indicates that there are 19 rows in the lookup table. The next line preceded by a "#" indicates that this lookup table corresponds to all of the waste packages/drip shields to be simulated (a fraction of 1). This is followed by one more comment line, which is used to specify column headers. The following 19 rows consist of temperature (°C) and RH (fraction) data pairs.

6.4.8.2 Relative Humidity Threshold Abstraction Model Validation

The Relative Humidity Threshold Abstraction Model (RHTAM) is an abstraction model. The validation method used in this section is to review the model parameters for reasonableness, or consistency in explanation of all relevant data. This results in an appropriate level of confidence in the RHTAM to consider it validated. As the RHTAM is an abstraction model, the only data relevant to this validation exercise is the process-level model being abstracted. The relative humidity threshold distribution used in the RHTAM (WDRHcrit.fil) was derived from the Analyses and Models Report entitled *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier* (CRWMS M&O 2000b, Section 6.4.1 and Table 8) (DTN: LL991212305924.108). This data is accepted data. The RHTAM conservatively assumes the presence of a $NaNO_3$ salt film (see Section 5.2) on the waste package and drip shield surfaces at all times. The fact that the relative humidity threshold distribution used in the RHTAM is derived from accepted experimental data provided by the process-level model (CRWMS M&O 2000b, Section 6.4.1 and Table 8) (DTN: LL991212305924.108) is considered sufficient to validate the model inputs (i.e., the abstracted model is consistent with the process-level model). The RHTAM is implemented within the WAPDEG software, which is fully qualified (see Section 3.1.2). Therefore, the RHTAM inputs are validated and the model is implemented within qualified software. This results in an appropriate level of confidence in the RHTAM to consider it validated.

6.4.9 Drip Shield Localized Corrosion Initiation Threshold and Rate Abstraction Model Implementation

As discussed in Section 5.2, there is no localized corrosion initiation threshold or localized corrosion rate model for the drip shield implemented in the WAPDEG conceptual model. As shown in Figure 2 (Section 4.1.6), localized corrosion of Titanium Grade 7 cannot initiate even at a pH of 14 based on the 3σ and 4σ confidence intervals.

6.4.10 Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model

6.4.10.1 Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model Implementation

Localized corrosion initiation for the waste package Alloy 22 outer barrier can only occur when the waste package surface is exposed to dripping water (see Section 5.4). During each time step, the WAPDEG DLL evaluates Equation 1 using the pH values read from the exposure file. If evaluation of Equation 1 yields a negative value (i.e., $Ecrit1 < Ecorr$), then localized corrosion can initiate. The rate of localized corrosion is given by the values listed in Table 2 (also see Section 5.3). As indicated by Figure 1 (Section 4.1.5), localized corrosion of Alloy 22 can not initiate at any pH based on the 4σ confidence interval.

6.4.10.2 Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model Validation

The localized corrosion initiation model used for the Alloy 22 waste package outer barrier is validated in the Analyses and Models Report entitled *Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier* (CRWMS M&O 2000d) (DTN: MO0003SPAPCC03.004).

The localized corrosion rate portion of the Waste Package Outer Barrier Localized Corrosion Initiation Threshold and Rate Abstraction Model (WPOBLCITRAM) is an abstraction model. The validation method used in this section is to review the model parameters for reasonableness, or consistency in explanation of all relevant data. This results in an appropriate level of confidence in the WPOBLCITRAM to consider it validated. As the WPOBLCITRAM is an abstraction model, the only data relevant to this validation exercise is the process-level model being abstracted. The localized corrosion rate distribution used in the WPOBLCITRAM (see Table 2) was presented in the Analyses and Models Report entitled *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000e, Section 6.6.6) (DTN: LL991213705924.109). This data is considered to be conservative bounding values to the Alloy 22 localized corrosion rates (see Section 5.4) and thus are considered verified for their intended use. Furthermore, the fact that the localized corrosion rate distribution used in the WPOBLCITRAM is directly provided by the process-level model (CRWMS M&O 2000e, Section 6.6.6) (DTN: LL991213705924.109) is considered sufficient to validate the model inputs (i.e., the abstracted model is consistent with the process-level model and the inputs are reasonable). The WPOBLCITRAM is implemented within the WAPDEG software, which is fully qualified (see Section 3.1.2). Therefore, the WPOBLCITRAM inputs are validated and the model is implemented within qualified software. This results in an appropriate level of confidence in the WPOBLCITRAM to consider it validated.

6.4.11 Manufacturing Defect Abstraction Model

6.4.11.1 Manufacturing Defect Abstraction Model Implementation

The MFD_External (in the GoldSim implementation, see Figure 6) consists of two containers as shown in Figure 11.

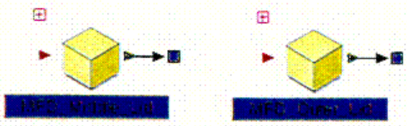

Figure 11. Contents of MFD_External Container in the GoldSim implementation (see Figure 6).

Each of these contains the inputs and parameters necessary to call the MFD subroutine, in the case of the Current WAPDEG Model, or the CWD subroutine, in the case of the Updated WAPDEG Model.

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The contents of the container MFD_Middle_Lid (used in the Current WAPDEG Model to provide input to modeling of the Alloy 22 waste package outer barrier flat closure lid) are presented in Figure 12. Note that throughout the GoldSim implementation figures, the Alloy 22 waste package outer barrier flat closure lid is referred to as the middle lid. The data element, thickness, is the lid thickness in mm. The extended closure lid is 25 mm thick while the flat closure lid is 10 mm thick. The data element lid_radius is 0.76 m for both the extended and flat closure lids. The non-detection probability parameters, b_ML and v_ML, uniformly range between 1.6 to 5 mm and 1 to 3 (see Section 4.1.7), respectively. The fraction of flaws considered, psi_ML, is sampled from a uniform distribution with bounding values of 0.3481 and 0.3632 (see Section 4.1.7). The data elements fileFlaws and fileSize are the file indices for the cumulative distribution functions representing the number of manufacturing defect flaws (file index 16) and their lengths (file index 17), respectively. These inputs are passed to the MFD DLL through the MFD_Mod element. The other call to the MFD DLL (contained in the container MFD_OuterLid) is similar, differing only in the file indexes used (11 and 12) and the lid thickness used (25 mm for the waste package extended closure lid). For further discussion of the MFD algorithm, refer to the *MFD Software Routine Report* (CRWMS M&O 2000s).

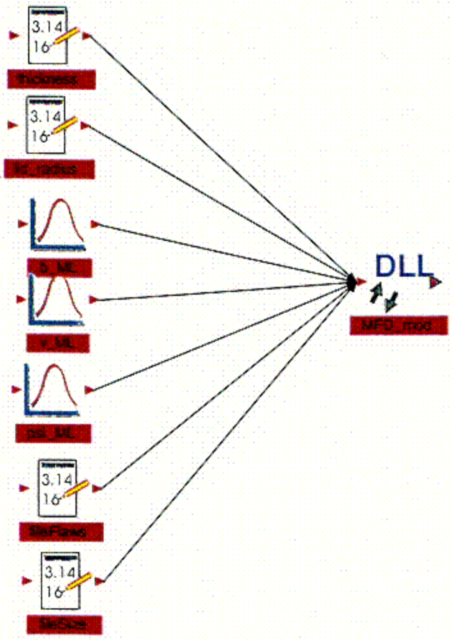

Figure 12. Contents of the MFD_MiddleLid Container in the Current WAPDEG Model GoldSim implementation (see Figure 6).

The contents of the container MFD_Middle_Lid (used in the Updated WAPDEG Model to provide input to modeling of the Alloy 22 waste package flat closure lid) are presented in Figure 13. The data element, thickness_ML, is the lid thickness in mm. The Alloy 22 waste package flat closure lid is 10 mm thick. The data element lid_radius_ML is 763.5 mm for the Alloy 22 waste package outer barrier flat closure lid. The non-detection probability parameters, b_ML and v_ML, uniformly range between 2.5 to 5 mm and 1 to 3 (see Section 4.1.7), respectively. The fraction of flaws considered, psi_ML, is sampled from a uniform distribution with bounding values of 0.3481 and 0.3632 (see Section 4.1.7), and the fraction of surface-breaking flaws, Fos_ML, is sampled from a uniform distribution with bounding values of 0.0013 and 0.0049. The data elements fileFlaws and fileSize are the file indices for the cumulative distribution

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functions representing the number of manufacturing defect flaws (file index 16) and their lengths (file index 17), respectively. These inputs are passed to the CWD DLL through the CWD_ML element. The other call to the CWD DLL (contained in the container MFD_OuterLid) is similar, differing only in the file indexes used (11 and 12), the lid thickness (25 mm for the Alloy 22 waste package outer barrier extended closure lid) and the lid radius used (770.5 mm for the Alloy 22 waste package outer barrier extended closure lid). For further discussion of the CWD algorithm, refer to the *CWD Software Routine Report* (CRWMS M&O 2000t).

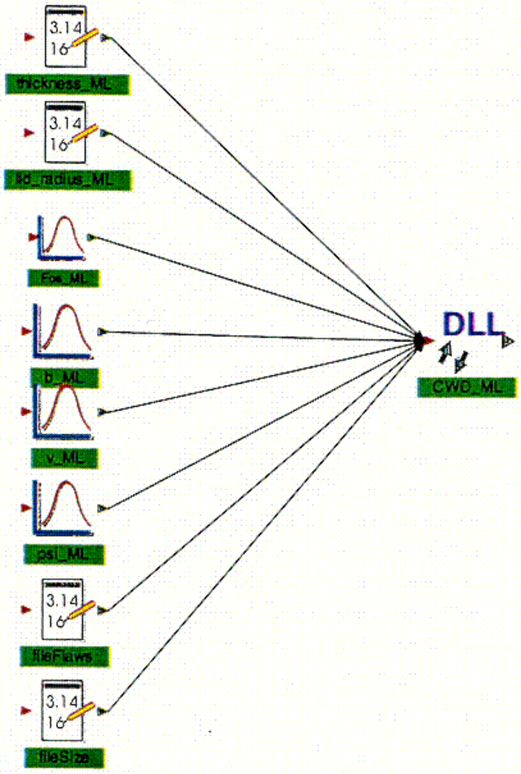

Figure 13. Contents of the MFD_MiddleLid Container in the Updated WAPDEG Model GoldSim implementation (see Figure 6).

All of the data and parameters discussed in this section were documented in the Analyses and Models Report entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i) and are tracked by DTN: MO0001SPASUP03.001 and DTN: MO0010SPASUP04.011 (see Table 4 for the Current WAPDEG Model and Table 5 for the Updated WAPDEG Model).

6.4.11.2 Manufacturing Defect Abstraction Model Validation

The Manufacturing Defect Abstraction Model (MDAM) is an abstraction model. The validation method used in this section is to review the model parameters for reasonableness, or consistency in explanation of all relevant data. This results in an appropriate level of confidence in the MDAM to consider it validated. As the MDAM is an abstraction model, the only data relevant to this validation exercise are the engineering analyses being abstracted (CRWMS M&O 2000o, Section 6.2.1 for the Current WAPDEG Model and CRWMS M&O 2000u, Section 6.2.1 for the Updated WAPDEG Model). The abstraction method used for the MDAM model is documented

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in the abstraction Analyses and Models Report (AMR) entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i, Section 6.2). Note that the MDAM uses the same model parameters and functional forms as its parent process-level models (CRWMS M&O 2000o, Section 6.2.1 for the Current WAPDEG Model and CRWMS M&O 2000u, Section 6.2.1 for the Updated WAPDEG Model). The MDAM model parameters and functional forms are technical product output developed using qualified methods per AP-3.10Q. The fact that the functional forms and model parameters used in the MDAM are identical to those provided in the process-level model is considered sufficient to validate the model inputs (i.e., the abstracted model is consistent with the process-level model). The MDAM is partially implemented within the WAPDEG software, which is fully qualified (see Section 3.1.2), and partially in the MFD software routine (for the Current WAPDEG Model) or CWD software routine (for the Updated WAPDEG Model) both of which are also fully qualified. Therefore, the MDAM inputs are validated and the model is implemented within qualified software. This results in an appropriate level of confidence in the MDAM to consider it validated.

6.4.12 Stress and Stress Intensity Factor Profile Abstraction Model

6.4.12.1 Stress and Stress Intensity Factor Profile Abstraction Model Implementation

The numerical manipulations discussed in Section 4.1.8 are implemented within the SCCD_External container which is called by the GoldSim implementation (see Figure 6). The contents of the SCCD_External container are shown in Figure 14.

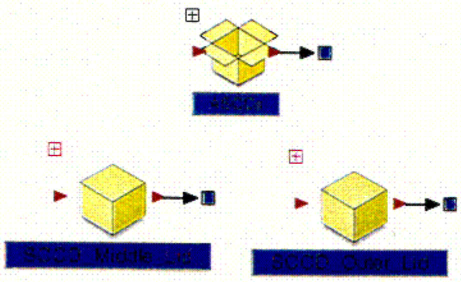

Figure 14. Contents of the SCCD_External Container in the GoldSim implementation (see Figure 6).

The contents of the container ASCCs are discussed in the next section. The contents of the container SCCD_Middle_Lid are shown in Figure 15. These data elements and functions implement the Stress and Stress Intensity Factor Profile Abstraction discussed in Section 4.1.8 and parts of the Slip Dissolution Model Abstraction discussed in Section 4.1.9. The data element idxinp contains the file index (15) for the input stress intensity factor (K_I) versus depth profiles listed in Table 7. The data elements A1_ML through A4_ML contain the stress coefficients for the flat closure lid listed in Table 8 for the Current WAPDEG Model and Table 9 for the Updated WAPDEG Model. The data element amp contains the amplitude of the stress variation used in Equation 6 (*17.236892*). The data element nangle contains the number of angles at which Equation 7 will be evaluated (5 or at each $\pi/5$ radians). The data elements YS_ML and fys_ML contain the yield strength and yield strength scaling factor (F), respectively, as listed in Table 10. The stochastic element z_ML represents the z argument to the $sz(z)$ function shown in Equation

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8. z_ML is sampled from a triangular distribution with a mean of zero, a lower bound of -3 and an upper bound of 3. The data element sinf contains the sine of the angle of projection that the crack path makes with the lid normal. The function Stress_ThreshML expression element takes the output of the Stress_ThreshMLfrac expression element (a value sampled from a uniform distribution between 0.2 and 0.3 for the Current WAPDEG Model and between 0.1 and 0.4 for the Updated WAPDEG Model) and multiplies it by the yield strength contained in the YS_ML data element to obtain the stress threshold for propagation of stress corrosion cracks (see Table 11 and Table 12). The data elements idxkin and idxstr contain the file indices for the output K_I and stress variability distributions (7 and 8, respectively). The Model_Number_ML data element contains the integer value 2 indicating that Uncertainty Model 2 (see CRWMS M&O 2000i, Section 6.3) is used to treat uncertainty in the stress and stress intensity factor profiles used for modeling stress corrosion cracking. For further discussion of the SCCD algorithm, refer to the *SCCD Software Routine Report* (CRWMS M&O 2000v). The other call to the SCCD DLL (contained in the container SCCD_Outer_Lid) is similar. For the Alloy 22 waste package outer barrier outer (extended closure) lid, the data element idxinp contains the file index (14), the stress coefficients for the extended closure lid from Table 8, for the Current WAPDEG Model, and Table 9, for the Updated WAPDEG Model, are used, the data element sinf is equal to one, and the file indices used for the output K_I and stress variability distributions are 4 and 5, respectively.

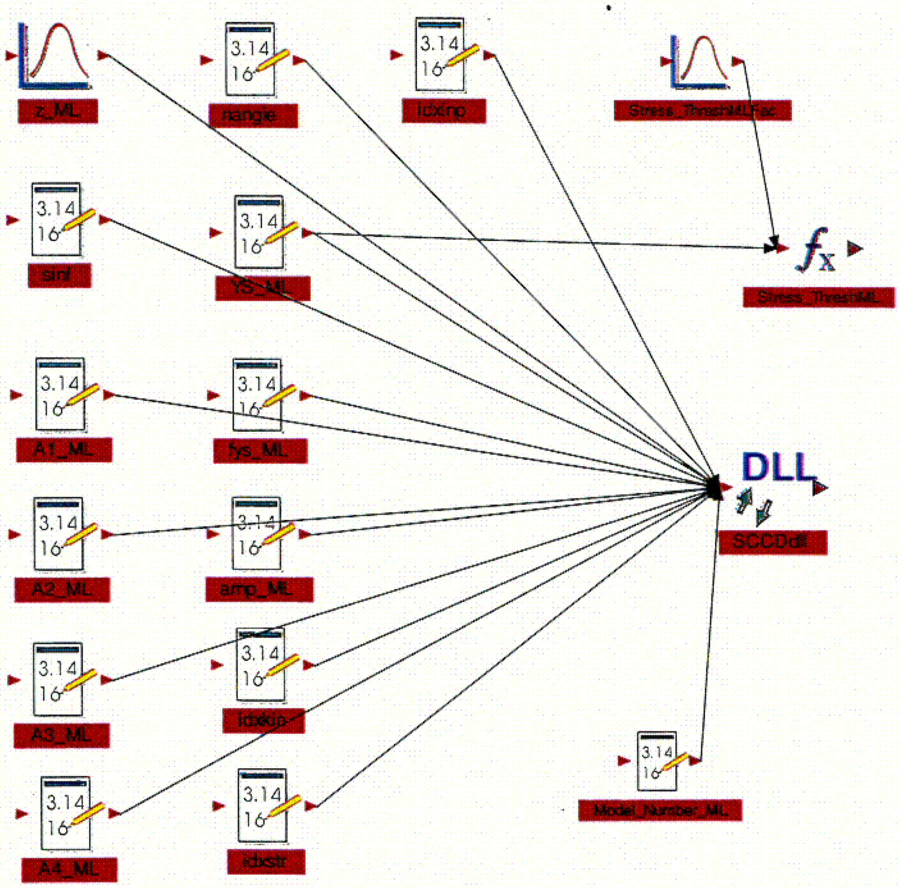

Figure 15. Contents of SCCD_Middle_Lid Container in the GoldSim implementation (see Figure 6).

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6.4.12.2 Stress and Stress Intensity Factor Profile Abstraction Model Validation

The Stress and Stress Intensity Factor Profile Abstraction Model (SSIFPAM) is an abstraction model. The validation method used in this section is to review the model parameters for reasonableness, or consistency in explanation of all relevant data. This results in an appropriate level of confidence in the SSIFPAM to consider it validated. As the SSIFPAM is an abstraction model, the only data relevant to this validation exercise is the process-level model being abstracted (CRWMS M&O 2000h, Section 6.2.2). The abstraction method used for the SSIFPAM model is documented in the abstraction Analyses and Models Report (AMR) entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i, Section 6.3) (DTN: MO0010MWDSUP04.010). This data is qualified. Note that the SSIFPAM uses the same model parameters and functional forms as its parent process-level model (CRWMS M&O 2000h, Section 6.2.2). The fact that the functional forms and model parameters used in the SSIFPAM are identical to those provided in the process-level model is considered sufficient to validate the model inputs (i.e., the abstracted model is consistent with the process-level model). The SSIFPAM is implemented within the qualified software routine SCCD DLL (CRWMS M&O 2000v). Therefore, the model inputs are validated and the model is implemented within qualified software. This results in an appropriate level of confidence in the model to consider it validated.

6.4.13 Slip Dissolution Abstraction Model

6.4.13.1 Slip Dissolution Abstraction Model Implementation

The contents of the ASCCs container (see Figure 14) are shown in Figure 16.

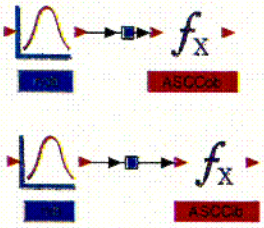

Figure 16. Contents of the ASCCs container in the SCCD_External container (see Figure 14) of the GoldSim implementation (see Figure 6).

The nob and nib stochastic elements sample the value of $\bar{n}$ (see Equation 13) to be used in modeling for the extended closure and flat closure lids, respectively. $\bar{n}$ is sampled from a uniform distribution between 3 and 3.36 in the Current WAPDEG Model and from a uniform distribution between 3.372 and 3.68 in the Updated WAPDEG Model. The expression elements ASCCob and ASCCib use the values of nob and nib (respectively) to evaluate Equation 12 (using Equation 13) for the extended closure and flat closure lids, respectively.

6.4.13.2 Slip Dissolution Abstraction Model Validation

The Slip Dissolution Abstraction Model (SDAM) is an abstraction model. The validation method used in this section is to review the model parameters for reasonableness, or consistency in explanation of all relevant data. This results in an appropriate level of confidence in the SDAM

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to consider it validated. As the SDAM is an abstraction model, the only data relevant to this validation exercise is the process-level model being abstracted (CRWMS M&O 2000h, Section 6.2.2). The abstraction method used for the SSIFPAM model is documented in the abstraction Analyses and Models Report (AMR) entitled *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i, Section 6.4) (DTN: MO0010MWDSUP04.010). This data is qualified. Note that the SDAM uses the same model parameters and functional forms as its parent process-level model (CRWMS M&O 2000h, Section 6.2.2). The fact that the functional forms and model parameters used in the SDAM are identical to those provided in the process-level model is considered sufficient to validate the model inputs (i.e., the abstracted model is consistent with the process-level model). The SDAM is implemented within the WAPDEG software, which is fully qualified (see Section 3.1.2). Therefore, the model inputs are validated and the model is implemented within qualified software. This results in an appropriate level of confidence in the model to consider it validated.

6.4.14 Waste Package Outer Barrier Microbial Induced Corrosion (MIC) Abstraction Model

6.4.14.1 Waste Package Outer Barrier Microbial Induced Corrosion (MIC) Abstraction Model Implementation

The Waste Package Outer Barrier MIC Model consists of a threshold relative humidity (RH) and a general corrosion rate multiplier. During each time step, the WAPDEG DLL reads the RH from the exposure file, and if this RH exceeds the threshold RH, MIC is allowed to occur. The effect of MIC is to increase the general corrosion rate by a multiplication factor that is sampled from a uniform distribution with a lower bound of 1 and an upper bound of 2 (see Table 13).

6.4.14.2 Waste Package Outer Barrier Microbial Induced Corrosion (MIC) Abstraction Model Validation

The Waste Package Outer Barrier Microbial Induced Corrosion Abstraction Model (WPOBMICAM) is an abstraction model. The validation method used in this section is to review the model parameters for reasonableness, or consistency in explanation of all relevant data. This results in an appropriate level of confidence in the WPOBMICAM to consider it validated. As the WPOBMICAM is an abstraction model, the only data relevant to this validation exercise is the process-level model being abstracted (CRWMS M&O 2000e, Sections 6.8 and 6.10). The WPOBMICAM parameters, consisting of a uniform distribution between 1 and 2, are technical product output information developed using qualified methods per AP-3.10Q and obtained from controlled and confirmed sources. Note that the WPOBMICAM uses the same model parameters as its parent process-level model (CRWMS M&O 2000e, Sections 6.8 and 6.10). The fact that the model parameters used in the WPOBMICAM are identical to those provided in the process-level model is considered sufficient to validate the model inputs (i.e., the abstracted model is consistent with the process-level model). The WPOBMICAM is implemented within the WAPDEG software, which is fully qualified (see Section 3.1.2). Therefore, the model inputs are validated and the model is implemented within qualified software. This results in an appropriate level of confidence in the model to consider it validated.

As noted in Section 6.3.3, the uncertainty treatment applied to the WPOBMICAM in this analysis is not identical to the uncertainty treatment recommended in the process-level model. However, the uncertainty treatment used in this analysis is more reasonable than that recommended in the process-level model. Therefore, this disagreement has no effect on the validation status of this model.

6.4.15 Waste Package Outer Barrier Aging and Phase Instability Abstraction Model

6.4.15.1 Waste Package Outer Barrier Aging and Phase Instability Abstraction Model Implementation

The Waste Package Outer Barrier Aging and Phase Instability Abstraction Model consists of a general corrosion rate multiplier distribution. Upon satisfaction of the relative humidity threshold for initiation of corrosion degradation (Section 6.4.8), the general corrosion rate is enhanced by a multiplier sampled from a uniform distribution with a lower bound of 1 and an upper bound of 2.5 (see Table 14).

6.4.15.2 Waste Package Outer Barrier Aging and Phase Instability Abstraction Model Validation

The Waste Package Outer Barrier Aging and Phase Instability Abstraction Model (WPOAPIAM) is an abstraction model. The validation method used in this section is to review the model parameters for reasonableness, or consistency in explanation of all relevant data. This results in an appropriate level of confidence in the WPOAPIAM to consider it validated. As the WPOAPIAM is an abstraction model, the only data relevant to this validation exercise is the process-level model being abstracted (CRWMS M&O 2000e, Sections 6.7.3 and 6.10) (DTN: LL000212405924.130). This data is qualified. The WPOAPIAM parameters, consisting of a uniform distribution between 1 and 2.5, are derived from qualified developed data. Note that the WPOAPIAM uses the same model parameters as its parent process-level model (CRWMS M&O 2000e, Sections 6.7.3 and 6.10). The fact that the model parameters used in the WPOAPIAM are identical to those provided in the process-level model is considered sufficient to validate the model inputs (i.e., the abstracted model is consistent with the process-level model). The WPOAPIAM is implemented within the WAPDEG software, which is fully qualified (see Section 3.1.2). Therefore, the model inputs are validated and the model is implemented within qualified software. This results in an appropriate level of confidence in the model to consider it validated.

As noted in Section 6.3.2, the uncertainty treatment applied to the WPOAPIAM in this analysis is not identical to the uncertainty treatment recommended in the process-level model. However, the uncertainty treatment used in this analysis is more reasonable than that recommended in the process-level model. Therefore, this disagreement has no effect on the validation status of this model.

6.4.16 Waste Package and Drip Shield Exposure Conditions (RH, T, Drips/No Drips, Seepage Water Chemistry, Etc.)

The exposure condition inputs to the WAPDEG analysis (see Section 4.1.12) are derived from three tables of pH data, two tables of Cl data, and multiple thermal hydrology infiltration bins containing data on temperature and relative humidity. The PREWAP routine extracts this data from these various tables (DTN: SN0007T0872799.014, MO0002SPALO046.010, MO9911SPACDP37.001) and prepares an output table that is used as input to the WAPDEG routine. For further discussion of the PREWAP algorithm, refer to Attachment I.

6.4.17 Variance Sharing

The WAPDEG DLL makes use of several variance sharing parameters. Variance sharing is similar to Gaussian Variance Partitioning between uncertainty and variability. However variance sharing is used to partition the variance of a variability distribution (perhaps resulting from a call to the GVP routine) between waste package to waste package variability and patch to patch variability on a given waste package (and/or crack to crack and pit to pit variability for localized degradation models). That is, given a variability distribution, e.g. a general corrosion cdf, and a variance share, the WAPDEG DLL samples a value for the general corrosion rate for a waste package patch based on the fraction of variance (one of the VarShar_x's).

The contents of the Variance_Share container is shown in Figure 17.

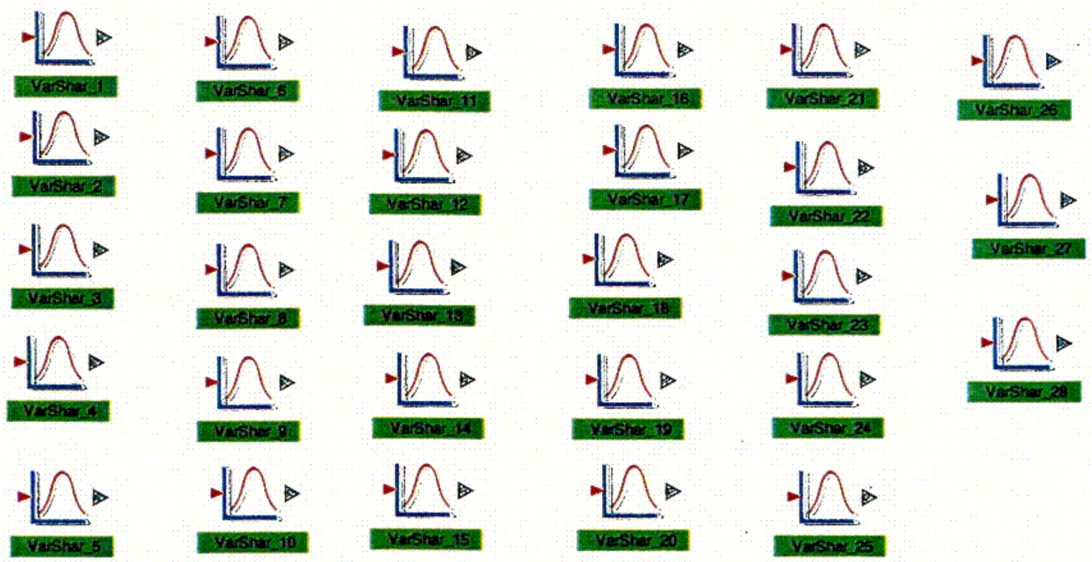

Figure 17. Contents of the Variance_Shares container in the GoldSim implementation (see Figure 6).

Each of the stochastic elements VarShar_1 through VarShar_28 are sampled from a uniform distribution with an upper bound of 1 and a lower bound of zero. These sampled values are used in a similar manner to the stochastic element, U, in the GVP routine discussed in Section 6.4.7.

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Var_Shar1 through Var_Shar8 are used to determine the fraction of variance allocated to waste package to waste package and patch to patch variance for the general corrosion models used during a simulation. Var_Shar9 through Var_Shar16 are used to determine the fraction of variance allocated to waste package to waste package, patch to patch, and pit to pit variance for the localized corrosion models used during a simulation. Var_Shar17 through Var_Shar22 are used to determine the fraction of variance allocated to waste package to waste package, patch to patch, and crack to crack variance for the stress corrosion cracking models used during a simulation. Var_Shar23 through Var_Shar28 are used determine the fraction of variance allocated to waste package to waste package and patch to patch variance for the microbially induced corrosion and aging and phase instability general corrosion enhancement factor models used during a simulation.

6.4.18 WAPDEG Model Validation

The WAste PAckage DEGradation (WAPDEG) Model is an abstraction model. The validation method used in this section is to review the model parameters for reasonableness, or consistency in explanation of all relevant data. This results in an appropriate level of confidence in the WAPDEG Model to consider it validated. As the WAPDEG Model is an abstraction model, the only data relevant to this validation exercise is the process-level models being abstracted. The WAPDEG conceptual model is discussed in Secion 6.2. The various abstraction models implemented within the WAPDEG Model have been validated throughout this Section (e.g., Sections 6.4.5, 6.4.6, 6.4.8, 6.4.10, 6.4.11, 6.4.12, 6.4.13, 6.4.14, and 6.4.15). These individual validations concluded that the abstracted models were consistent with their parent process-level models. The WAPDEG Model is implemented within the WAPDEG software, which is fully qualified (see Section 3.1.2). Therefore, the WAPDEG Model inputs (the abstracted models and parameters) are validated and the WAPDEG Model is implemented within qualified software. This results in an appropriate level of confidence in the WAPDEG Model to consider it validated.

6.5 ANALYSIS RESULTS

6.5.1 Current WAPDEG Model Nominal-Case Results

The previous Sections have documented the inputs to the WAPDEG nominal-case analysis. In this section, the results of the WAPDEG nominal-case analysis for waste package and drip shield degradation are presented. As discussed in Section 6.1, the waste package and drip shield degradation analyses to be presented in this Section are for 100 realizations of WAPDEG to account for the uncertainty analysis of the uncertain corrosion parameters. Each WAPDEG realization corresponds to a complete WAPDEG run to represent the degradation variability for a given number of waste package and drip shield pairs. The major simulation parameters used in the analysis are summarized below.

- Temperature, relative humidity, and contacting solution pH histories without the use of backfill (see Section 6.4.16)
- 400 waste package and drip shield pairs
- 20 mm thick waste package outer barrier (Alloy 22)

- 15 mm thick drip shield (Titanium grade 7)
- 1000 patches per waste package
- 500 patches per drip shield
- The MFD DLL (see Section 3.1.4) is used for the treatment of manufacturing defects in the Alloy 22 waste package outer barrier closure weld regions.
- The conservative (see Table 10) yield strength scaling factor of ±30% is used to treat uncertainty in the stress and stress intensity factor profiles
- The stress threshold is uniformly distributed between 20 and 30% of the yield strength

Sensitivities using other choices of the last two parameters are discussed in the next section.

A complete list of input parameters and their values used is given in the input file, bsr20.xls (DTN: MO0010MWDWAP01.009). The WAPDEG analysis results (i.e., waste package and drip shield failure time and number of crack, pit and patch penetrations) are reported as a group of "degradation profile curves" that represent the potential range of the output parameters. All input files used in this analysis and output files produced from this analysis are tracked by DTN: MO0010MWDWAP01.009. The analysis results are presented for the upper and lower bounds, mean, and 95th, 75th, 25th and 5th percentiles as a function of time for the following output parameters:

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

Note that localized corrosion does not initiate for either the waste package (Alloy 22 outer barrier) or the drip shield, because the exposure conditions on the drip shield and waste package surface are not severe enough to initiate localized corrosion (i.e., the corrosion potential is less than the threshold corrosion potential) (see Sections 6.3.9 and 6.3.10). Also note that the drip shield is assumed not to be subject to stress corrosion cracking (see Section 6.2), thus no crack penetration failure of the drip shield is calculated. Thus, for the drip shield, the first patch breach time profile is the same as the failure time profile.

The upper and lower bounds, mean, and 95th, 75th, 25th and 5th percentile curves do not correspond to single realizations. They are summary statistics related to consideration of all 100 realizations. In the bullets below, the origin of the upper and lower bound, mean, and 95th, 75th, 25th and 5th percentile curves for first breach of the waste package are discussed. Similar wording (not included for the sake of brevity) could be applied for discussion of origins of the drip shield first breach curves, waste package first crack penetration curves, etc.

- At each point in time the upper bound curve shows the realization with the greatest fraction of waste packages failed calculated in any one of the 100 realizations. This may not be the same realization at each point in time. The upper bound curve becomes non-zero at the time of failure of first waste package in all of the 100 realizations.

- At each point in time the 95th percentile curve shows the realization with the 95th greatest fraction of waste packages failed, i.e., 95 realizations out of 100 have smaller fraction of waste packages failed calculated in any one of the 100 realizations. This may not be the same realization at each point in time. The 95th percentile curve becomes non-zero at the time when at least 5 realizations have at least one waste package failure.

- At each point in time the 75th percentile curve shows the realization calculated in any one of the 100 realizations with the 75th greatest fraction of waste packages failed, i.e., 75 realizations out of 100 have smaller fraction of waste packages failed. This may not be the same realization at each point in time. The 75th percentile curve becomes non-zero at the time when at least 25 realizations have at least one waste package failure.

- At each point in time the 25th percentile curve shows the realization calculated in any one of the 100 realizations with the 25th greatest fraction of waste packages failed, i.e., 25 realizations out of 100 have smaller fraction of waste packages failed. This may not be the same realization at each point in time. The 25th percentile curve becomes non-zero at the time when at least 75 realizations have at least one waste package failure.

- At each point in time the 5th percentile curve shows the realization calculated in any one of the 100 realizations with the 5th greatest fraction of waste packages failed, i.e., 5 realizations out of 100 have smaller fraction of waste packages failed. This may not be the same realization at each point in time. The 5th percentile curve becomes non-zero at the time when at least 95 realizations have at least one waste package failure.

- At each point in time the mean curve shows the mean of all the fractions of waste packages failed in all of the 100 realizations. The mean curve becomes non-zero at the time of failure of first waste package in all of the 100 realizations.

Figure 18 shows the upper and lower bounds, mean, and 95th, 75th, 25th and 5th percentile confidence intervals of the first breach profile for the waste packages with time. The upper bound profile, which is the upper extreme of the probable range of the first breach time, indicates that the earliest possible first breach time for a waste package is about 10,000 years. Note that the estimated earliest possible first breach time has a very low probability. It can be shown by comparing with the upper bound profile in Figure 21 (showing the first crack breach profiles of waste packages with time) that the first breach is by SCC crack penetration (see the discussion of the results in Figure 19 and Figure 20 later in this Section). The median estimate (50% of waste packages failed) of the first breach time of the upper bound profile is about 34,000 years. The median estimate of the first breach time of the mean profile is about 97,000 years. The time to fail 10 percent of waste packages for the two profiles is about 23,000 and 49,500 years, respectively.

Figure 19 shows the first breach profiles of drip shields with time. Because the drip shields are not subject to stress corrosion cracking and localized corrosion, the first breach profiles shown in the figure are all by general corrosion only. As discussed in Section 6.2, both the upper and under sides of the drip shield are exposed to the exposure conditions in the emplacement drift and are subject to corrosion. In addition, both sides experience the same exposure conditions regardless of whether the drip shields are dripped on or not. Thus, in the analysis, the general corrosion rate for the drip shields is sampled twice independently, once for the patches on the upper side and the once for the patches on the under side. This results in reduced variability in the degradation profiles and thus a fast failure rate (i.e., many drip shields failing over a short time period). This is shown in the upper bound profile, in which the drip shield first breach starts at about 20,000 years and 50 percent of the drip shields fail within a couple of thousand years after the initial failure. Similar trends are also seen with the 95th, 75th and mean profiles. In terms of the number of patch penetration openings per failed drip shield with time in Figure 20, the upper bound profile shows that as the drip shields fail, a large number of patches are perforated over a relatively short time period (a few thousand years). A similar trend is seen for the 95th percentile profile. However, the profile shows a larger spread for the other profiles.

Figure 21 and Figure 22 show respectively the first crack penetration and patch penetration profiles of the waste packages with time. The first crack breach times of the upper bound and 95th percentile profiles are about 10,000 and 20,000 years respectively (Figure 21), and the first patch breach times of the upper and 95th percentile profiles are about 36,500 and 41,000 years, respectively (Figure 22). Comparison of the first crack and patch breach profiles with the first breach profiles in Figure 18 indicates that the initial breach (or failure) of the waste packages is likely by SCC crack penetration in the Alloy 22 waste package outer barrier closure lid welds. For the 75th percentile profiles in the figures, the first crack and patch penetration times are about 30,000 and 50,000 years, respectively.

Figure 23 shows the profile for the average number of crack penetrations per failed waste package. As discussed for Figure 22, the upper bound and 95th percentile profiles show the first crack penetration at about 10,000 and 20,000 years, respectively. The mean profile never develops more than 25 cracks. SCC cracks in passive alloys such as Alloy 22 tend to be very tight (i.e., small crack opening displacement) by nature (CRWMS M&O 2000h, Section 6.5.5). The opposing sides of through-wall SCC cracks will continue to corrode at very low passive corrosion rates until the gap region of the tight crack opening is "plugged" by the corrosion product particles and precipitates such as carbonate present in the water. Any water transport through this oxide/salt filled crack area will be mainly by diffusion-type transport processes (CRWMS M&O 2000h). Thus, both the effective water flow rate into the waste packages and the radionuclide release rate from the waste packages through the SCC cracks would be expected to be extremely low and should not contribute significantly to the overall radionuclide release rate from the repository.

Figure 24 presents the profile for the average number of patch openings per failed waste package. For the upper bound profile, which again represents an extremely low probability case, the first patch breach occurs at about 36,500 years (see also Figure 22), and about 15 patches of the failed waste packages (about 1.5 percent of the waste package surface area) are breached by 100,000 years. For the mean profile, there will be only 2.5 patch openings in each of the failed waste packages by 100,000 years.

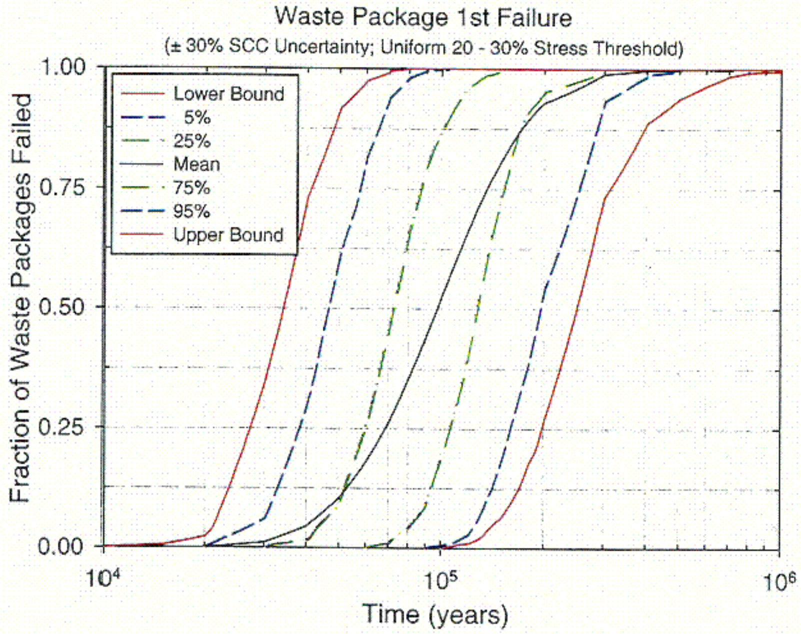

Figure 18. The Upper and Lower Bounds, Mean, and 95[th], 75[th], 25[th] and 5[th] Percentile Confidence Intervals of the First Breach Profile of Waste Packages with Time for the Current WAPDEG Model

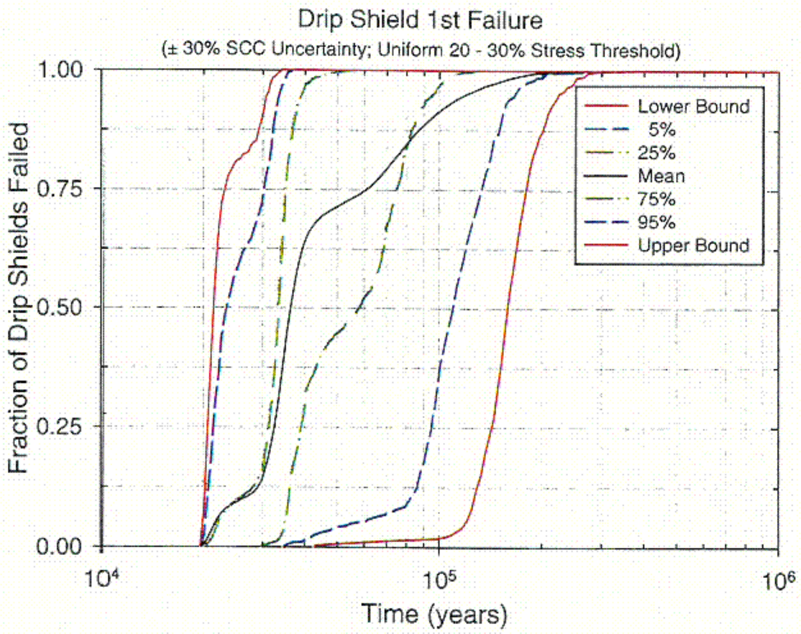

Figure 19. The Upper and Lower Bounds, Median, and 95[th], 75[th], 25[th] and 5[th] Percentile Confidence Intervals of the First Breach Profile of Drip Shield with Time for the Current WAPDEG Model

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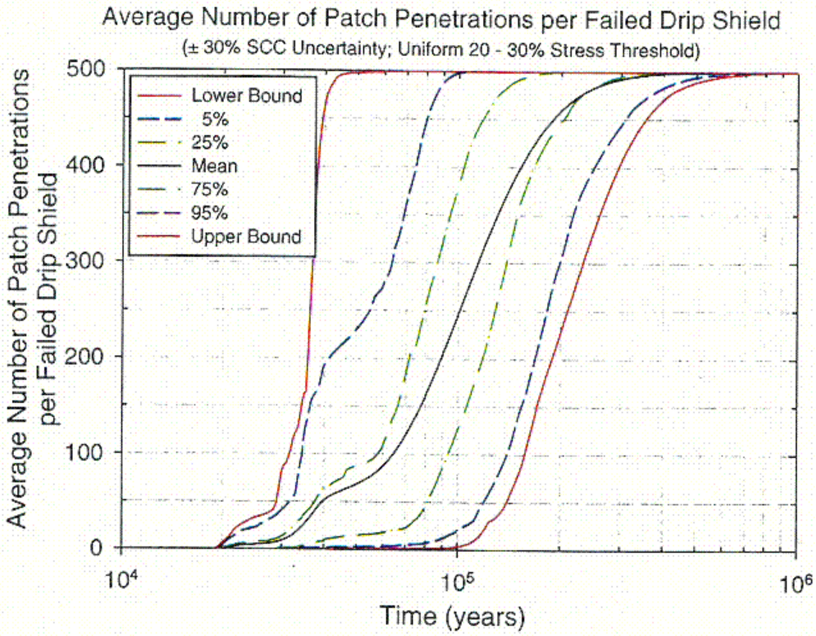

Figure 20. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Average Number of Patch Penetrations per Failed Drip Shield Profile with Time for the Current WAPDEG Model

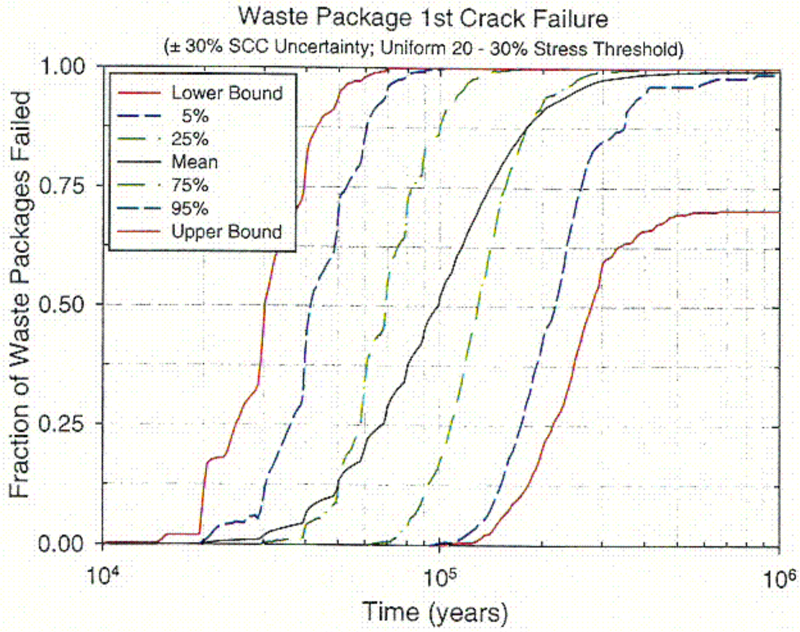

Figure 21. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Crack Breach Profile of Waste Packages with Time for the Current WAPDEG Model

C15

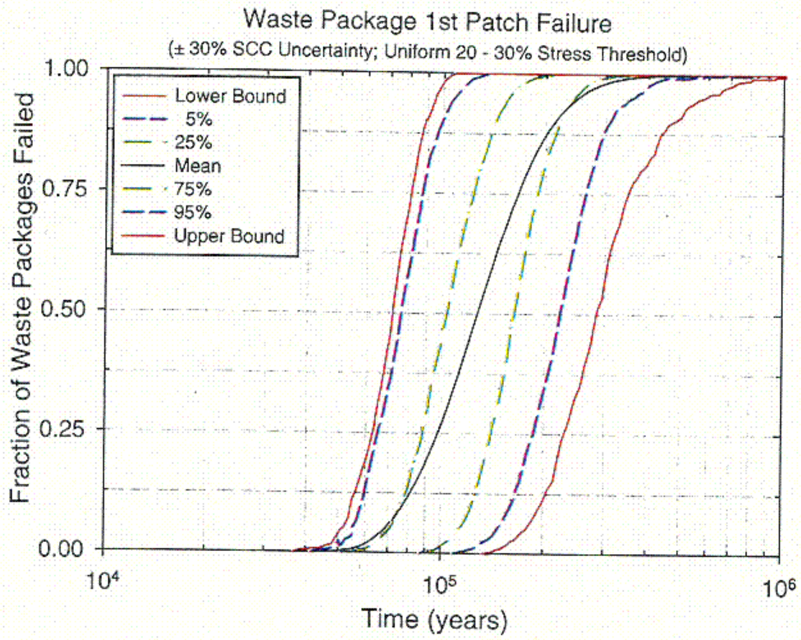

Figure 22. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Patch Breach Profile of Waste Packages with Time for the Current WAPDEG Model

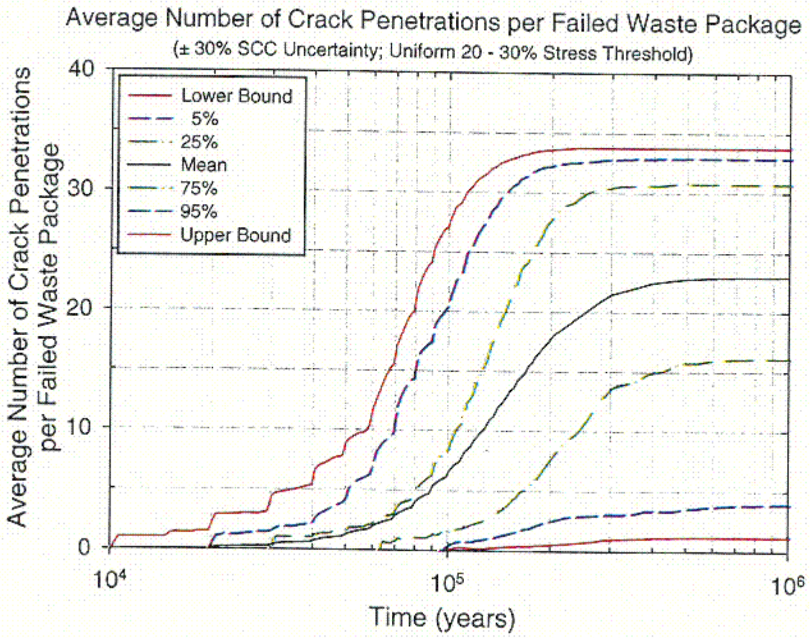

Figure 23. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Average Number of Crack Penetrations per Failed Waste Package Profile with Time for the Current WAPDEG Model

C16

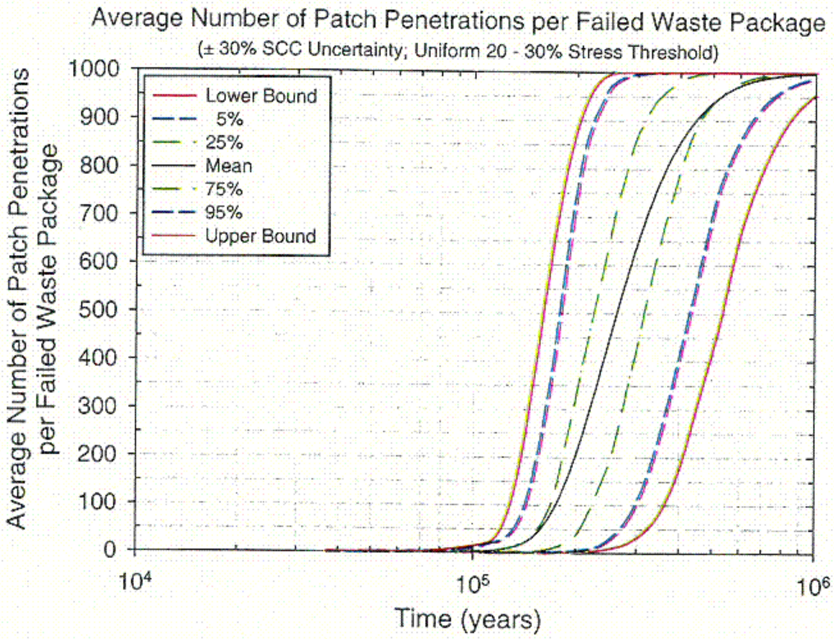

Figure 24. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Average Number of Patch Penetrations per Failed Waste Package Profile with Time for the Current WAPDEG Model

6.5.2 Sensitivities Using the Current WAPDEG Model

Four sensitivities were conducted using the Current WAPDEG Model. The first two of these utilize the optimum (±5%) and realistic (±10%) choices for the yield strength scaling factor (see Table 10). All other parameters used are the same as those for the Current WAPDEG Model nominal case. The drip shield failure and waste package patch breach profiles are similar to those discussed in the nominal case since only SCC crack modeling parameters are being changed in these sensitivities. Therefore, only the waste package first breach and first crack time profiles are discussed.

In Figure 25 the upper and lower bounds, mean, and 95th, 75th, 25th and 5th percentile confidence intervals of the first breach profile for the waste packages with time using the optimum yield strength scaling factor are presented. The upper bound profile, which is the upper extreme of the probable range of the first breach time, indicates that the earliest possible first breach time for a waste package is about 20,000 years (10,000 years later than in the nominal case). It can be shown by comparing with the upper bound profile in Figure 26 (showing the first crack breach profiles of waste packages with time) that the first breach is by SCC crack penetration. The median estimate (50% of waste packages failed) of the first breach time of the upper bound profile is about 51,000 years (17,000 years later than in the nominal case). The median estimate of the first breach time of the mean profile is about 91,000 years (6,000 years earlier than in the nominal case). The time to fail 10 percent of waste packages for the two profiles is about 36,000 and 56,000 years, respectively.

C17

Figure 26 shows the first crack penetration profiles of the waste packages with time. The first crack breach times of the upper bound and 95th percentile profiles are about 19,500 and 22,000 years, respectively. These times are about 9,500 and 2,000 years later, respectively, than the conservative case. For the 75th percentile profiles in the figure, the first crack penetration time is about 71,500 years (about 41,500 years later than in the nominal case).

In Figure 27 the upper and lower bounds, mean, and 95th, 75th, 25th and 5th percentile confidence intervals of the first breach profile for the waste packages with time using the realistic yield strength scaling factor are presented. The upper bound profile, which is the upper extreme of the probable range of the first breach time, indicates that the earliest possible first breach time for a waste package is about 20,000 years (10,000 years later than in the nominal case). It can be shown by comparing with the upper bound profile in Figure 28 (showing the first crack breach profiles of waste packages with time) that the first breach is by SCC crack penetration. The median estimate (50% of waste packages failed) of the first breach time of the upper bound profile is about 50,500 years (16,500 years later than in the nominal case). The median estimate of the first breach time of the mean profile is about 93,700 years (4,300 years earlier than in the nominal case). The time to fail 10 percent of waste packages for the two profiles is about 35,000 and 55,500 years, respectively.

Figure 28 shows the first crack penetration profiles of the waste packages with time. The first crack breach times of the upper bound and 95th percentile profiles are about 19,500 and 20,500 years, respectively. These times are about 9,500 and 500 years later, respectively, than the nominal case. For the 75th percentile profile in the figure, the first crack penetration time is about 30,000 years (about the same time as in the nominal case).

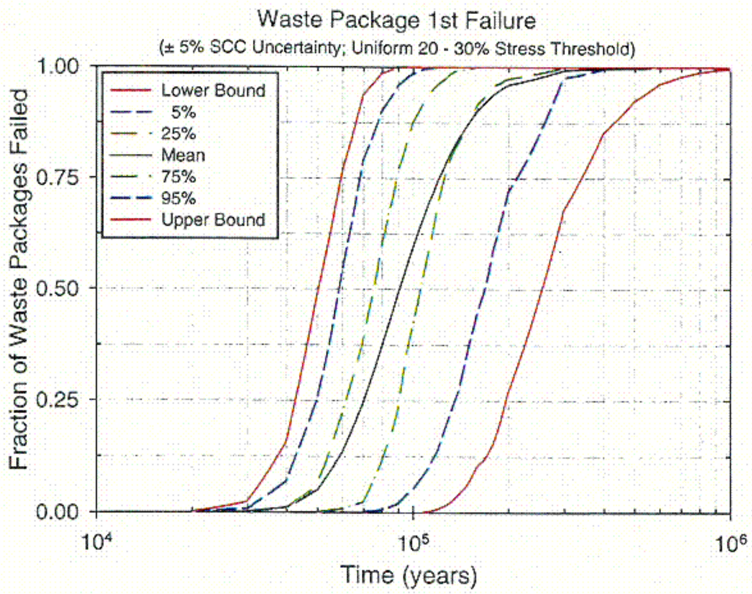

Figure 25. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Breach Profile of Waste Packages with Time using Optimum (±5%) Yield Strength Scaling Factor.

C18

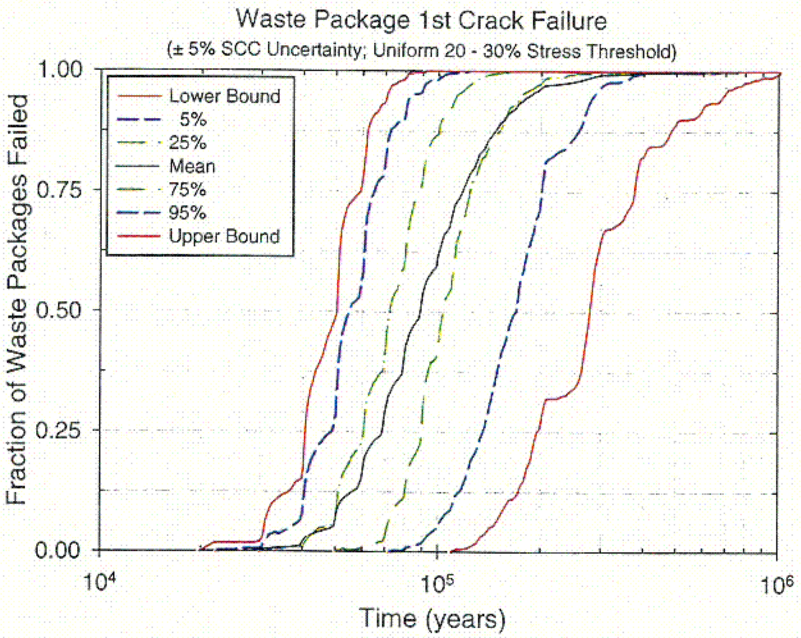

Figure 26. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Crack Breach Profile of Waste Packages with Time using Optimum (±5%) Yield Strength Scaling Factor.

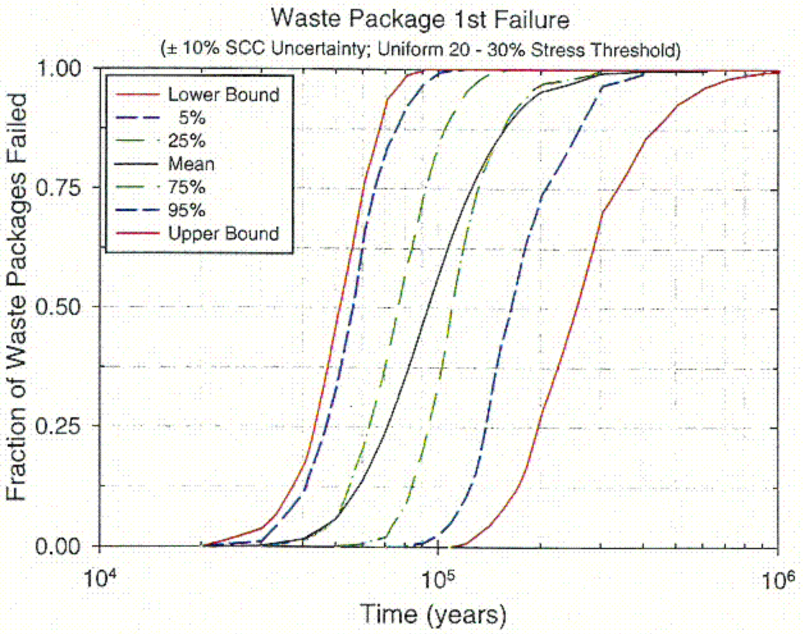

Figure 27. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Breach Profile of Waste Packages with Time using Realistic (±10%) Yield Strength Scaling Factor.

C19

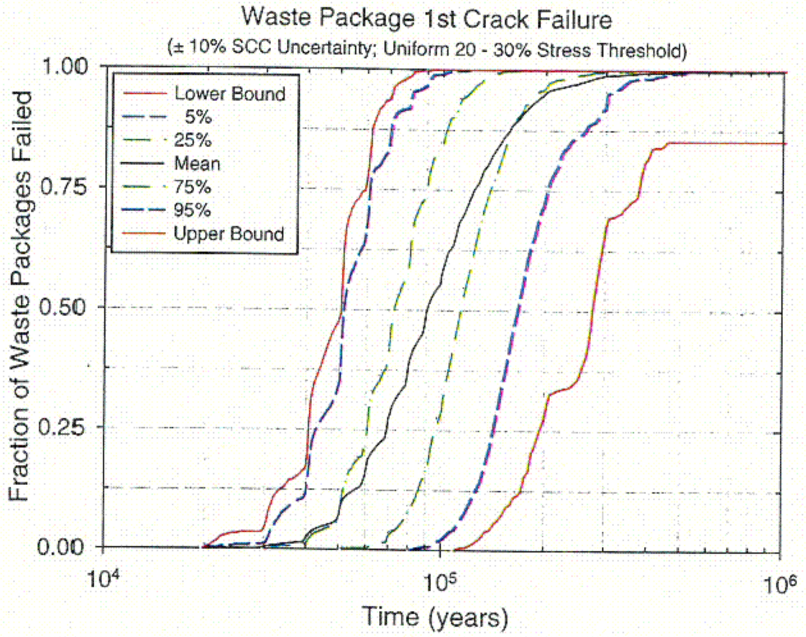

Figure 28. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Crack Breach Profile of Waste Packages with Time using Realistic (±10%) Yield Strength Scaling Factor.

The third sensitivity study conducted using the Current WAPDEG Model involved changing the stress threshold from a uniform distribution between 20 and 30% of the yield strength used in the nominal case to a wider range between 10 and 40% of the yield strength. All other parameters used are the same as those for the Current WAPDEG Model nominal case. The drip shield failure and waste package patch breach profiles are similar to those discussed in the nominal case since only SCC crack modeling parameters are being changed in these sensitivities. Therefore, only the waste package first breach and first crack time profiles are discussed.

In Figure 29 the upper and lower bounds, mean, and 95th, 75th, 25th and 5th percentile confidence intervals of the first breach profile for the waste packages with time using the modified stress threshold distribution are presented. The upper bound profile, which is the upper extreme of the probable range of the first breach time, indicates that the earliest possible first breach time for a waste package is about 15,000 years (5,000 years later than in the nominal case). It can be shown by comparing with the upper bound profile in Figure 30 (showing the first crack breach profiles of waste packages with time) that the first breach is by SCC crack penetration. The median estimate (50% of waste packages failed) of the first breach time of the upper bound profile is about 34,000 years (about the same time as in the nominal case). The median estimate of the first breach time of the mean profile is about 97,000 years (about the same time as in the nominal case). The time to fail 10 percent of waste packages for the two profiles is about 23,000 and 36,000 years, respectively.

Figure 30 shows the first crack penetration profiles of the waste packages with time. The first crack breach times of the upper bound and 95th percentile profiles are about 15,000 and 20,000

C20

years, respectively. The upper bound first crack breach time is about 5,000 years later than the nominal case. The 95th percentile first crack breach time is about the same as the nominal case. For the 75th percentile profile in the figure, the first crack penetration time is about 30,000 years (about the same time as in the nominal case).

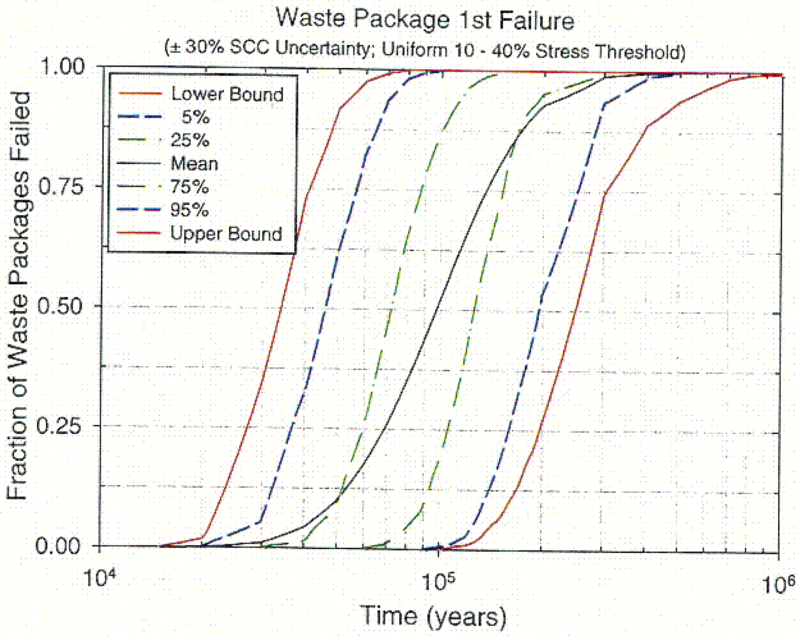

Figure 29. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Breach Profile of Waste Packages with Time using Conservative (±30%) Yield Strength Scaling Factor and Modified Stress Threshold Distribution.

C21

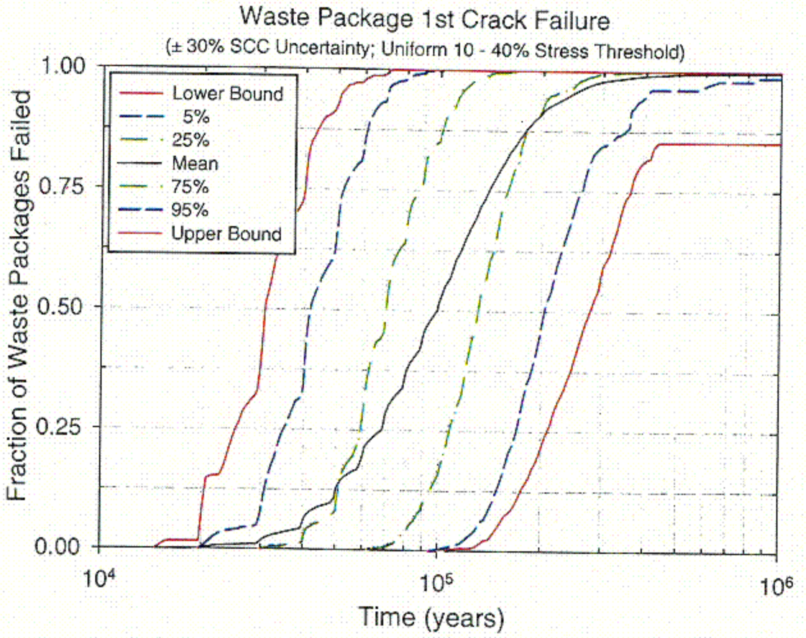

Figure 30. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Crack Breach Profile of Waste Packages with Time using Conservative (±30%) Yield Strength Scaling Factor and Modified Stress Threshold Distribution.

The fourth sensitivity study conducted using the Current WAPDEG Model involved changing the fraction of flaws considered from a uniform distribution between 0.3481 and 0.3632 used in the nominal case to a uniform distribution between 0.003481 and 0.003632, i.e., only 1% of the flaws are considered capable of propagation in the radial direction in the presence of hoop stresses. This less conservative choice of parameters is consistent with analyses of flaw orientations presented in the *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier and the Stainless Steel Structural Material* AMR (CRWMS M&O 2000h, Section 6.5.1) and the *Analysis of Mechanisms for Early Waste Package Failure* AMR (CRWMS M&O 2000u, Section 6.2.1). All other parameters used are the same as those for the Current WAPDEG Model nominal case. The drip shield failure and waste package patch breach profiles are similar to those discussed in the nominal case since only SCC crack modeling parameters are being changed in these sensitivities. Therefore, only the waste package first breach and first crack time profiles are discussed.

In Figure 31 the upper and lower bounds, mean, and 95th, 75th, 25th and 5th percentile confidence intervals of the first breach profile for the waste packages with time using the modified stress threshold distribution are presented. The upper bound profile, which is the upper extreme of the probable range of the first breach time, indicates that the earliest possible first breach time for a waste package is about 20,000 years (about 10,000 years earlier than the nominal case). It can be shown by comparing with the upper bound profile in Figure 32 (showing the first crack breach profiles of waste packages with time) that the first breach is by SCC crack penetration. The median estimate (50% of waste packages failed) of the first breach time of the upper bound profile is about 55,000 years (about 25,000 years later than the nominal case). The median

C22

estimate of the first breach time of the mean profile is about 115,000 years (about 18,000 years later than in the nominal case). The time to fail 10 percent of waste packages for the two profiles is about 40,000 and 66,000 years, respectively.

Figure 32 shows the first crack penetration profiles of the waste packages with time. The first crack breach times of the upper bound and 95th percentile profiles are about 20,000 and 29,000 years, respectively. The upper bound first crack breach time is about 10,000 years later than the nominal case. The 95th percentile first crack breach time is about 19,000 years later than in the nominal case. For the 75th percentile profile in the figure, the first crack penetration time is about 45,000 years (about 15,000 years later than in the nominal case).

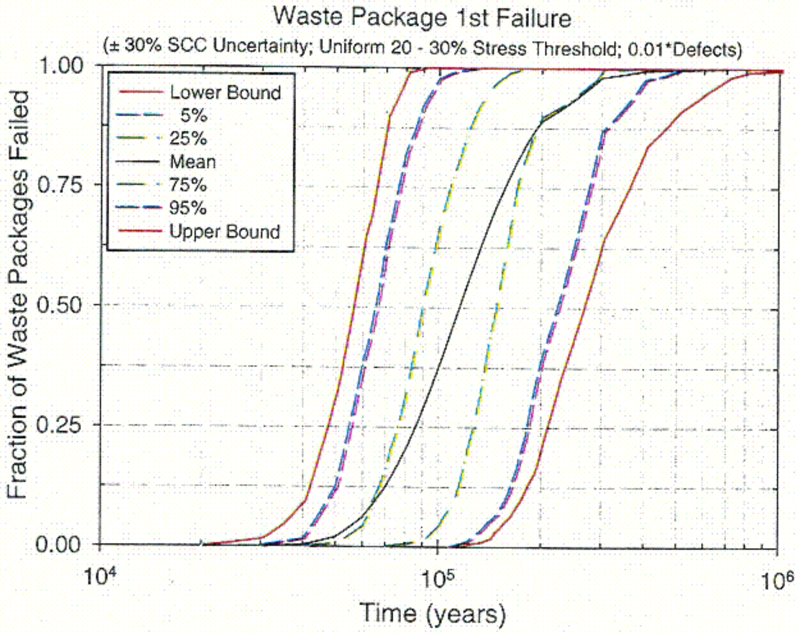

Figure 31. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Breach Profile of Waste Packages with Time Considering only 1% of the Flaws Capable of Propagation in Radial Direction

C23

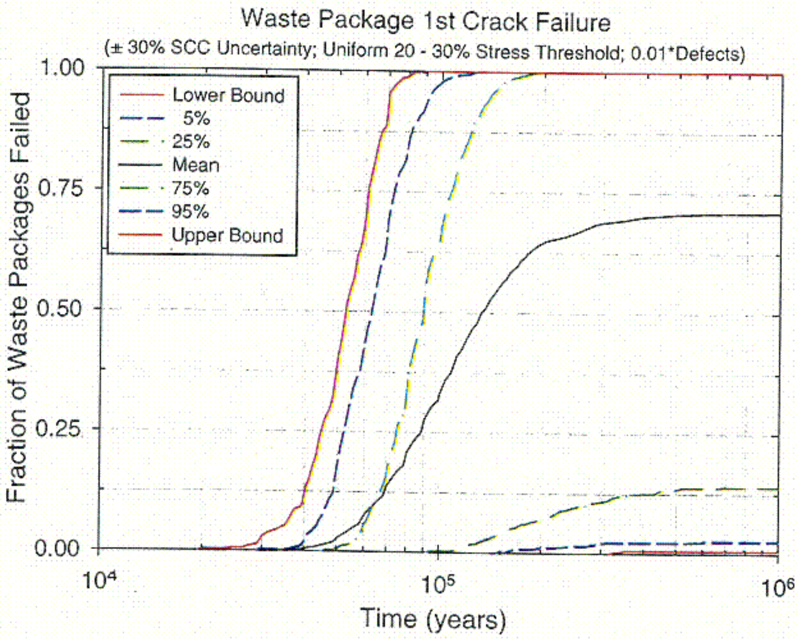

Figure 32. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Crack Breach Profile of Waste Packages with Time Considering only 1% of the Flaws Capable of Propagation in Radial Direction

6.5.3 Updated WAPDEG Model Results

As mentioned in Section 1, two WAPDEG models are documented in this report. The Updated WAPDEG Model differs from the Current WAPDEG Model due to changes to a few model inputs. These differences are summarized below:

- The Updated WAPDEG Model uses the CWD DLL (CRWMS M&O 2000t) (the Current WAPDEG Model uses the MFD DLL (CRWMS M&O 2000s)) in its treatment of the Manufacturing Defects Abstraction Model.
- The lid radii used in the Updated WAPDEG Model and the lower bound on the distribution for the location parameter for the probability of non-detection (*b*) are larger than those used in the Current WAPDEG Model.
- The Updated WAPDEG Model also uses one more input than the Current WAPDEG Model in its treatment of the Manufacturing Defects Abstraction Model, F_{os}, the fraction of surface-breaking flaws.
- The Updated WAPDEG Model uses a stress threshold for the initiation of stress corrosion cracking processes that is uniformly distributed between 10% and 40% of the yield strength (the Current WAPDEG Model uses a stress threshold uniformly distributed between 20% and 30% of the yield strength).

C24

- The Updated WAPDEG Model has a different distribution than the Current WAPDEG Model for n, the crack growth exponent. This distribution is uniform between 0.843 and 0.92 in the Updated WAPDEG Model and is uniform between 0.75 and 0.84 in the Current WAPDEG Model.

- The Updated WAPDEG Model uses slightly different coefficients to calculate the stress profile than does the Current WAPDEG Model.

Figure 33 shows the upper and lower bounds, mean, and 95th, 75th, 25th and 5th percentile confidence intervals of the first breach profile for the waste packages with time. The upper bound profile, which is the upper extreme of the probable range of the first breach time, indicates that the earliest possible first breach time for a waste package is about 15,000 years. Note that the estimated earliest possible first breach time has a very low probability. It can be shown by comparing with the upper bound profile in Figure 36 (showing the first crack breach profiles of waste packages with time) that the first breach is by SCC crack penetration (see the discussion of the results in Figure 34 and Figure 35 later in this Section). The median estimate (50% of waste packages failed) of the first breach time of the upper bound profile is about 34,000 years. The median estimate of the first breach time of the mean profile is about 97,000 years. The time to fail 10 percent of waste packages for the two profiles is about 23,000 and 49,500 years, respectively.

Figure 34 shows the first breach profiles of drip shields with time. Because the drip shields are not subject to stress corrosion cracking and localized corrosion, the first breach profiles shown in the figure are all by general corrosion only. As discussed in Section 6.2, both the upper and under sides of the drip shield are exposed to the exposure conditions in the emplacement drift and are subject to corrosion. In addition, both sides experience the same exposure conditions regardless of whether the drip shields are dripped on or not. Thus, in the analysis, the general corrosion rate for the drip shields is sampled twice independently, once for the patches on the upper side and the once for the patches on the under side. This results in reduced variability in the degradation profiles and thus a fast failure rate (i.e., many drip shields failing over a short time period). This is shown in the upper bound profile, in which the drip shield first breach starts at about 20,000 years and 50 percent of the drip shields fail within a couple of thousand years after the initial failure. Similar trends are also seen with the 95th, 75th and median profiles. In terms of the number of patch penetration openings per failed drip shield with time in Figure 35, the upper bound profile shows that as the drip shields fail, a large number of patches are perforated over a relatively short time period (a few thousand years). A similar trend is seen for the 95th percentile profile. However, the profile shows a larger spread for the other profiles.

Figure 36 and Figure 37 show respectively the first crack penetration and patch penetration profiles of the waste packages with time. The first crack breach times of the upper bound and 95th percentile profiles are about 15,000 and 20,000 years respectively (Figure 36), and the first patch breach times of the upper and 95th percentile profiles are about 33,000 and 43,000 years, respectively (Figure 37). Comparison of the first crack and patch breach profiles with the first breach profiles in Figure 33 indicates that the initial breach (or failure) of the waste packages is likely by SCC crack penetration in the Alloy 22 waste package outer barrier closure lid welds. For the 75th percentile profiles in the figures, the first crack and patch penetration times are about 32,500 and 58,000 years, respectively.

Figure 38 shows the profile for the average number of crack penetrations per failed waste package. As discussed for Figure 36, the upper bound and 95th percentile profiles show the first crack penetration at about 15,000 and 20,000 years, respectively. The mean profile never develops more than 25 cracks. SCC cracks in passive alloys such as Alloy 22 tend to be very tight (i.e., small crack opening displacement) by nature (CRWMS M&O 2000h). The opposing sides of through-wall SCC cracks will continue to corrode at very low passive corrosion rates until the gap region of the tight crack opening is "plugged" by the corrosion product particles and precipitates such as carbonate present in the water. Any water transport through this oxide/salt filled crack area will be mainly by diffusion-type transport processes (CRWMS M&O 2000h). Thus, both the effective water flow rate into the waste packages and the radionuclide release rate from the waste packages through the SCC cracks would be expected to be extremely low and should not contribute significantly to the overall radionuclide release rate from the repository.

Figure 39 presents the profile for the average number of patch openings per failed waste package. For the upper bound profile, which again represents an extremely low probability case, the first patch breach occurs at about 36,500 years (see also Figure 37), and about 12 patches of the failed waste packages (about 1.2 percent of the waste package surface area) are breached by 100,000 years. For the mean profile, there will be only about 2 patch openings in each of the failed waste packages by 100,000 years.

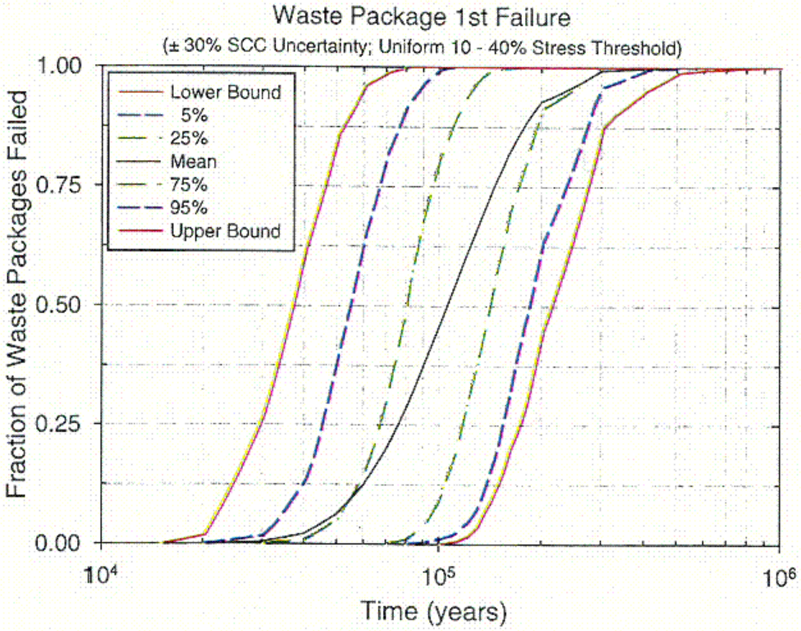

Figure 33. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Breach Profile of Waste Packages with Time for the Updated WAPDEG Model

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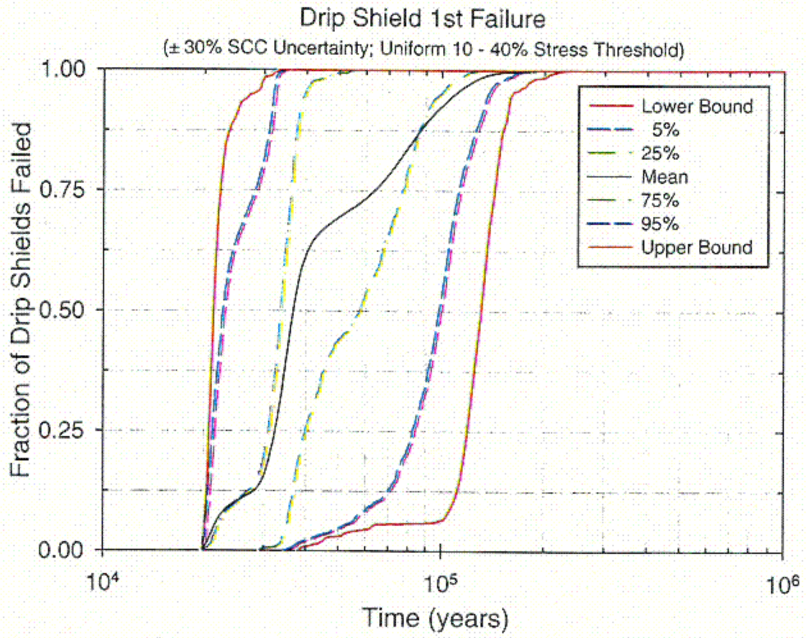

Figure 34. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Breach Profile of Drip Shield with Time for the Updated WAPDEG Model

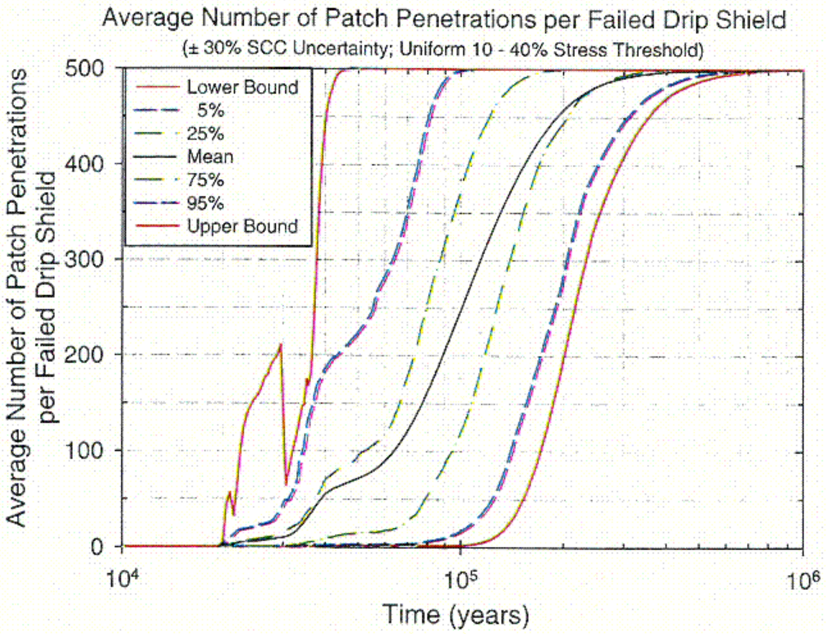

Figure 35. The Upper and Lower Bounds, Mean, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Average Number of Patch Penetrations per Failed Drip Shield Profile with Time for the Updated WAPDEG Model

C26

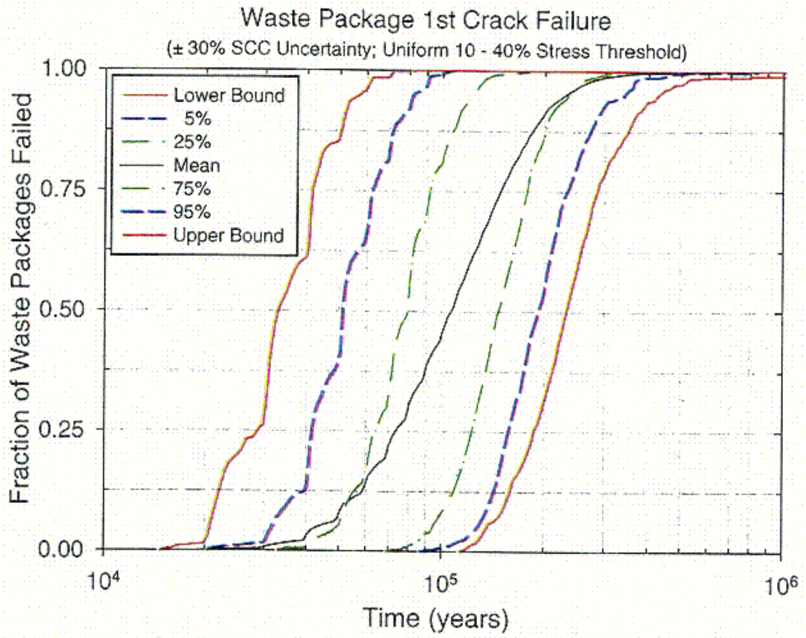

Figure 36. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Crack Breach Profile of Waste Packages with Time for the Updated WAPDEG Model

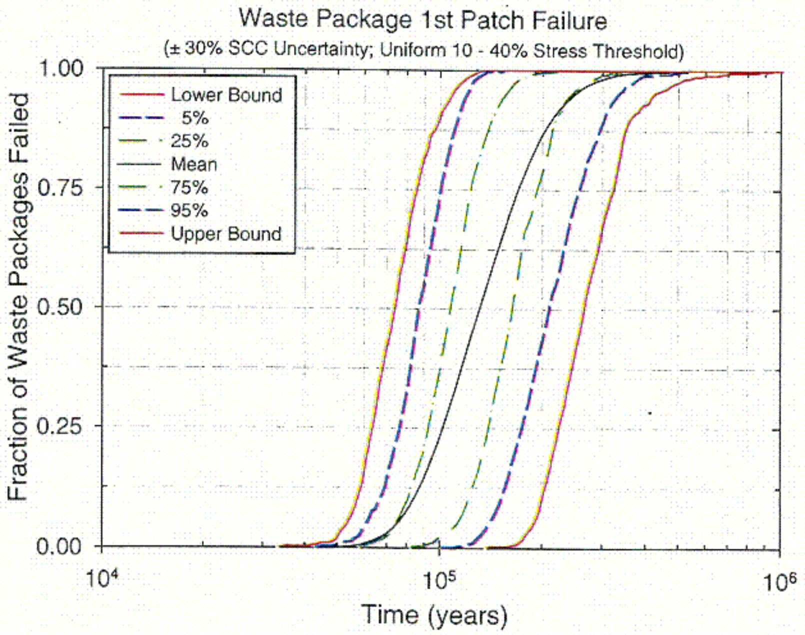

Figure 37. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the First Patch Breach Profile of Waste Packages with Time for the Updated WAPDEG Model

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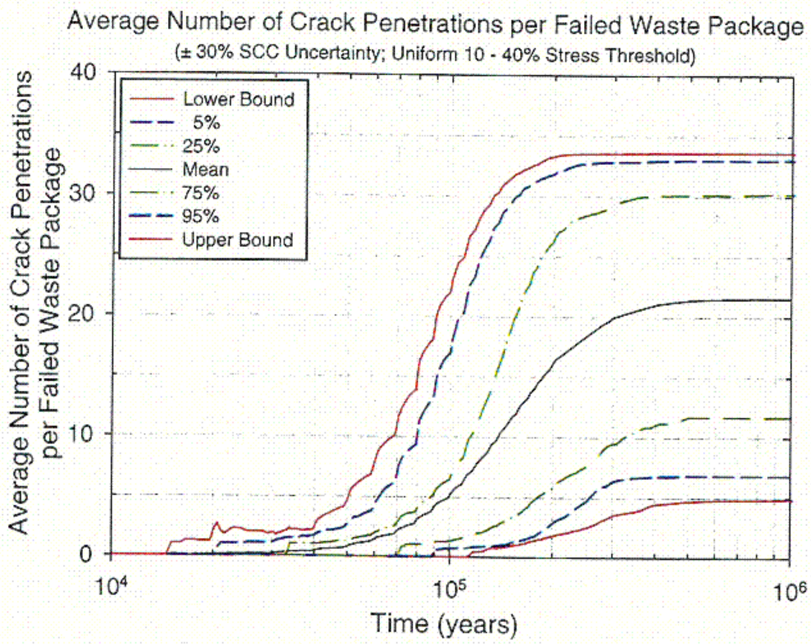

Figure 38. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Average Number of Crack Penetrations per Failed Waste Package Profile with Time for the Updated WAPDEG Model

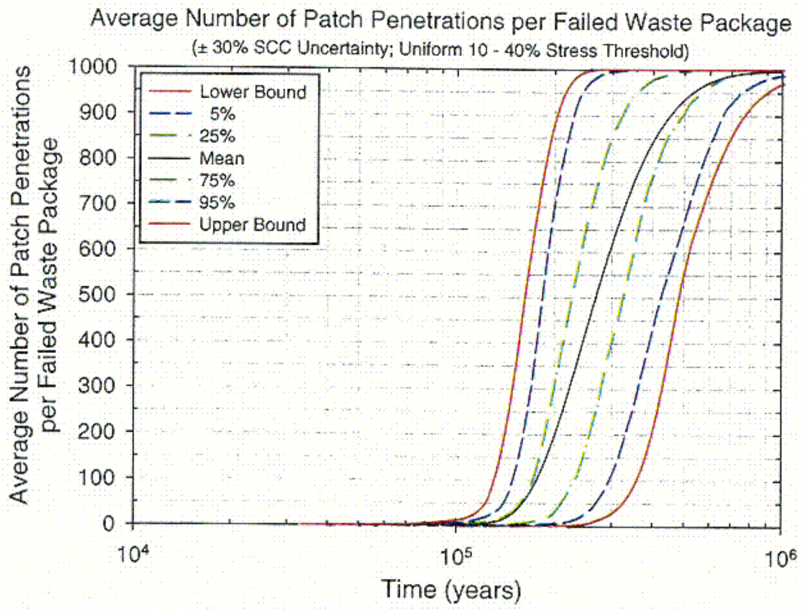

Figure 39. The Upper and Lower Bounds, Median, and 95th, 75th, 25th and 5th Percentile Confidence Intervals of the Average Number of Patch Penetrations per Failed Waste Package Profile with Time for the Updated WAPDEG Model

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7. CONCLUSIONS

The results of all analyses documented in this AMR are tracked by DTN: MO0010MWDWAP01.009.

A conceptual model for the nominal case analysis of degradation of drip shield and waste package in the Yucca Mountain repository was developed, incorporating the data and analyses of the individual degradation processes documented in the companion process-level analysis AMRs (CRWMS M&O 2000b-o, u). The conceptual model and the abstractions of the process-level models and their parameters were incorporated into the integrated waste package degradation model (WAPDEG). Incorporating the exposure conditions (temperature, relative humidity and pH of contacting solution) of the waste packages and drip shields in the repository, the WAPDEG analysis was conducted to develop a detailed description of waste package and drip shield degradation and to develop the degradation abstractions as input to the total system performance assessment (TSPA) analysis.

The waste package and drip shield degradation analyses have shown that based on the current corrosion model abstractions and assumptions, neither the drip shields nor the waste packages fail within the regulatory time period (10,000 years). The candidate materials for the drip shield (Titanium Grade 7) and the waste package outer barrier (Alloy 22) are highly corrosion resistant and, under the repository exposure conditions, are not expected to be subject to the degradation processes that, if initiated, could lead to failure in a short time period. Those degradation modes are localized corrosion (pitting and crevice corrosion), stress corrosion cracking (SCC), and hydrogen induced cracking (HIC) (applicable to drip shield only). Both the drip shield and waste package degrade by general corrosion at very low passive dissolution rates. The current experimental data and detailed process-level analyses, upon which the model abstractions incorporated in the WAPDEG analysis are based, are consistent with this conclusion. Only the closure-lid welds of the waste package, for which complete stress mitigation may not be possible, may be subject to rapidly penetrating corrosion modes under the expected repository conditions (CRWMS M&O 2000e, 2000f, 2000h, and 2000j). Because of the potential residual stresses, the closure-lid welds would be subject to SCC. As discussed in *Abstraction of Models of Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield* (CRWMS M&O 2000i), once a SCC crack initiates, it penetrates the closure-lid thickness in a very short time. The analysis also demonstrated the importance of stress mitigation in the closure-lid welds to avoid premature failures of waste packages by SCC.

To mitigate the SCC threat to potential early failure of the waste package, a dual closure-lid design for the waste package outer barrier has been used, and different stress mitigation techniques have been proposed for the dual closure-lid welds: induction heating solution annealing for the Alloy 22 waste package outer barrier extended closure-lid welds and laser peening for the flat closure-lid welds (CRWMS M&O 2000p, Section 6.4). The numerical modeling-based analyses have shown that the hoop stress (driving radial cracks) is the dominant stress in the closure-lid welds that could cause SCC failure of waste package. The analyses also have shown that the above stress mitigation techniques can achieve a substantial stress relief for the closure-lid welds (CRWMS M&O 2000h). According to the analyses abstraction (CRWMS M&O 2000i, Section 6.3.1), mitigation of the hoop stress in the Alloy 22 waste package outer barrier extended closure-lid welds has resulted in a stress state such that the corresponding stress intensity factor for the radial crack is negative to a depth of 6 to 10-mm from the surface. For the Alloy 22 waste package outer barrier flat closure-lid welds, the stress intensity factor is negative to a depth of 1.5 to 3-mm. In the waste package degradation analysis, for a smooth surface without the presence of manufacturing defects, no SCC cracks, no SCC cracks initiate in the closure-lid welds until the compressive layer is removed by general corrosion.

The predicted long life-time of the waste packages in the current analysis is attributed mostly to 1) the stress mitigation to the substantial depths in the dual closure-lid welds and 2) the very low general-corrosion rate applied to the closure-lid welds to remove the compressive stress zones, providing a long delay time before initiating SCC crack growth. One of the major uncertainties associated with the current analysis is the technical challenge and demonstration to achieve the stress mitigation in the closure-lid welds as dictated from the numerical analyses. In addition, because of a large number of waste packages (12,000 or more) to be emplaced in the repository and because the closure-lid welding will be conducted remotely, the quality control and quality assurance (QC and QA) in the welding and subsequent stress mitigation would be another major uncertainty. The uncertainties associated with the hoop stress and stress intensity factor used in the current analyses need to be closely re-evaluated for the future analysis. Another uncertainty in the current analysis is the general corrosion rate used for the closure lid welds. Additional testing and analyses will provide more confidence in the general corrosion rates used.

Other uncertainties associated with the current analysis have to do with the modeling assumption that the non-closure lid weld area of the waste package is fully annealed and no significant stress state is expected to develop during the life-time in the repository. This assumption will be evaluated as additional data and/or analysis is developed. In addition, there are uncertainties in the current analysis from the use of conservative assumptions. One example is the hoop stress and corresponding (radial crack) stress intensity factor profiles used in the current analysis, which are for the condition at the time of manufacturing. As a crack propagates in the closure-lid welds and/or the welds are thinned by general corrosion, stresses in the welds may re-distribute in such a way that the SCC initiation and crack growth are mitigated (see Section 5.6 and CRWMS M&O 2000h, Section 6.2.2). Such a stress re-distribution or relaxation is not considered in the current abstraction.

Additionally, because of the conservatism in the current threshold RH to initiate corrosion of the drip shield and waste package, no benefit of the drip shield is captured in the WAPDEG analysis for waste package degradation. As discussed in Section 6.2, the threshold RH is based on the deliquescence point of $NaNO_3$ salt as a function of temperature (this effectively incorporates any effect of dust deposition on the waste package surface from any preclosure activities). The same threshold RH is used for both the dripping and non-dripping cases. Realistically, while the drip shield is operative, it will keep the corrosive dripping water from contacting the underlying waste package and provide more benign (or less corrosive) exposure conditions for the waste package. A more realistic model for the corrosion initiation threshold is needed.

Analyses documented in this AMR are limited to the Enhanced Design Alternative (EDA) II and the waste-package outer barrier dual-lid design. The results may not be applicable to other design considerations.

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

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9. ATTACHMENTS

I PREWAP Software Routine Report

ATTACHMENT I

PREWAP SOFTWARE ROUTINE REPORT

1. SOFTWARE ROUTINE IDENTIFICATION

Software Name and Version Number: PREWAP Version 1.0

This routine was developed using Microsoft Developer Studio 97 with Visual Fortran 6.0, Professional Edition.

SRR Document Identification Number: N/A

SRR Media Number (If Applicable): N/A

2. DESCRIPTION AND TESTING

2.1 OVERVIEW

Corrosion of the drip shields and waste packages is accounted for in the Total System Performance Assessment-Site Recommendation (TSPA-SR) model by the WAPDEG routine, which runs as a DLL under the TSPA-SR software (Golder Associates 2000). As input, WAPDEG requires T-H data (temperatures, relative humidities, etc.), as well as seepage chemistry information (pH, chloride concentration, etc.). T-H data are taken from CRWMS M&O 2000k. Seepage chemistry in-drift is characterized in the AMR entitled *In-Drift Precipitates/Salts Analysis* (CRWMS M&O 2000l). In-package chemistry is characterized in the AMR entitled *In-Package Chemistry Abstraction* (CRWMS M&O 2000m).

The PREWAP routine calculates the seepage chemistry associated with the T-H data. The T-H and seepage chemistry data are then written to output files that are used as input to the WAPDEG software (CRWMS M&O 2000a).

The PREWAP routine extracts this data from these various tables and prepares an output table that is used as input to the WAPDEG software.

The PREWAP routine is a stand-alone executable.

2.2 INPUTS

The input to PREWAP consist of in-drift drip and no-drip chemistry pH and Cl data, in-package pH and Cl data, and T-H data (for low, mean, and high infiltration cases) (CRWMS M&O 2000k) for Commercial Spent Nuclear Fuel (CSNF) and Co-Disposed Waste Package (CDSP) waste packages. Information is also passed to PREWAP regarding input and output file names, as well as an RH corrosion limit.

2.2.1 In-Drift Chemistry Data (Drip Conditions)

In-drift pH and Chloride Concentration (Cl) under dripping conditions are dependent on RH and the abstracted time period. Within a given set of RH and time period, they can also be dependent on temperature (T), invert evaporation rate (Q_e), and seepage rate (Q_s) into the drift. The break-down of cases and their independent parameters are given in Table 1.

Table 1. Classification of In-Drift pH and Cl Data Sets for Dripping Conditions

	RH	time period(s)*	additional independent parameters
case 1	RH<50.3%	all	none
case 2	50.3%<RH<85%	2, 3, 4, 5	none
case 3	RH>85%	2, 3, 5	1-Qe/Qs
case 4	RH>85%	4	1-Qe/Qs, T

*time periods:
1 0 to 50 years from initial opening of the repository
2 50 to 1000 years from initial opening of the repository
3 1000 to 2000 years from initial opening of the repository
4 2000 to 100,000 years from initial opening of the repository
5 > 100,000 years from initial opening of the repository

Case 1 conditions have no pH and Cl (Molal) data. For this case, the pH and Cl are hardwired in the PREWAP code to be equal to -9.99E-02 (the default 'does not exist' value for WAPDEG input).

Case 2 data for pH and Cl are contained in files **phTable1.dat** and **ClTable1.dat**, respectively. The contents of these files are shown in Table 2 and Table 3. The value in the first row indicates the number of rows of data to follow. The data are organized as a set of 1-D look-up tables. The 1st column contains the RH independent parameter values. Columns 2, 3, and 4 contain the dependent parameter values (pH or Cl) for time periods 2, 3/5, and 4, respectively. The remaining information in the file below the look-up table (column headings and descriptive text) is not used by PREWAP.

Case 3 data for pH and Cl are contained in files **phTable2.dat** and **ClTable2.dat**, respectively. The contents of these files are shown in Table 4 and Table 5. The value in the first row indicates the number of rows of data to follow. The data are organized as a set of 1-D look-up tables. The 1st column contains the $1\text{-}Q_e/Q_s$ independent parameter values. Columns 2, 3, and 4 contain the dependent parameter values (pH or Cl) for time periods 2 and 3/5, respectively. The remaining information in the file below the look-up table (column headings and descriptive text) is not used by PREWAP.

Case 4 data for pH and Cl are contained in files **phTable3.dat** and **ClTable3.dat**, respectively. The contents of these files are shown in Table 6 and Table 7. The values in the first row indicate the number of rows and columns that make up the dependent data set (pH or Cl values) in the 2-D look-up table that follows. The next row contains the independent parameter temperature values. In the remaining rows, the 1st column contains the 1-Q_e/Q_s independent parameter values. Columns 2, 3, and 4 contain the dependent parameter values (pH or Cl) for temperatures of 25 C, 50 C, and 75 C, respectively. The remaining information in the file below the look-up table (column headings and descriptive text) is not used by PREWAP.

Table 2. Case 2 pH Look-Up Table (In-Drift Dripping Conditions)

10			
50.3	9.40	7.64	7.02
51.0	9.40	7.64	7.02
53.1	9.40	7.64	7.02
55.2	9.40	7.64	7.02
60.5	9.40	7.64	7.02
65.7	9.40	7.64	7.02
71.0	9.40	7.64	7.02
76.2	9.40	7.64	7.02
81.5	9.40	7.64	7.02
85.0	9.40	7.64	7.02
	2	3/5 4	

; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; 1st independent variable (columns) = Abstracted Period
; 2nd independent variable (rows) = relative humidity (RH)
; dependent parameter = pH

Table 3 Case 2 Cl Look-Up Table (In-Drift Dripping Conditions)

10			
50.3	-2.431	-2.428	-2.415
51.0	-1.246	-1.244	-1.231
53.1	-0.389	-0.391	-0.380
55.2	-0.164	-0.169	-0.159
60.5	0.225	0.211	0.216
65.7	0.380	0.358	0.359
71.0	0.420	0.396	0.396
76.2	0.428	0.403	0.403
81.5	0.418	0.394	0.394
85.0	0.407	0.382	0.382
	2	3/5	4

; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; 1st independent variable (columns) = Abstracted Period
; 2nd independent variable (rows) = relative humidity (RH)
; dependent parameter = log Cl (i.e., log of Cl concentration (molal))

Table 4. Case 3 pH Look-Up Table (In-Drift Dripping Conditions)

7		
0.000999	9.40	7.64
0.001	9.41	7.64
0.01	9.28	7.58
0.1	9.21	7.45
0.5	8.87	7.64
0.9	8.62	7.71
1.0	8.58	7.72
	2	3/5

; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; 1st independent variable (columns) = Abstracted Period
; 2nd independent variable (rows) = 1-Qe/Qs (Qe = evaporation rate, Qs = incoming seepage rate)
; condition: relative humidity (RH) > 85 percent
; dependent parameter = pH

Table 5. Case 3 Cl Look-Up Table (In-Drift Dripping Conditions)

7		
0.000999	0.387	0.382
0.001	0.190	0.373
0.01	-0.752	-0.502
0.1	-1.745	-1.496
0.5	-2.445	-2.194
0.9	-2.699	-2.449
1.0	-2.745	-2.496
	2	3/5

; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; 1st independent variable (columns) = Abstracted Period
; 2nd independent variable (rows) = 1-Qe/Qs (Qe = evaporation rate, Qs = incoming seepage rate)
; condition: relative humidity (RH) > 85 percent
; dependent parameter = log Cl (i.e., log of Cl concentration (molal))

Table 6. Case 4 pH Look-Up Table (In-Drift Dripping Conditions)

7	3		
25		50	75
0.0011999	7.02	7.02	7.02
0.0012	6.78	6.86	7.02
0.01	6.986	6.95	7.02
0.1	7.11	7.03	6.97
0.5	7.23	7.18	7.14
0.9	7.09	7.22	7.18
1.0	7.05	7.22	7.19

; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; condition: Period 4
; 1st independent variable (columns) = temperature ('C)
; dependent parameter = pH

Table 7. Case 4 Cl Look-Up Table (In-Drift Dripping Conditions)

7	3		
25		50	75
0.0011999	0.38202	0.38202	0.38202
0.0012	0.39094	0.38202	0.38202
0.01	-0.48798	-0.48872	-0.48945
0.1	-1.4828	-1.48216	-1.48214
0.5	-2.18053	-2.18052	-2.18059
0.9	-2.43581	-2.43581	-2.43581
1.0	-2.48149	-2.48149	-2.48162

; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; dependent parameter = log Cl (i.e., log of Cl concentration (Molal))

2.2.2 In-Drift Chemistry Data (No-Drip Conditions)

In-drift pH under no-dripping conditions is dependent on CO2 fugacity and temperature. No-drip pH data are contained in file **phTable4.data**. The contents of this file are shown in Table 8. The values in the first row indicate the number of rows and columns that make up the dependent data set (pH values) in the 2-D look-up table that follows. The next row contains the independent parameter temperature values. In the remaining rows, the 1st column contains the independent parameter log CO2 fugacity values. Columns 2, 3, 4, and 5 contain the dependent parameter values (pH) for temperatures of 25 C, 45 C, 75 C, and 95 C, respectively. The remaining information in the file below the look-up table (column headings) is not used by PREWAP.

There are no data for Cl under no-dripping conditions; hence the no-drip Cl is hardwired in the PREWAP code to be equal to the default 'does not exist' value of -9.99E-02.

Table 8. pH Look-Up Table (In-Drift No-Dripping Conditions)

```
7         4
25        45     75     95
-1  4.41  4.47   4.60   4.70
-3  5.41  5.49   5.73   6.02
-4  5.91  6.03   6.41   6.70
-5  6.39  6.57   6.88   6.96
-6  6.80  6.92   6.99   7.00
-7  6.97  6.99   7.00   7.00
-9  7.00  7.00   7.00   7.00
log
fCO2
```

2.2.3 In-Package Chemistry Data (Drip and No-Drip Conditions)

In-Package chemistry is dependent upon the waste type (CSNF or CDSP) in the waste package. Bounding values for the pH and Cl are read into PREWAP from the file **InPkgChem.dat**. The 1st row contains the bounding pH values for CSNF and CDSP, respectively. The 2nd row contains the bounding Cl value used for both CSNF and CDSP.

Table 9. pH and Cl In-Package Chemistry Data

```
7.60   9.83
2.014E-04
```

For CSNF, the in-package chemistry is a function of cladding coverage and seepage flow rate. Inspection of Figures 4.3 and 4.4 in the *In-Package Chemistry Abstraction* (CRWMS M&O 2000m) finds that the >1000 year post-breach period has the potential to have the highest pH within the bounds of the response surface data-set. Using the appropriate equation from Table 4.6 (CRWMS M&O 2000m) yields the upper bound on pH for CSNF.

$$pH = 6.0668 - 0.5395\log(cc) + 4.0479\left[\frac{yr}{mm}\right]Q$$

$$pH = 6.0668 - 0.5395\log(0.02) + 4.0479\left[\frac{yr}{mm}\right]\left(0.15\frac{mm}{yr}\right) = 7.60$$

The terms *cc* and *Q* represent cladding coverage fraction and flow rate (mm/yr), respectively. For CDSP the in-package chemistry is a function of relative glass rate and seepage flow rate. The glass rate is a relative dissolution rate and is described in further detail in the *In-Package Chemistry Abstraction* (CRWMS M&O 2000m). Inspection of Figures 4.5 and 4.6 in the *In-Package Chemistry Abstraction* (CRWMS M&O 2000m) finds that the >1000 year post-breach period has the potential to have the highest pH within the bounds of the response surface data-set. Using the appropriate equation from Table 4.11 (CRWMS M&O 2000m) yields the upper bound on pH for CSNF.

$$pH = 8.4247 - 3.4173\left[\frac{yr}{mm}\right]Q + 0.1403GR$$

$$pH = 8.4247 - 3.4173\left[\frac{yr}{mm}\right]\left(0.0015\frac{mm}{yr}\right) + 0.1403(10.0) = 9.83$$

The terms Q and GR represent the seepage and glass rate, respectively. A chloride value of 2.014E-04 mol/kg (equal to that of J-13 water) is specified for both CSNF and CDSP waste package (CRWMS M&O 2000m).

2.2.4 T-H Data

The T-H data sets are broken down into five 'bins' based on infiltration rate. Furthermore, there are separate sets of T-H data for each infiltration scenario (low, mean, or high). Table 10 shows the relationship between infiltration bins, infiltration scenario, and the T-H data files.

Table 10 Relationship Between Infiltration Bins, Infiltration Scenario, and T-H Data Files

	infiltration scenario		
infiltration bin	**low**	**mean**	**high**
bin 1 (< 3.4 mm/yr)	CSNF_low_Bin1.in HLW_low_Bin1.in	CSNF_mean_Bin1.in HLW_mean_Bin1.in	n/a n/a
bin 2 (3.4 to 10 mm/yr)	CSNF_low_Bin2.in HLW_low_Bin2.in	CSNF_mean_Bin2.in HLW_mean_Bin2.in	CSNF_high_Bin2.in HLW_high_Bin2.in
bin 3 (10 to 20 mm/yr)	n/a n/a	CSNF_mean_Bin3.in HLW_mean_Bin3.in	CSNF_high_Bin3.in HLW_high_Bin3.in
bin 4 (20 to 60 mm/yr)	n/a n/a	CSNF_mean_Bin4.in HLW_mean_Bin4.in	CSNF_high_Bin4.in HLW_high_Bin4.in
bin 5 (> 60 mm/yr)	n/a n/a	CSNF_mean_Bin5.in HLW_mean_Bin5.in	CSNF_high_Bin5.in HLW_high_Bin5.in

The format of the T-H files is illustrated in Table 11.

Table 11 T-H File CSNF_mean_Bin5.in

line(s)	T-H file information	comment
1	Infiltration Bin:	not used
2	qinf > 60.0 mm/yr	not used
3	RIP_csnf_d0010500_bin-60_mean	not used
4	data column headers (see below)	not used
5	The number of Rows = 83	numeric value read in
6	The fraction of this history = 0.000576	numeric value read in
7	Coordinate Location:	not used
8	The easting coordinate = 170208.78 m	not used
9	The northing coordinate = 234316.70 m	not used
10	Infiltration rate:	not used
11	qinf = 61.00266 mm/yr	not used
12 to 94	T-H data	read in
95	The number of Rows = 84	numeric value read in
96	The fraction of this history = 0.000960	numeric value read in
97	Coordinate Location:	not used
98	The easting coordinate = 170228.75 m	not used
99	The northing coordinate = 234315.60 m	not used
100	Infiltration rate:	not used
101	qinf = 60.79187 mm/yr	not used
102 to 195	T-H data	read in
196	The number of Rows = 87	numeric value read in
197	The fraction of this history = 0.001153	numeric value read in
198	Coordinate Location:	not used
199	The easting coordinate = 170256.20 m	not used
200	The northing coordinate = 234314.20 m	not used
201	Infiltration rate:	not used
202	qinf = 60.37322 mm/yr	not used
203 to 290	T-H data	read in

Each T-H data file contains time-histories from zero to one-million years for the following parameters at a given number of spatial locations:

Waste Package Temperature [C]
Drip Shield Temperature [C]
Drift Wall Temperature [C]
Invert Temperature [C]
Waste Package RH [-]
Drip Shield RH [-]
Drift Wall RH [-]

Backfill RH [-]
Invert RH [-]
Liquid Saturation at the Drip Shield [-]
Liquid Saturation at the Invert [-]
Air Mass Fraction [-]
Water Vapor Flux at Drift Wall [kg/yr/m of drift]
Air Flux at Drift Wall [kg/yr/m of drift]
Drip Shield Water Evaporation Rate [m3/yr]
Backfill Water Evaporation Rate [m3/yr]
Invert Water Evaporation Rate [m3/yr]
Percolation Flux at 5 m [mm/yr]
Volume flow at the Drip Shield Top [m3/yr]
Volume flow at the Invert [m3/yr]
Top of the Drip Shield Temperature [C]

2.2.5 Input/Output Control Files

The **InMaster.in** and **OutMaster.in** files pass file-name information to PREWAP. The 1st row in **InMaster.in** contains the RH corrosion limit; the 2nd row contains the number of file names. The remaining rows list the names of the T-H files that are to be read by PREWAP. **OutMaster.in** contains the names of the WAPDEG input files that PREWAP results are to be written.

Table 12 InMaster.in File

```
0.501
22
CSNF_nbf_low_bin1.in
CSNF_nbf_low_bin2.in
HLW_nbf_low_bin1.in
HLW_nbf_low_bin2.in
CSNF_nbf_mean_bin1.in
CSNF_nbf_mean_bin2.in
CSNF_nbf_mean_bin3.in
CSNF_nbf_mean_bin4.in
CSNF_nbf_mean_bin5.in
HLW_nbf_mean_bin1.in
HLW_nbf_mean_bin2.in
HLW_nbf_mean_bin3.in
HLW_nbf_mean_bin4.in
HLW_nbf_mean_bin5.in
CSNF_nbf_high_bin2.in
CSNF_nbf_high_bin3.in
CSNF_nbf_high_bin4.in
CSNF_nbf_high_bin5.in
HLW_nbf_high_bin2.in
HLW_nbf_high_bin3.in
HLW_nbf_high_bin4.in
HLW_nbf_high_bin5.in
```

Table 13 OutMaster.in File

```
CSNF_nbf_low_bin1.ou
CSNF_nbf_low_bin2.ou
HLW_nbf_low_bin1.ou
HLW_nbf_low_bin2.ou
CSNF_nbf_mean_bin1.ou
CSNF_nbf_mean_bin2.ou
CSNF_nbf_mean_bin3.ou
CSNF_nbf_mean_bin4.ou
CSNF_nbf_mean_bin5.ou
HLW_nbf_mean_bin1.ou
HLW_nbf_mean_bin2.ou
HLW_nbf_mean_bin3.ou
HLW_nbf_mean_bin4.ou
HLW_nbf_mean_bin5.ou
CSNF_nbf_high_bin2.ou
CSNF_nbf_high_bin3.ou
CSNF_nbf_high_bin4.ou
CSNF_nbf_high_bin5.ou
HLW_nbf_high_bin2.ou
HLW_nbf_high_bin3.ou
HLW_nbf_high_bin4.ou
HLW_nbf_high_bin5.ou
```

2.3 DESCRIPTION OF SOFTWARE ROUTINE INCLUDING THE EXECUTION ENVIRONMENT

2.3.1 Development and Execution Environment

The PREWAP routine is a FORTRAN executable. The code was developed and tested in the Windows NT 4.0 operating system. It was compiled with Digital FORTRAN Professional 6.0 as a stand-alone executable (exe) program. The routine operates in a Windows 95/98 or Windows NT environment

2.3.2 Main Program

The PREWAP program begins by calling a subroutine (**ReadMasterFiles**) that reads in the T-H input and WAPDEG output file names. Next it calls a subroutine (**ReadChemData**) to read in the in-drift chemistry lookup tables and in-package chemistry data. The program then initiates a loop that calls subroutines that; read in the T-H data, perform the necessary calculations, and generate the WAPDEG input files.

The program loop first calls a subroutine to count the data sets(**CountDataSets**) in the selected T-H file. It then calls a subroutine to allocate arrays (**AllocateArays**) to hold the data during processing. Next a subroutine (**ReadInputFile**) reads the T-H data. The data are then processed by a subroutine (**DoCalculations**) that performs the necessary calculations. The next subroutine (**CullDataPoints**) checks the data set resulting from the calculations and eliminates (based on a threshold RH value) those portions that will not contribute to corrosion of the EBS. This modified dataset is in turn checked by the **AddDataPoints** subroutine to determine if minimum time-step size requirements are met. If they are not, interpolated data points are added back to the data set between the times that do not meet the minimum time-step requirements. The data set is then written to an output file by the **WriteOutputFile** subroutine. Finally it calls a subroutine (**DeallocateArrays**) to deallocate the arrays allocated earlier in the loop.

2.3.4 Subroutine ReadMasterFiles

The **ReadMasterFiles** subroutine opens the files **InMaster.in** and **OutMaster.in**. The RH corrosion limit and the number of T-H and WAPDEG input files are read in. A do-loop is then initiated that reads in the input file names (T-H files) from **InMaster.in** and the output file names (WAPDEG files) from **OutMaster.in**.

2.3.5 Subroutine ReadChemData

This subroutine reads in the Cl and pH look-up tables from files **CLtable1.dat, CLtable2.dat, Cltable3.dat, pHtable1.dat, pHtable2.dat, pHtable3.dat,** and **pHtable4.dat**. In-package chemistry data are read in from the file **InPkgChem.dat**. The data contained in these files are described Section 2.2.

2.3.6 Subroutine CountDataSets

This subroutine counts the number of data sets in each of the T-H files. It initializes the number of data sets (**nDataSets**) counter to 1 and the maximum number of rows (**maxRows**) variable to 0. The subroutine then reads past the 1st four rows of header information to the 5th row. It then reads past the header information in row 5 and reads the number of rows listed for that data set. This value is assigned to the variable **rows**. It then sets the value of **maxRows** equal to the number of rows just read.

The subroutine then reads past the next six rows of header information to the 1st data set. It then initiates a do-loop that executes **rows** number of times to read past the 1st data set.

It then begins to read the rest of the file with a do-loop. It reads the 1st header row for the next data set. If the end of file is reached the subroutine exits the do loop. If not, the subroutine reads the number of rows in the next data set as **rows**. It then increments the counter, **nDataSets**, by 1 and tests to see if the number of rows in this data set is greater than **maxrows**. If so, **maxrows** is set equal to **rows**. It then reads through this data set and restarts the loop. This loop is repeated until the end of file is reached. When the end of file is reached, the subroutine exits the do loop and closes the data file. The subroutine is then exited back to the main program.

2.3.7 Subroutine AllocateArays

This subroutine sets the bounds on dynamic arrays to match the maximum number of rows (**maxRows**) and number of data sets (**nDataSets**) counted in the subroutine **CountDataSets**.

2.3.8 Subroutine ReadInputFile

This subroutine reads the data from the T-H file to the dynamic arrays established in the previous subroutine.

2.3.9 Subroutine DoCalculations

This subroutine calculates pH and pH^2 for the waste package and the drip shield under drip and no drip conditions. Source Code is included for calculating Cl chemistry, but it is commented out. It also sets the in-package and barrier interface pH values for drip and no drip conditions.

The subroutine begins with a do-loop that sequentially processes each data set read from the TH file. Inside this loop is another do-loop that sequentially processes each row of data in the data set to calculate pH and pH^2 for the waste package and the drip shield. First it calculates the waste package pH and pH^2 for both drip and no drip conditions by calling the **InDriftCalc** subroutine using arguments that are specific to the waste package. Next it calculates the drip shield pH and pH^2 for both drip and no drip conditions by again calling the **InDriftCalc** subroutine, but using arguments that are specific to the drip shield.

After these calculations the subroutine sets the in-package pH for drip conditions for the waste package to the appropriate bounding value (pH of 7.6 for CSNF, 9.8 for Defense High Level Waste, and 9.83 for CDSP). It then sets the in-package pH for no-drip conditions equal to the default 'does not exist' value of -9.99E-02. Values for pH^2 are calculated from the pH values.

This process is repeated for each row of data in the data set. After all rows in a data set have been processed, the code processes the next data set until all data sets have been processed.

2.3.10 Subroutine InDriftCalc

The **InDriftCalc** subroutine is called by the **DoCalculations** subroutine. It performs the pH and pH^2 calculations for drip and no drip conditions for each row of data in the data set. The subroutine begins by first checking to see if the temperature is less than zero or if the seep rate is less than –99. If either condition applies, the pH for drip and no drip conditions is set to the default 'does not exist' value of -9.99E-02. If neither condition applies, the routine calculates 1-Q_e/Q_s for the row of data.

An **if-then-else** statement is used to determine which of the time periods is applicable. Values of drip and no-drip pH in the >50 year time period are set equal to the default 'does not exist' value of –9.99E-02. For the remaining time periods, an **if-then-else** statement is used to determine the applicable pH data-set based on RH. Table 14 shows the relationships between time periods, RH ranges, the potential independent parameters, and the pH data-sets.

Table 14 In-Drift Chemistry

time period	RH	drip condition	log(fCO2)	$1-Q_e/Q_s$	T	applicable point-value or data-set
>50 yrs	n/a	drip	n/a	n/a	n/a	-9.99E-02
		no drip				-9.99E-02
50 to 1000 yrs	RH < 50	drip	n/a	n/a	n/a	-9.99E-02
		no drip				-9.99E-02
	50<= RH <=85	drip	n/a	n/a	n/a	9.40
		no drip	**-6.5**		**T**	phTable4
	RH > 85	drip	n/a	**$1-Q_e/Q_s$**	n/a	phTable2a
		no drip	**-6.5**	n/a	**T**	phTable4
1000 to 2000 yrs	RH < 50	drip	n/a	n/a	n/a	-9.99E-02
		no drip				-9.99E-02
	50<= RH <=85	drip	n/a	n/a	n/a	7.64
		no drip	**-3.0**	n/a	**T**	phTable4
	RH > 85	drip	n/a	**$1-Q_e/Q_s$**	n/a	phTable2b
		no drip	**-3.0**	n/a	**T**	phTable4
2000 to 100,000 yrs	RH < 50	drip	n/a	n/a	n/a	-9.99E-02
		no drip				-9.99E-02
	50<= RH <=85	drip	n/a	n/a	n/a	7.02
		no drip	**-2.0**	n/a	**T**	phTable4
	RH > 85	drip	n/a	**$1-Q_e/Q_s$**	**T**	phTable3
		no drip	**-2.0**	n/a	**T**	phTable4
<100,000 yrs	RH < 50	drip	n/a	n/a	n/a	-9.99E-02
		no drip				-9.99E-02
	50<= RH <=85	drip		n/a	n/a	7.64
		no drip	**-3.0**	n/a	**T**	phTable4
	RH > 85	drip		**$1-Q_e/Q_s$**	n/a	phTable2b
		no drip	**-3.0**	n/a	**T**	phTable4

As an example, the subroutine **Interp1D** is used to select pH values from the pH data-sets **phTable2a** and **phTable2b**, while subroutine **Interp2D** is used to select pH values from the pH data-sets **phTable3** and **phTable4**. In Table 14 the independent parameters associated with the pH data sets are denoted by **bold-face** type.

After these tests and calculations are performed to determine the values for pH under drip and no drip conditions, the values for pH^2 for drip and no drip conditions are calculated.

2.3.11 Subroutine Interp1D

This subroutine is called by the **InDriftCalc** subroutine to interpolate thermophysical properties such as pH values, from one-dimensional arrays (e.g. **phTable2a** and **phTable2b**) created when the in-drift chemistry data from and **phTable2.dat** file were read. The subroutine is passed the value of the independent variable, the independent and dependent variable vectors, and the number of rows in the passed vectors. The subroutine passes back the interpolated dependent variable value.

The subroutine first checks to see if the independent variable value is within the upper and lower bounds of the independent variable vector. If it is above the upper bound, the dependent variable value is set equal to its upper bound; if it is below the lower bound the dependent variable is set equal to its lower bound. If neither condition is met, the subroutine linearly interpolates the dependent variable value between the independent vector values bounding the independent variable.

2.3.12 Subroutine Interp2D

This subroutine is called by the **InDriftCalc** subroutine to interpolate thermophysical properties such as pH values from two dimensional arrays (e.g. **phTable3** and **phTable4**) created when the in-drift chemistry data from the **phTable3.dat** and **phTable4.dat** files were read. The subroutine is passed the values of the two independent variable, the two independent variable vectors, the dependent variable array, and the number of rows and columns passed array. The subroutine passes back the interpolated dependent variable value.

This subroutine first checks the value of the 1st independent variable to see if it is within the range of the 1st independent variable vector. If it is outside the range of the independent vector, a flag is set denoting whether it is above or below the range of the 1st independent vector. If the value of the 1st independent variable is within the range of the 1st independent vector, the subroutine loops through the 1st independent vector to identify the first row where the value of the 1st independent vector is less than the 1st independent variable.

Next the subroutine checks the value of the 2nd independent variable to see if it is within the range of the 2nd independent variable vector. If it is outside the range of the independent vector, a flag is set denoting whether it is above or below the range of the 2nd independent vector. If the value of the 2nd independent variable is within the range of the 2nd independent vector, the subroutine loops through the 2nd independent vector to identify the first row where the value of the 2nd independent vector is less than the 2nd independent variable.

The subroutine then checks to see if the 1st independent variable lower bound flag is set. If so, it then checks to see if the 2nd independent variable lower or upper bound flag is set. If this condition is satisfied, the dependent variable is assigned the value of the applicable corner point in the 2D array. If the 2nd independent variable is within the bounds of the 2nd independent vector, the subroutine linearly interpolates the dependent variable value between the 2nd independent vector values bounding the independent variable (i.e. along the lower edge of the array).

If the 1st independent variable is not outside the lower bound, the same process is repeated to determine if it is outside the upper bound. If this condition is satisfied, the dependent variable is set to the value at the upper corner points of the array or along the upper edge of the array.

The same logic is then repeated to identify values that are outside the upper and lower bounds of the 2nd independent variable.

If the 1st and 2nd independent variables are both within the bounds of their respective vectors, the program linearly interpolates the j-th column value between the i and i+1 rows. It then linearly interpolates the i-th row value between the j-th and j+1 columns. The results of these calculations are then used to linearly interpolate the dependent variable value.

2.3.13 Subroutine CullDataPoints

This subroutine removes rows of data where the waste package or drip shield temperature or RH are outside predetermined values. The subroutine loops through each data set. In turn each data-set is looped through (excepting the last row). A flag (**corFlag**) is set, based on a series of tests, to indicate whether or not that row of data is to be retained.

The **corFlag** is initialized to zero, as is the counter **nnRows()** which keeps track of the number of rows that are retained from each data-set.

The subroutine first checks to see if the waste package temperature or drip shield temperature is less than zero (values less than zero denote temperatures that 'do not exist'). If the condition is satisfied, the subroutine skips the remaining tests with **corFlag** set to zero. If the conditions are not satisfied, then the next test is performed with the **corFlag** variable still equal to zero.

Next the waste package and drip shield RH are checked to see if they are greater than the **corLim** value. If either is greater than **corLim**, **corFlag** is set to one and the remaining tests are skipped. Otherwise, **corFlag** remains at zero and the next test is performed.

Next the waste package RH for this row of data is checked to see if it is less than **corLim,** and the waste package RH for the next row of data is checked to see if it is greater than **corLim**. If both conditions are met, **corFlag** is set to one and the remaining tests are skipped. Otherwise, **corFlag** remains at zero, and the next test is performed.

Next the drip shield RH for this row of data is checked to see if it is less than **corLim,** and the drip shield RH for the next row of data is checked to see if it is greater than **corLim**. If both conditions are met, **corFlag** is set to one, and the remaining tests are skipped. Otherwise, it remains at zero, and the next test is performed.

Next the waste package RH for this row of data is checked to see if it is less than **corLim,** and the waste package RH for the previous row of data is checked to see if it is greater than **corLim**. If both conditions are met, **corFlag** is set to one, and the remaining tests are skipped. Otherwise, **corFlag** remains at zero, and the next test is performed.

Next the drip shield RH for this row of data is checked to see if it is less than **corLim,** and the drip shield RH for the previous row of data is checked to see if it is greater than **corLim**. If both conditions are met, **corFlag** is set to one, and the remaining tests are skipped. Otherwise, **corFlag** remains at zero and the next test is performed.

Next the waste package RH for the current row of data, the preceding row of data, and the next row of data are checked to see if they are all less than **corLim**. If these conditions are met, the remaining tests are skipped, with **corFlag** remaining at zero. If these conditions are not met, the next test is performed.

Next the drip shield RH for the current row of data, the preceding row of data, and the next row of data, are checked to see if they are all less than **corLim**. If these conditions are met, the final test is skipped, with **corFlag** remaining at zero. If these conditions are not met, **corFlag** is set to one.

If **corFlag** is set to one by any of the preceding tests, the row of data is written to a temporary file (**temp.dat**) and **nnRows()** is incremented by one.

The last row of data is written to the temporary file for all of the data sets.

When all of the data-sets have been processed, the temporary file is closed.

2.3.14 Subroutine AddDataPoints

This subroutine steps through the time histories in the temporary file (**temp.dat**) created by the **CullDataPoints** subroutine and determines if time-step sizes above 50,000 years are sufficiently small. This is accomplished in two parts. For time periods from 50,000 to 200,000 years, the time-step interval should be no greater than 10,000 years. For time periods greater than 200,000 years, the time-step interval should be no greater than 100,000 years.

First the subroutine opens the temporary data file (**temp.dat**) created by the **CullDataPoints** subroutine and creates a new temporary data file (**temp2.dat**).

A **do-loop** is used to cycle through all of the time histories. The current time history is read from **temp.dat** and stored in the dynamically allocated **TempStorage** array.

A nested do-loop is then used to cycle through all of the rows in the current time history.

First the time for the current row of data is checked to see if it is greater than 50,000 years and less than 200,000 years. If so, the interval between it and the next time step is evaluated to determine if it is greater than 10,000 years. If so, the current row of data is written to the **temp2.dat** file, and the **AddPoints1** subroutine is called to generate a sufficient number of 10,000 year-spaced interpolated data sets such that no time interval is greater than 10,000 years. If the time interval is less than 10,000 years, the current row of data is written to the **temp2.dat** file.

Next the subroutine checks to see if the time history is greater than 200,000 years. If so, the interval between it and the next time step is checked to determine if it is greater than 100,000 years. If so, the current row of data is written to the **temp2.dat** file and the **AddPoints2** subroutine is called to generate a sufficient number of 100,000 year-spaced interpolated data sets such that no time interval is greater than 100,000 years. If the time interval is less than 100,000 years, the current row of data is written to the **temp2.dat** file.

If the time history is less than 50,000 years, the data is written to the temp2.dat file.

This process is repeated until all rows up to the last one have been checked. When the last row of data is reached, it is written to the **temp2.dat** file.

2.3.15 Subroutine AddPoints1

This subroutine interpolates data between time steps. It begins by checking to see if the time for the next row of data is greater than 200,000 years. If not, it skips forward to generate points for 10,000 year intervals. If so, it then sets two time steps, one for less than 200,000 years (**delTime1** = 200,000 years – current time step) and one for greater than 200,000 years (**delTime2** = 800,000 years). It then calculates the number of extra time steps needed for less than 200,000 years (**numExtraPoints1**) by dividing **delTime1** by 10,000 years. The number of time steps required above 200,000 years (**numExtraPoints2**) is determined by dividing **delTime2** by 100,000 years.

If **numExtraPoints1** is greater than zero, a **do-loop** is initiated that interpolates data points at 10,000 year intervals and writes them to the **TempStorage** array.

If **numExtraPoints2** is greater than zero, a **do-loop** is initiated that interpolates data points at 100,000 year intervals and writes them to the **TempStorage** array.

If the time step checked at the beginning of the routine is less than 200,000 years this, section of the subroutine calculates the time interval between the current time history and the next time history (**delTime**). It then divides **delTime** by 10,000 years to determine **numExtraPoints**. Next a **do-loop** is initiated that interpolates data points at 10,000 year intervals and writes them to the **TempStorage** array.

2.3.16 Subroutine AddPoints2

This subroutine interpolates data for time steps above 200,000 years. It begins by calculating the time interval between the current time step and the next time step (**delTime**). It then divides **delTime** by 100,000 years to determine **numExtraPoints**. Next a **do-loop** is initiated that interpolates data points at 100,000 year intervals and writes them to the **TempStorage** array.

2.3.17 Subroutine WriteOutputFile

This subroutine writes the output file from the **PREWAP** routine. It begins by opening the current output file (**outfile**) and the **temp2.dat** file. It then writes the initial comment lines and number of data sets to **outfile**. A **do-loop** is used to write each data set to the **outfile**. Within the **do-loop** the number of rows of data, the fraction of packages this data set is applicable to, and the header line for the data set are written to the **outfile**. Then a nested **do-loop** is used to read the data-set values from the **temp2.dat** file and write them to the **outfile**.

Finally the subroutine closes the **outfile** and **temp2.dat** files.

2.3.18 Subroutine DeallocateArrays

This subroutine deallocates all of the arrays allocated at the beginning of the program.

2.4 DESCRIPTION OF TEST CASES

PREWAP was validated using EXCEL spreadsheets to replicate PREWAP calculations and logic functions.

The interpolation subroutines were verified by running them independently of the overall program. A separate program was written containing the interpolate subroutines. This program was then compiled and run using an input deck that exercised all of the subroutine's calculations and logic functions. The output was written to output file. These results were then compared to an EXCEL spreadsheet that replicated the subroutine's calculations. These files are presented in Section 3.3 COMPUTER LISTING OF TEST DATA INPUT AND OUTPUT. Visual inspections of these files show that the outputs from both methods agree, thus validating the operation of the interpolation subroutines.

Next the overall program was verified by comparing the output from the program using a limited input deck covering the full range of values expected for the input to the output from an EXCEL spreadsheet that replicated the programs calculations and logic functions. This was accomplished by copying the test data input file to an EXCEL spreadsheet. Additional columns were then added to the spreadsheet containing equations or logic functions performed by the PREWAP program. This included columns for intermediate and final output. The output from the PREWAP program, using the test file as input, was compared to the results obtained from the spreadsheet. These files are presented in Section 3.3 COMPUTER LISTING OF TEST DATA INPUT AND OUTPUT. Visual inspection of these files shows that the output from the PREWAP program is consistent with the results generated by the spreadsheet.

2.5 DESCRIPTION OF TEST RESULTS

The results of these tests demonstrate that the output from the PREWAP program agrees with the test cases, verifying that the program correctly performs its intended functions.

2.6 RANGE OF INPUT VALUES FOR WHICH RESULTS WERE VERIFIED

Inputs to PREWAP are those physical parameters contained in the pH, Cl, and T-H files. Ranges for these parameters are those that are physically plausible for the parameter. For example RH cannot exceed 100%, pH and Cl concentrations values cannot be negative. No other limitations exist on the range of input parameter values.

2.7 LIMITATIONS ON SOFTWARE ROUTINE APPLICATIONS OR VALIDITY

This is a stand alone executable program that can be run under the Windows 95/98 and Windows NT operating environments on any PC platform with 100 megabytes of disk space and 64 megabytes of RAM.

3. SUPPORTING INFORMATION:

3.1 DIRECTORY LISTING OF EXECUTABLE AND DATA FILES

The PREWAP executable and the associated input files must be contained in the same directory. There are no other restrictions on directory names or structure that will affect the operation of the code.

3.2 COMPUTER LISTING OF SOURCE CODE

```
program prewap

! define dynamic variables
real(8), allocatable :: etime(:,:), wpT(:,:), dsT(:,:), dwT(:,:), iT(:,:)
real(8), allocatable :: wpRH(:,:), dsRH(:,:), dwRH(:,:), bfRH(:,:), iRH(:,:)
real(8), allocatable :: dsLS(:,:), iLS(:,:), massFracAir(:,:)
real(8), allocatable :: dwFluxWV(:,:), dwFluxAir(:,:)
real(8), allocatable :: dsEvapRate(:,:), bfEvapRate(:,:), iEvapRate(:,:)
real(8), allocatable :: PercFlux5m(:,:), tdsPercFlux(:,:), iPercFlux(:,:)
real(8), allocatable :: tdsT(:,:)

real(8), allocatable :: fract(:)

real(8), allocatable :: wpPHnd(:,:), wpCLnd(:,:), wpPHd(:,:), wpCLd(:,:)
real(8), allocatable :: dsPHnd(:,:), dsCLnd(:,:), dsPHd(:,:), dsCLd(:,:)
real(8), allocatable :: ipkPHnd(:,:), ipkCLnd(:,:), ipkPHd(:,:), ipkCLd(:,:)
real(8), allocatable :: barPHnd(:,:), barCLnd(:,:), barPHd(:,:), barCLd(:,:)

real(8), allocatable :: TempStorage(:,:)

integer(4), allocatable :: nRows(:), nnRows(:), nnnRows(:)

! define fixed variables

real(8) RHvector(10), Qvector(7), Tvector3(3), Tvector4(4), fCO2vector(7)
real(8) CLtable1a(10), CLtable1b(10), CLtable1c(10)
real(8) CLtable2a(7), CLtable2b(7)
real(8) CLtable3(7,3)
real(8) PHtable1a(10), PHtable1b(10), PHtable1c(10)
real(8) PHtable2a(7), PHtable2b(7)
real(8) PHtable3(7,3)
real(8) PHtable4(7,4)

real(8) ReadVector(22)
real(8) newValue(22)
```

```
integer(4) nRowsTable1, nRowsTable2, nRowsTable3, nColsTable3
integer(4) nRowsTable4, nColsTable4

real(8) ipkPHbounding, CorLim

real(8) pHCSNFinpk, pHCDSPInpk, Clinpk

integer(4) l, j, k
integer(4) iFile, nFile
integer(4) rows, maxRows, nDataSets, maxnnRows
integer(4) corFlag

character*6 dummy1
character*6 dummy2(6)
character*25 infile, outfile
character*25 InFileNames(100)
character*25 OutFileNames(100)

open(unit=99, file='debug.dat')        ! open debug file

! read in TH input and WAPDEG output file names
call ReadMasterFiles

! read in data for in-drift chemistry lookup tables
call ReadChemData

maxnnRows=0        ! initialize counter

! main program loop
! calls the subroutines that read in TH data, perform the necessary
! calculations, and generate the WAPDEG input files
do iFile=1,nFile

  infile=InFileNames(iFile)
  outfile=OutFileNames(iFile)

  write(*,*) "processing file: ", infile

  call CountDataSets
  call AllocateArrays
  call ReadInputFile
  call DoCalculations
  call CullDataPoints
  call AddDataPoints
  call WriteOutputFile
  call DeallocateArrays

end do

write(99,*) maxnnRows

close(99)    ! close debug file

contains
```

```
! this is the end of the "prewap" main program logic

! subroutines between the "contains" line and the "end subroutine prewap"
! line are internal to the "prewap" main program

!*****************************************************************************
!*****************************************************************************
subroutine ReadMasterFiles

! open 'InMaster.in' and 'OutMaster.in' files
open(unit=11, file='InMaster.in')
open(unit=12, file='OutMaster.in')

! read in the RH corrosion limit
read(11,*) CorLim

! read in the number of file names in the files
read(11,*) nFile

! read in input and output file names
do i=1,nFile
 read(11,*) InFileNames(i)
 read(12,*) OutFileNames(i)
end do

! close files
close(unit=11)
close(unit=12)

end subroutine ReadMasterFiles
!*****************************************************************************
!*****************************************************************************
subroutine ReadChemData

! read in log[Cl] data as a function of RH
open(unit=80, file='CLtable1.dat')
read(80,*) nRowsTable1     ! number of rows in the table
do m=1,nRowsTable1
 read(80,*) RHvector(m), CLtable1a(m), CLtable1b(m), CLtable1c(m)
end do
close(80)

! read in log[Cl] data as a function of 1-Qe/Qs
open(unit=80, file='CLtable2.dat')
read(80,*) nRowsTable2     ! number of rows in the table
do m=1,nRowsTable2
 read(80,*) Qvector(m), CLtable2a(m), CLtable2b(m)
end do
close(80)

! log[Cl] data as a function of 1-Qe/Qs and temperature(C)
open (unit=80, file='CLtable3.dat')

! number of rows and columns in the table
read(80,*) nRowsTable3, nColsTable3
```

```
! read in the temperature data
read(80,*) (Tvector3(n), n=1,nColsTable3)
do m=1,7
 read(80,*) Qvector(m), (CLtable3(m,n), n=1,nColsTable3)
end do
close(80)

! pH data as a function of RH
open(unit=80, file='PHtable1.dat')
do m=1,10
 read(80,*) RHvector(m), PHtable1a(m), PHtable1b(m), PHtable1c(m)
end do
close(80)

! pH data as a function of 1-Qe/Qs
open(unit=80, file='PHtable2.dat')
do m=1,nRowsTable2
 read(80,*) Qvector(m), PHtable2a(m), PHtable2b(m)
end do
close(80)

! pH data as a function of 1-Qe/Qs and temperature(C)
open (unit=80, file='PHtable3.dat')
read(80,*) (Tvector3(n), n=1,nColsTable3)
do m=1,nRowsTable3
 read(80,*) Qvector(m), (PHtable3(m,n), n=1,nColsTable3)
end do
close(80)

! pH data as a function of fCO2 and temperature(C)
open (unit=80, file='PHtable4.dat')
read(80,*) nRowsTable4, nColsTable4
read(80,*) (Tvector4(n), n=1,nColsTable4)
do m=1,nRowsTable4
 read(80,*) fCO2vector(m), (PHtable4(m,n), n=1,nColsTable4)
end do
close(80)

open (unit=80, file='InPkgChem.dat')
read(80,*) pHCSNFinpk, phCDSPinpk
read(80,*) Clinpk
close(80)


end subroutine ReadChemData
!***************************************************************************
!
!***************************************************************************
subroutine CountDataSets

open(unit=70, file=infile)

nDataSets=1        ! initialize # of data sets to 1
maxRows=0          ! initialize the max number of rows to 0

! read past 1st four rows of header information
do i=1,4
```

```
 read(70,*) dummy1
end do

! read past header info in line 5 to get number of rows of data
read(70,*) (dummy2(i), i=1,5), rows
write(99,*) rows, "  rows"

! set max number of rows equal to the # of rows in 1st data set
maxRows=rows

! read past next six rows of header information
do i=1,6
 read(70,*) dummy1
end do

! read past the 1st data set
do i=1,rows
 read(70,*) dummy
end do

! read through the rest of the file until the end of the file is reached
do

! read the 1st row header information for the next data set
! if this read occurs at the end of the file, the 'eof' error
! causes the do loop to be exited
 read(70,*,end=100) (dummy2(i), i=1,5), rows
 !write(99,*) rows, "  rows"

! if an 'eof' error did not occur, increment the data set counter
! and read through the given data set
 nDataSets=nDataSets+1

! if the # of rows in the current data set are greater than the current
! max rows value, set max rows equal to the # of rows in the current data set
 if (rows .gt. maxRows) then
  maxRows=rows
 end if

! read through the current data set
 do i=1,(6+rows)
  read(70,*) dummy1
 end do

end do

! line that the 'eof' error causes the do-loop to bails out to
100 continue

! close the data file
close(unit=70)

! write the number of data sets to debug.dat
write(99,*) nDataSets, "  # of data sets"

end subroutine CountDataSets
```

```
!***********************************************************************************
!***********************************************************************************
subroutine AllocateArrays

! set bounds on dynamic arrays whose size is dependent upon the current TH file
allocate (etime(1:maxRows, 1:nDataSets))
allocate (wpT(1:maxRows, 1:nDataSets))
allocate (dsT(1:maxRows, 1: nDataSets))
allocate (dwT(1:maxRows, 1:nDataSets))
allocate (iT(1:maxRows, 1:nDataSets))
allocate (wpRH(1:maxRows, 1:nDataSets))
allocate (dsRH(1:maxRows, 1:nDataSets))
allocate (dwRH(1:maxRows, 1:nDataSets))
allocate (bfRH(1:maxRows, 1:nDataSets))
allocate (iRH(1:maxRows, 1:nDataSets))
allocate (dsLS(1:maxRows, 1:nDataSets))
allocate (iLS(1:maxRows, 1:nDataSets))
allocate (massFracAir(1:maxRows, 1:nDataSets))
allocate (dwFluxWV(1:maxRows, 1:nDataSets))
allocate (dwFluxAir(1:maxRows, 1:nDataSets))
allocate (dsEvapRate(1:maxRows, 1:nDataSets))
allocate (bfEvapRate(1:maxRows, 1:nDataSets))
allocate (iEvapRate(1:maxRows, 1:nDataSets))
allocate (PercFlux5m(1:maxRows, 1:nDataSets))
allocate (tdsPercFlux(1:maxRows, 1:nDataSets))
allocate (iPercFlux(1:maxRows, 1:nDataSets))
allocate (tdsT(1:maxRows, 1:nDataSets))

allocate (nRows(1:nDataSets))
allocate (nnRows(1:nDataSets))
allocate (nnnRows(1:nDataSets))
allocate (fract(1:nDataSets))

end subroutine AllocateArrays
!***********************************************************************************
!***********************************************************************************
subroutine ReadInputFile

open(unit=70, file=infile)      ! open input file

j=1       ! column index for 1st data set

! read past 1st four rows of header information
do i=1,4
 read(70,*) dummy1
end do

! read past header info in line 5 to get number of rows of data
read(70,*) (dummy2(i), i=1,5), nRows(j)

! read past header info in line 6 to get "fraction of this history" value
read(70,*) (dummy2(i), i=1,6), fract(j)

! read past next five rows of header information
do i=1,5
 read(70,*) dummy1
```

```
end do

! read in data from 1st data set
do i=1, nRows(j)
 read(70,*) etime(i,j),      &     ! time [yr]
        wpT(i,j),         & ! temperature - waste package [C]
             dsT(i,j),         & ! temperature - drip shield [C]
             dwT(i,j),         & ! temperature - drift wall [C]
             iT(i,j),         &  ! temperature - invert [C]
             wpRH(i,j),         &    ! rel. humidity - waste package [-]
             dsRH(i,j),         &    ! rel. humidity - drip shield [-]
             dwRH(i,j),         &    ! rel. humidity - drift wall [-]
             bfRH(i,j),         & ! rel. humidity - backfill [-]
             iRH(i,j),          & ! rel. humidity - invert [-]
             dsLS(i,j),         & !
        iLS(i,j),         &  !
             massFracAir(i,j),  & ! mass frac. air [
             dwFluxWV(i,j),     & ! water vapor flux - drift wall [
             dwFluxAir(i,j),    & ! air flux - drift wall [
             dsEvapRate(i,j),   & ! evap. rate - drip shield [m3/yr]
             bfEvapRate(i,j),   & ! evap. rate - backfill [m3/yr]
             iEvapRate(i,j),    &
             PercFlux5m(i,j),   & ! perc flux @ 5m [mm/yr]
             tdsPercFlux(i,j),  & ! perc flux -  drip shield top [mm/yr]
             iPercFlux(i,j),    & ! perc flux - invert [mm/yr]
             tdsT(i,j)            ! temperature -  drip shield top [C]
end do

! now read in data for data sets 2 to nDataSets
do j=2,nDataSets

! read past header info in line 5 to get number of rows of data
 read(70,*) (dummy2(i), i=1,5), nRows(j)

! read past header info in line 6 to get "fraction of this history" value

 read(70,*) (dummy2(i), i=1,6), fract(j)

! read past next five rows of header information
 do i=1,5
  read(70,*) dummy1
 end do

! read in data from the j-th data set
 do i=1, nRows(j)
  read(70,*) etime(i,j),                                    &
        wpT(i,j), dsT(i,j), dwT(i,j), iT(i,j),               &
        wpRH(i,j), dsRH(i,j), dwRH(i,j), bfRH(i,j), iRH(i,j), &
        dsLS(i,j), iLS(i,j),                                 &
        massFracAir(i,j),                                    &
        dwFluxWV(i,j), dwFluxAir(i,j),                       &
        dsEvapRate(i,j), bfEvapRate(i,j), iEvapRate(i,j),    &
             PercFlux5m(i,j), tdsPercFlux(i,j), iPercFlux(i,j),  &
             tdsT(i,j)
 end do
```

```
end do

close(unit=70)   ! close the data file

end subroutine ReadInputFile
!*********************************************************************************
!*********************************************************************************
subroutine DoCalculations

allocate (wpPHnd(1:maxRows, 1:nDataSets))
allocate (wpCLnd(1:maxRows, 1:nDataSets))

allocate (wpPHd(1:maxRows, 1:nDataSets))
allocate (wpCLd(1:maxRows, 1:nDataSets))

allocate (dsPHnd(1:maxRows, 1:nDataSets))
allocate (dsCLnd(1:maxRows, 1:nDataSets))

allocate (dsPHd(1:maxRows, 1:nDataSets))
allocate (dsCLd(1:maxRows, 1:nDataSets))

allocate (ipkPHnd(1:maxRows, 1:nDataSets))
allocate (ipkCLnd(1:maxRows, 1:nDataSets))

allocate (ipkPHd(1:maxRows, 1:nDataSets))
allocate (ipkCLd(1:maxRows, 1:nDataSets))

allocate (barPHnd(1:maxRows, 1:nDataSets))
allocate (barCLnd(1:maxRows, 1:nDataSets))

allocate (barPHd(1:maxRows, 1:nDataSets))
allocate (barCLd(1:maxRows, 1:nDataSets))

! perform calculations at each "i" time for all "j" data sets
do j=1,nDataSets
 do i=1,nRows(j)

! NOTE: CL chemistry is NOT calculated in this code version. Instead, pH^2 is
! reported in the wpCLd, wpCLnd, dsCLd, and dsCLnd variables

! calculate waste package in-drift pH and pH^2 for drip and no drip conditions
  call InDriftCalc(etime(i,j), wpT(i,j), wpRH(i,j),          &
            dsEvapRate(i,j), tdsPercFlux(i,j),        &
                RHvector, Qvector, Tvector3, Tvector4,      &
            CLtable1a, CLtable1b, CLtable1c,          &
            CLtable2a, CLtable2b,                 &
            CLtable3,                &
            PHtable1a, PHtable1b, PHtable1c,          &
            PHtable2a, PHtable2b,                 &
            PHtable3, PHtable4,                 &
            nRowsTable1, nRowsTable2,                 &
                nRowsTable3, nColsTable3,                 &
                nRowsTable4, nColsTable4,                 &
                wpPHd(i,j), wpCLd(i,j), wpPHnd(i,j), wpCLnd(i,j),  &
                i, j, infile)
```

```
! calculate drip shield in-drift pH and pH^2 for drip and no drip conditions
 call InDriftCalc(etime(i,j), dsT(i,j), dsRH(i,j),            &
            dsEvapRate(i,j), tdsPercFlux(i,j),           &
                 RHvector, Qvector, Tvector3, Tvector4,     &
            CLtable1a, CLtable1b, CLtable1c,             &
            CLtable2a, CLtable2b,                    &
            CLtable3,                             &
            PHtable1a, PHtable1b, PHtable1c,             &
            PHtable2a, PHtable2b,                    &
            PHtable3, PHtable4,                      &
                 nRowsTable1, nRowsTable2,                &
                 nRowsTable3, nColsTable3,                &
                 nRowsTable4, nColsTable4,                &
                 dsPHd(i,j), dsCLd(i,j), dsPHnd(i,j), dsCLnd(i,j),  &
                 i, j, infile)

! set bounding in-package pH for CSNF or HLW
if (infile(1:4) .eq. 'CSNF') then
 ipkPHbounding=phCSNFinpk        ! CSNF bounding pH value
else
 ipkPHbounding=phCDSPinpk        ! HLW bounding pH value
end if

! in-package drip pH is set equal to bounding values

  ipkPHd(i,j)=ipkPHbounding
  ipkCLd(i,j)=ipkPHd(i,j)*ipkPHd(i,j)
!  ipkCLd(i,j)=CLinpk              ! mol/kg

! in-package no drip pH is set equal to -9.99E-02
! (default 'don't exist' values)
  ipkPHnd(i,j)=-9.99E-02
  ipkCLnd(i,j)=ipkPHnd(i,j)*ipkPHnd(i,j)
!  ipkCLd(i,j)=-9.99E-02           ! mol/kg

! barrier drip and no drip pH are set equal to -9.99E-02
! (default 'don't exist' values)
  barPHd(i,j)=-9.99E-02
  barCLd(i,j)=barPHd(i,j)*barPHd(i,j)
!  barCLd(i,j)=-9.99E-02
  barPHnd(i,j)=-9.99E-02
  barCLnd(i,j)=barPHnd(i,j)*barPHnd(i,j)
!  barCLnd(i,j)=-9.99E-02

 end do
end do

end subroutine DoCalculations
!*******************************************************************************
!*******************************************************************************
subroutine CullDataPoints

open(unit=72, file='temp.dat')        ! open temporary storage file

! loop through all of the data sets
do j=1,nDataSets
```

```
! initialize counter for number of rows that will get written
! to temporary storage file
nnRows(j)=0

do i=1,nRows(j)-1

 corFlag=0     ! initialize corrosion flag to 0 (no corrosion)

 ! skip row if wpT or dsT 'do not exist'
 if(wpT(i,j) .le. 0.0 .or. dsT(i,j) .le. 0.0) then
  ! write to debug file
  !write(99,*) etime(i,j), "  trapped on no wpT or dsT"

 ! write row if wpRH or dsRH is equal or above corrosion limit
 elseif( (wpRH(i,j) .ge. CorLim) .or. (dsRH(i,j) .ge. CorLim) ) then
  corFlag=1
  !write(99,*) etime(i,j), "  RH above corrosion limit"

 ! write row for wp no corrosion/corrosion transition
 elseif( (wpRH(i,j) .lt. 0.501) .and. (wpRH(i+1,j) .ge. 0.501) ) then
  corFlag=1
  !write(99,*) etime(i,j), "  wp no cor/cor transition"

 ! write row for ds no corrosion/corrosion transition
 elseif( (dsRH(i,j) .lt. 0.501) .and. (dsRH(i+1,j) .ge. 0.501)  ) then
  corFlag=1
  !write(99,*) etime(i,j), "  ds no cor/cor transition"

 ! write row for wp corrosion/no corrosion transition
 elseif( (wpRH(i,j) .lt. 0.501) .and. (wpRH(i-1,j) .ge. 0.501) ) then
  corFlag=1
  !write(99,*) etime(i,j), "  wp cor/no cor transition"

 ! write row for ds corrosion/no corrosion transition
 elseif( (dsRH(i,j) .lt. 0.501) .and. (dsRH(i-1,j) .ge. 0.501) ) then
  corFlag=1
  !write(99,*) etime(i,j), "  ds cor/no cor transition"

 ! skip row if in middle of no corrosion
 elseif( (wpRH(i,j) .lt. 0.501) .and.  &
       (wpRH(i-1,j) .lt. 0.501) .and.  &
       (wpRH(i+1,j) .lt. 0.501) ) then

  !write(99,*) etime(i,j), "  trapped on middle of no corrosion (wp)"
  ! trap

 elseif( (dsRH(i,j) .lt. 0.501) .and.  &
       (dsRH(i-1,j) .lt. 0.501) .and.  &
            (dsRH(i+1,j) .lt. 0.501) ) then

  !write(99,*) etime(i,j), "  trapped on middle of no corrosion (ds)"
  ! trap

 else
 ! middle of corrosion
```

```
corFlag=1
!write(99,*) etime(i,j), "  default"

end if

! write the i-th row of data to the temp file if corFlag=1
if(corFlag .eq. 1) then
 write(72,1020) etime(i,j), wpT(i,j), wpRH(i,j), dsT(i,j), dsRH(i,j),  &
        wpPHnd(i,j), wpCLnd(i,j), wpPHd(i,j), wpCLd(i,j),    &
            dsPHnd(i,j), dsCLnd(i,j), dsPHd(i,j), dsCLd(i,j),    &
            ipkPHnd(i,j), ipkCLnd(i,j), ipkPHd(i,j), ipkCLd(i,j),  &
            barPHnd(i,j), barCLnd(i,j), barPHd(i,j), barCLd(i,j),  &
            PercFlux5m(i,j)
 1020 format(22(ES10.3, "  "))

 ! increment the number of rows stored for the j-th time history
 nnRows(j)=nnRows(j)+1

end if

end do

! write the last time history to the temp file
i=nRows(j)
write(72,1020) etime(i,j), wpT(i,j), wpRH(i,j), dsT(i,j), dsRH(i,j),  &
        wpPHnd(i,j), wpCLnd(i,j), wpPHd(i,j), wpCLd(i,j),    &
            dsPHnd(i,j), dsCLnd(i,j), dsPHd(i,j), dsCLd(i,j),    &
            ipkPHnd(i,j), ipkCLnd(i,j), ipkPHd(i,j), ipkCLd(i,j),  &
            barPHnd(i,j), barCLnd(i,j), barPHd(i,j), barCLd(i,j),  &
            PercFlux5m(i,j)

! increment the number of rows stored for the j-th time history
nnRows(j)=nnRows(j)+1

write(99,*) j, nnRows(j)


if(nnRows(j) .gt. maxnnRows) then
 maxnnRows=nnRows(j)
end if

end do

close(72)

end subroutine CullDataPoints
!*************************************************************************
!*************************************************************************
subroutine AddDataPoints

open(unit=72, file='temp.dat')        ! open temporary storage files
open(unit=73, file='temp2.dat')


do j=1, nDataSets        ! loop through the time histories
```

```
allocate (TempStorage(1:nnRows(j), 1:22))       ! set TempStorage array size

! initialize counter for number of rows to be written to the WAPDEG input file
! for the j-th time history
nnnRows(j)=nnRows(j)

! read j-th time history from temp.dat file
do i=1,nnRows(j)
 read(72,*) (TempStorage(i,m), m=1,22)
end do

 do i=1,nnRows(j)-1 ! loop through all but the last row of data

 ! check times between 50,000 and 200,000 years to see
 ! if time steps are <= 10,000 years
 if((TempStorage(i,1) .ge. 50000.0)  .and.   &
   (TempStorage(i,1) .lt. 200000.0)) then

  ! if time step is greater than 10,000 years write current row of data
  ! to temp2.dat and call subroutine to add interpolated data and times
  ! at 10,000 year intervals between the i-th and i-th+1 rows
  if(TempStorage(i+1,1)-TempStorage(i,1) .gt. 10000.0) then
   write(73,1020) (TempStorage(i,m), m=1,22)
       1020 format(22(ES10.3, "  "))
   call AddPoints1

  else
   ! if time step is <= 10,000 years write current row of data to temp2.dat
   write(73,1020) (TempStorage(i,m), m=1,22)

  endif

 ! check times after 200,000 years to see
 ! if time steps are <= 100,000 years
 elseif(TempStorage(i,1) .ge. 200000.0) then

  ! if time step is greater than 100,000 years write current row of data
  ! to temp2.dat and call subroutine to add interpolated data and times
  ! at 100,000 year intervals between the i-th and i-th+1 rows
  if(TempStorage(i+1,1)-TempStorage(i,1) .gt. 100000.0) then
   write(73,1020) (TempStorage(i,m), m=1,22)
       call AddPoints2

  else
   ! if time step is <= 100,000 years write current row of data to temp2.dat
   write(73,1020) (TempStorage(i,m), m=1,22)

  endif

 else
 ! if time is <= 50,000 years write current row of data to temp2.dat
  write(73,1020) (TempStorage(i,m), m=1,22)

 endif

 end do
```

```
! write the last row of data to the temp2.dat file
write(73,1020) (TempStorage(nnRows(j),m), m=1,22)

deallocate (TempStorage)      ! deallocate the TempStorage array

end do

close(72)       ! close temporary files
close(73)

end subroutine AddDataPoints
!*******************************************************************************
!*******************************************************************************
subroutine WriteOutputFile

open(unit=71, file=outfile)         ! open output file
open(unit=73, file='temp2.dat')  ! open temporary storage file

! write initial comment lines
write(71,1011)
1011 format('! 1st comment line')
write(71,1012)
1012 format('! 2nd comment line')
write(71,1013)
1013 format('! 3rd comment line')

write(71,1014) nDataSets
1014 format('# ', I4, ' 21')      ! # of datasets and # of columns of data
                                  ! WAPDEG guys don't want 22nd column
do j=1,nDataSets
 write(71,1015) nnnRows(j)
 1015 format('# ', I4)            ! # of rows in the j-th dataset

 write(71,1016) fract(j)
 1016 format('# ', ES10.3)           ! fraction of packages

 write(71,1018)                      ! writes header line
 1018 format('! t        ',' wpT      ',' wpRH      ',  &
        ' dsT      ',' dsRH      ',' wpPHnd   ',   &
             ' wpCLnd   ',' wpPHd    ',' wpCLd     ',   &
             ' dsPHnd   ',' dsCLnd   ',' dsPHd     ',   &
             ' dsCLd    ',' ipkPHnd  ',' ipkCLnd   ',   &
             ' ipkPHd   ',' ipkCLd   ',' barPHnd   ',   &
             ' barCLnd  ',' barPHd   ',' barCLd    ',   &
             ' PercFlux5m')

 1020 format(22(ES10.3, "  "))
 do i=1,nnnRows(j)
  read(73,*) (ReadVector(m), m=1,22)
  write(71,1020) (ReadVector(m), m=1,22)
 end do


end do
```

```
write(99,*)

close(unit=71)  ! close output file
close(unit=73)  ! close temporary storage file

end subroutine WriteOutputFile
!*****************************************************************************
!*****************************************************************************
subroutine DeallocateArrays

! deallocate arrays
deallocate (etime, wpT,  dsT, dwT, iT, wpRH, dsRH, dwRH, bfRH, iRH)
deallocate (dsLS, iLS, massFracAir, dwFluxWV, dwFluxAir)
deallocate (dsEvapRate, bfEvapRate, iEvapRate)
deallocate (PercFlux5m, tdsPercFlux, iPercFlux, tdsT)

deallocate (fract)

deallocate (wpPHnd, wpCLnd, wpPHd,  wpCLd)
deallocate (dsPHnd,  dsCLnd,  dsPHd, dsCLd)
deallocate (ipkPHnd,  ipkCLnd,  ipkPHd,  ipkCLd)
deallocate (barPHnd,  barCLnd,  barPHd,  barCLd)

deallocate (nRows, nnRows, nnnRows)

end subroutine DeallocateArrays
!*****************************************************************************
!*****************************************************************************
subroutine AddPoints1

! check for time step spanning across 200,000 years
if (TempStorage(i+1,1) .gt. 200000.0) then
 ! if it does set two time steps
 ! one for <= 200,000 and one for > 200,000 years
 delTime1=200000.0-TempStorage(i,1)
 delTime2=800000.0

 ! calculate the number of extra points to be added
 numExtraPoints1 = ceiling(delTime1/10000)
 numExtraPoints2 = ceiling(delTime2/100000)-1


 if (numExtraPoints1 .ne. 0) then
 ! generate interpolated data for the extra points to be added
  do ii=1,numExtraPoints1
   do jj=2,22
    delDep=TempStorage(i+1,jj)-TempStorage(i,jj)
    newValue(jj)=TempStorage(i,jj) + delDep*(10000*ii/delTime1)
   end do
   1021 format(22(ES10.3, " "))
   ! write the interpolated data to the temp2.dat file
   write(73,1021) TempStorage(i,1)+10000*ii, (newValue(m), m=2,22)
  end do
 end if

 if (numExtraPoints2 .ne. 0) then
```

```
! generate interpolated data for the 1st extra point to be added
do jj=2,22
 delDep=TempStorage(i+1,jj)-TempStorage(i,jj)
 newValue(jj)=TempStorage(i,jj) + &
        delDep*(200000-TempStorage(i,1))/(TempStorage(i+1,1)-TempStorage(i,1))
end do
! write the interpolated data to the temp2.dat file
write(73,1021) 300000.0, (newValue(m), m=2,22)

! generate interpolated data for the remaining extra points to be added
do ii=2,numExtraPoints2
 do jj=2,22
  delDep=TempStorage(i+1,jj)-TempStorage(i,jj)
  newValue(jj)=TempStorage(i,jj) + delDep*(100000*ii/delTime2)
 end do
 ! write the interpolated data to the temp2.dat file
 write(73,1021) 200000.0+100000.0*ii, (newValue(m), m=2,22)
end do
end if

! increment the number of rows of the j-ht time history by the number of points added
nnnRows(j)=nnnRows(j)+numExtraPoints1+numExtraPoints2

else
! time step doesn't span 200,000 years

! calculate the number of extra points to be added
delTime=TempStorage(i+1,1)-TempStorage(i,1)
numExtraPoints = ceiling(delTime/10000)-1

if (numExtraPoints .eq. 0) then
 return
end if

! generate interpolated data for the points to be added
do ii=1,numExtraPoints
 do jj=2,22
  delDep=TempStorage(i+1,jj)-TempStorage(i,jj)
  newValue(jj)=TempStorage(i,jj) + delDep*(10000*ii/delTime)
 end do
 ! write the interpolated data to the temp2.dat file
 write(73,1021) TempStorage(i,1)+10000*ii, (newValue(m), m=2,22)
end do

! increment the number of rows of the j-ht time history by the number of points added
nnnRows(j)=nnnRows(j)+numExtraPoints

end if

end subroutine AddPoints1
!***************************************************************************
!***************************************************************************
subroutine AddPoints2

delTime=TempStorage(i+1,1)-TempStorage(i,1)
```

```
numExtraPoihts = ceiling(delTime/100000)-1

if (numExtraPoints .eq. 0) then
 return
end if

do ii=1,numExtraPoints
 do jj=2,22
  delDep=TempStorage(i+1,jj)-TempStorage(i,jj)
  newValue(jj)=TempStorage(i,jj) + delDep*(100000*ii/delTime)
 end do
 write(73,1022) TempStorage(i,1)+100000*ii, (newValue(m), m=2,22)
 1022 format(22(ES10.3, "  "))
end do

nnnRows(j)=nnnRows(j)+numExtraPoints

end subroutine AddPoints2
!******************************************************************************
!******************************************************************************
end program prewap

! subroutines past this point are external to the "prewap" main program

!******************************************************************************
!******************************************************************************
! calualate the pH and Cl under drip and no drip conditions

! NOTE: CL chemistry is NOT calculated in this code version. Instead, pH^2 is
! reported in the wpCLd, wpCLnd, dsCLd, and dsCLnd variables

subroutine InDriftCalc(etime, T, RH, EvapRate, SeepRate,      &
                RHvector, Qvector, Tvector3, Tvector4,    &
          CLtable1a, CLtable1b, CLtable1c,          &
          CLtable2a, CLtable2b,                 &
          CLtable3,                  &
          PHtable1a, PHtable1b, PHtable1c,          &
          PHtable2a, PHtable2b,                 &
          PHtable3, PHtable4,                  &
                nRowsTable1, nRowsTable2,              &
                nRowsTable3, nColsTable3,              &
                nRowsTable4, nColsTable4,              &
          PHd, CLd, PHnd, CLnd,                  &
               i, j, infile)

 real(8) RHvector(nRowsTable1), Qvector(nRowsTable2), fCO2vector(nRowsTable4)
 real(8) Tvector3(nColsTable3), Tvector4(nColsTable4)
 real(8) CLtable1a(nRowsTable1), CLtable1b(nRowsTable1), CLtable1c(nRowsTable1)
 real(8) CLtable2a(nRowsTable2), CLtable2b(nRowsTable2)
 real(8) CLtable3(nRowsTable3,nColsTable3)
 real(8) PHtable1a(nRowsTable1), PHtable1b(nRowsTable1), PHtable1c(nRowsTable1)
 real(8) PHtable2a(nRowsTable2), PHtable2b(nRowsTable2)
 real(8) PHtable3(nRowsTable3,nColsTable3)
 real(8) PHtable4(nRowsTable4,nColsTable4)

 real(8) etime, T, RH, Qratio, EvapRate, SeepRate
```

```
real(8) PHd, CLd, PHnd, CLnd, logCLd, logfCO2

integer(4) nRowsTable1, nRowsTable2, nRowsTable3, nColsTable3
integer(4) i, j

character*15 infile

! trap for temperatures and seep rates that "don't exist"
if( (T .lt. 0.0) .or. (SeepRate .lt. -99.0)) then

! drip and no drip pH are set equal to -9.99E-02
! (default 'don't exist' values)
 PHd=-9.99E-02
 PHnd=-9.99E-02

! place holder for CL calculations
!  CLd=-9.99E-02
!  CLnd=-9.99E-02

else

! calculate 1-Qe/Qs
 if( SeepRate .eq. 0.0) then        ! sets 1-Qe/Qs equal to 0.0 when Qs=0
  Qratio=0.0
 else
  Qratio=1.0 - abs(EvapRate/SeepRate)
 end if

! determine what range of in-drift chemistry data is applicable, then
! calculate pH and pH^2

! 1st period (< 50 years -- pre-closure) ****************************************
 if(etime .lt. 50.0) then

  ! drip and no drip pH are set equal to -9.99E-02
  ! (default 'don't exist' values)
  PHd=-9.99E-02
  PHnd=-9.99E-02

! place holder for CL calculations
   ! drip and no drip CL are set equal to -9.99E-02
   ! (default 'don't exist' values)
!  CLd=-9.99E-02
!  CLnd=-9.99E-02

! 2nd time period (50 to 1000 years) ******************************************
 elseif( (etime .gt. 50.0) .and. (etime .le. 1000.0) ) then

  logfCO2=-6.5

  ! 1st range (RH <= 50)
  if (100*RH .le. 50.0) then
   !!write(99,*) "1st range"

   ! drip and no drip pH are set equal to -9.99E-02
   ! (default 'don't exist' values)
```

```
  PHd=-9.99E-02
  PHnd=-9.99E-02

! place holder for CL calculations
  ! drip and no drip CL are set equal to -9.99E-02
  ! (default 'don't exist' values)
!  CLd=-9.99E-02
!  CLnd=-9.99E-02

 ! 2nd range (50 <= RH <= 85)
 elseif( (100*RH .ge. 50.0) .and.  &
       (100*RH .le. 85.0) ) then

  !!write(99,*) "2nd range"

  PHd=9.40     ! drip pH is constant in this range
  call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
            nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!   call Interp1D(100*RH, RHvector, CLtable1a, nRowsTable1, logCLd)
!   CLd=10**logCLd
!   CLnd=-9.99E-02

 ! 3rd range (RH > 85)
 elseif(100*RH .gt. 85.0) then

  !!write(99,*) "3rd range"

  call Interp1D(Qratio, Qvector, PHtable2a, nRowsTable2, PHd)
  call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
            nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!  call Interp1D(Qratio, Qvector, CLtable2a, nRowsTable2, logCLd)
!  CLd=10**logCLd
!  CLnd=-9.99E-02

  else
   !!write(99,*) "failed all 2nd period tests"
  end if

 ! 3rd time period (1000 years to 2000 years) ***************************
 elseif( (etime .gt. 1000.0) .and. (etime .le. 2000.0) ) then

  logfCO2=-3.0

 ! 1st range (RH < 50)
  if (100*RH .lt. 50.0) then
   !!write(99,*) "1st range"

   ! drip and no drip pH are set equal to -9.99E-02
   ! (default 'don't exist' values)
   PHd=-9.99E-02
   PHnd=-9.99E-02
```

```
! place holder for CL calculations
  ! drip and no drip CL are set equal to -9.99E-02
  ! (default 'don't exist' values)
!  CLd=-9.99E-02
!  CLnd=-9.99E-02

 ! 2nd range (50 <= RH <= 85)
 elseif( (100*RH .ge. 50.0) .and.  &
        (100*RH .le. 85.0) ) then

  !!write(99,*) "2nd range"


  PHd=7.64    ! drip pH is constant in this range
  call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
           nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!  call Interp1D(100*RH, RHvector, CLtable1b, nRowsTable1, logCLd)
!  CLd=10**logCLd
!  CLnd=-9.99E-02

 ! 3rd range (RH > 85)
 elseif(100*RH .gt. 85.0) then

  !!write(99,*) "3rd range"
  call Interp1D(Qratio, Qvector, PHtable2b, nRowsTable2, PHd)
  call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
           nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!  call Interp1D(Qratio, Qvector, CLtable2b, nRowsTable2, logCLd)
!  CLd=10**logCLd
!  CLnd=-9.99E-02

 else
  !!write(99,*) "failed all 3nd period tests"
 end if

 ! 4th time period (2000 year to 100,000 years) ********************
 elseif( (etime .gt. 2000.0) .and. (etime .le. 100000.0) ) then

  logfCO2=-2.0

  ! 1st range (RH < 50)
  if (100*RH .lt. 50.0) then
   !!write(99,*) "1st range"

   PHd=-9.99E-02
   PHnd=-9.99E-02

! place holder for CL calculations
!  CLd=-9.99E-02
!  CLnd=-9.99E-02

  ! 2nd range (50 <= RH <= 85)
```

```
elseif( (100*RH .ge. 50.0) .and.  &
     (100*RH .le. 85.0) ) then

 !!write(99,*) "2nd range"

 PHd=7.02    ! drip pH is constant in this range
 call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
          nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!  call Interp1D(100*RH, RHvector, CLtable1b, nRowsTable1, logCLd)
!  CLd=10**logCLd
!  CLnd=-9.99E-02

 ! 3rd range (RH > 85)
 else

  !!write(99,*) "3rd range"

  call Interp2D(Qratio, T, Qvector, Tvector3, PHtable3, &
          nRowsTable3, nColsTable3, PHd)
  call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
          nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!  call Interp2D(Qratio, T, Qvector, Tvector, CLtable3, &
!           nRowsTable3, nColsTable3, logCLd)
!  CLd=10**logCLd
!  CLnd=-9.99E-02

 end if

! 5th time period (>100,000 years) ******************
else

 logfCO2=-3.0

 ! 1st range (RH < 50)
 if (100*RH .lt. 50.0) then
  !!write(99,*) "1st range"

  PHd=-9.99E-02
  PHnd=-9.99E-02

! place holder for CL calculations
!  CLd=???
!  CLnd=-9.99E-02

 ! 2nd range (50 <= RH <= 85)
 elseif( (100*RH .ge. 50.0) .and.  &
      (100*RH .le. 85.0) ) then

  !!write(99,*) "2nd range"

  PHd=7.64    ! drip pH is constant in this range
  call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
```

```
            nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!  call Interp1D(100*RH, RHvector, CLtable1b, nRowsTable1, logCLd)
!  CLd=10**logCLd
!  CLnd=-9.99E-02

 ! 3rd range (RH > 85)
 elseif(100*RH .gt. 85.0) then

  !!write(99,*) "3rd range"
  call Interp1D(Qratio, Qvector, PHtable2b, nRowsTable2, PHd)
  call Interp2D(logfCO2, T, fCO2vector, Tvector4, PHtable4, &
            nRowsTable4, nColsTable4, PHnd)

! place holder for CL calculations
!  call Interp1D(Qratio, Qvector, CLtable2b, nRowsTable2, logCLd)
!  CLd=10**logCLd
!  CLnd=-9.99E-02

 end if

 end if

end if

! substitute pH^2 values in place of CL values
CLd=PHd*PHd
CLnd=PHnd*PHnd

  !!write(99,*) etime, " etime"
  !!write(99,*) j, i, " j-th dataset, i-th time"
  !!write(99,*) T, " temp"
  !!write(99,*) RH, " RH"
  !!write(99,*) EvapRate, " evap rate"
  !!write(99,*) SeepRate, " seep rate"
  !!write(99,*) Qratio, " Qe/Qs"
  !!write(99,*)

end subroutine InDriftCalc
!**********************************************************************************
!**********************************************************************************
! 1-D interpolation routine
subroutine Interp1D(ind, IndData, DepData, nRows, dep)

! number of rows in 1-D table
integer(4) nRows

! independent and dependent variable vectors
real(8) IndData(nRows), DepData(nRows)

! independent and dependent variables
real(8) ind, dep

! check for independent variable outside of data set range
if (ind .le. IndData(1)) then
```

```
 dep=DepData(1)              ! value is below lower bound, set equal to floor
elseif (ind .ge. IndData(nRows)) then
 dep=DepData(nRows)          ! value is above upper bound, set equal to ceiling
else

 do i=1,nRows-1              ! value is within the range of the data set
  if ((ind .ge. IndData(i)) .and. (ind .lt. IndData(i+1))) then

   ! linear interpolation
   ! y = y(i) + [x-x(i)]/[x(i+1)-x(i)] * [y(i+1)-y(i)]
   dep=DepData(i) &
       + (ind-IndData(i))/(IndData(i+1)-IndData(i)) &
         *(DepData(i+1)-DepData(i))
  end if
 end do
end if

end subroutine Interp1D
!*****************************************************************************
!*****************************************************************************
subroutine Interp2D(ind1, ind2, IndData1, IndData2, DepData, nRows, nCols, dep)

! number of rows and columns in 2-D table
integer(4) nRows, nCols

! independent variable vectors and dependent variable array
real(8) IndData1(nRows), IndData2(nCols), DepData(nRows,nCols)

! independent variables, intermediate dependent variables, and dependent variable
real(8) ind1, ind2, dep1, dep, dep2

! flags for independent variable values beyond upper and lower bounds
integer(4) iflag_lb, iflag_ub, jflag_lb, jflag_ub

!!write(99,*) "in Interp2D"
!!write(99,*) ind1, " ind1"
!!write(99,*) ind2, " ind2"

! initialize flags
iflag_lb = 0
iflag_ub = 0
jflag_lb = 0
jflag_ub = 0

! determine i-index
if (ind1 .le. IndData1(1)) then
 i=1             ! ind1 less than lower bound
 iflag_lb = 1
elseif (ind1 .ge. IndData1(nRows)) then
 i=nRows         ! ind1 greater than upper bound
 iflag_ub = 1

else

 do ii=1,nRows-1
  if ((ind1 .ge. IndData1(ii)) .and. (ind1 .lt. IndData1(ii+1))) then
```

```
   i=ii      ! ind1 is between IndData1(ii) and IndData1(ii+1)
  end if
 end do

end if

!!write(99,*) i, " i"


! determine j-index
if (ind2 .le. IndData2(1)) then
 j=1           ! ind2 less than lower bound
 jflag_lb = 1

elseif (ind2 .ge. IndData1(nCols)) then
 j=nCols      ! ind2 greater than upper bound
 jflag_ub = 1

else

 do jj=1,nCols-1
  if ((ind2 .ge. IndData2(jj)) .and. (ind2 .lt. IndData2(jj+1))) then
   j=jj         ! ind2 is between IndData2(jj) and IndData2(jj+1)
  end if
 end do

end if

!!write(99,*) j, " j"

! logic trap to catch points below the lower bound of the table
if(iflag_lb .eq. 1) then     ! outside lower bound
 if( (jflag_lb .eq. 1) .or. (jflag_ub .eq. 1) ) then
 dep=DepData(i,j)          ! corner point
 else
 ! linearly interpolate along lower edge
  dep=DepData(i,j)  &
    + (ind2-IndData2(j))/(IndData2(j+1)-IndData2(j))  &
          *(DepData(i,j+1)-DepData(i,j))
 end if
end if

! logic trap to catch points above the upper bound of the table
if(iflag_ub .eq. 1) then    ! outside upper bound
 if( (jflag_lb .eq. 1) .or. (jflag_ub .eq. 1) ) then
  dep=DepData(i,j)          ! corner point
 else
 ! linearly interpolate along upper edge
  dep=DepData(i,j)  &
    + (ind2-IndData2(j))/(IndData2(j+1)-IndData2(j))  &
          *(DepData(i,j+1)-DepData(i,j))
 end if
end if

! logic trap to catch points beyond the left and right bound of the table
if( (jflag_lb .eq. 1) .or. (jflag_ub .eq. 1) ) then
```

```
! outside right or left bound
if( (iflag_lb .eq. 1) .or. (iflag_ub .eq. 1) ) then
 ! trap for corner points (already calculated)
else
 ! linearly interpolate along left or right edge
 dep=DepData(i,j)  &
   + (ind1-IndData1(i))/(IndData1(i+1)-IndData1(i))  &
     *(DepData(i+1,j)-DepData(i,j))
 end if
end if

! logic trap to catch points in the table
if( (iflag_lb .eq. 0) .and. (iflag_ub .eq. 0) .and.  &
   (jflag_lb .eq. 0) .and. (jflag_ub .eq. 0) ) then

! interpolate in j-th column between the i-th and (i+1)-th row
dep1i=DepData(i,j)  &
   + (ind1-IndData1(i))/(IndData1(i+1)-IndData1(i))  &
     *(DepData(i+1,j)-DepData(i,j))

! interpolate in (j+1)-th column between the i-th and (i+1)-th row
dep2i=DepData(i,j+1)  &
   + (ind1-IndData1(i))/(IndData1(i+1)-IndData1(i))  &
     *(DepData(i+1,j+1)-DepData(i,j+1))

! interpolate the results above results between
! the j-th and (j+1)-th columns
dep=dep1i          &
 +(ind2-IndData2(j))/(IndData2(j+1)-IndData2(j))    &
  *(dep2i-dep1i)

end if

end subroutine Interp2D
!*********************************************************************************
!*********************************************************************************
```

3.3 COMPUTER LISTING OF TEST DATA INPUT AND OUTPUT

3.3.1 Source Code For Testing The Interpolation Subroutines

```
program PWinterp

real(8) CLvector(10), CLtable1a(10)
real(8) Tvector(3), Qvector(7), PHtable3(7,3)
real(8) nInput1D, nInput2D
real(8) indVar1, indVar2
real(8) dep

integer(4) nRows1
integer(4) nRows2, nCols2
```

```
call ReadChemData

open(unit=90, file='input1D.dat')
open(unit=91, file='output1D.dat')
read(90,*) nInput1D
do i=1,nInput1D
 read(90,*) indVar1
 call Interp1D(indVar1, CLvector, CLtable1a, nRows1, dep)
 write(91,*) indVar1, dep
end do
close(90)
close(91)

open(unit=90, file='input2D.dat')
open(unit=91, file='output2D.dat')
read(90,*) nInput2D
do i=1,nInput2D
 read(90,*) indVar1, indVar2
 call Interp2D(indVar1, indVar2, Qvector, Tvector, PHtable3, nRows2, nCols2, dep)
 write(91,*) indVar1, indVar2, dep
end do
close(90)
close(91)

contains

!*******************************************************************************
subroutine ReadChemData

! CL data as a function of RH (1-D table)
open(unit=80, file='CLtable1.dat')
read(80,*) nRows1

do m=1,nRows1
 read(80,*) CLvector(m), CLtable1a(m)
end do
close(80)

! pH data as a function of 1-Qe/Qs and temperature(C) (2-D table)
open (unit=80, file='PHtable3.dat')
read(80,*) nRows2, nCols2
read(80,*) (Tvector(n), n=1,nCols2)
do m=1,nRows2 .
 read(80,*) Qvector(m), (PHtable3(m,n), n=1,nCols2)
end do
close(80)

end subroutine ReadChemData
!*******************************************************************************

end program PWinterp

!*******************************************************************************
!*******************************************************************************
! 1-D interpolation routine
subroutine Interp1D(ind, IndData, DepData, nRows, dep)
```

```
! number of rows in 1-D table
integer(4) nRows

! independent and dependent variable vectors
real(8) IndData(nRows), DepData(nRows)

! independent and dependent variables
real(8) ind, dep

! check for independent variable outside of data set range
if (ind .le. IndData(1)) then
 dep=DepData(1)              ! value is below lower bound, set equal to floor
elseif (ind .ge. IndData(nRows)) then
 dep=DepData(nRows)          ! value is above upper bound, set equal to ceiling
else

 do i=1,nRows-1            ! value is within the range of the data set
  if ((ind .ge. IndData(i)) .and. (ind .lt. IndData(i+1))) then

   ! linear interpolation
   ! y = y(i) + [x-x(i)]/[x(i+1)-x(i)] * [y(i+1)-y(i)]
   dep=DepData(i)  &
       + (ind-IndData(i))/(IndData(i+1)-IndData(i))  &
           *(DepData(i+1)-DepData(i))
  end if
 end do
end if

end subroutine Interp1D
!*************************************************************************************
!*************************************************************************************
subroutine Interp2D(ind1, ind2, IndData1, IndData2, DepData, nRows, nCols, dep)

! number of rows and columns in 2-D table
integer(4) nRows, nCols

! independent variable vectors and dependent variable array
real(8) IndData1(nRows), IndData2(nCols), DepData(nRows,nCols)

! independent variables, intermediate dependent variables, and dependent variable
real(8) ind1, ind2, dep1, dep, dep2

! flags for independent variable values beyond upper and lower bounds
integer(4) iflag_lb, iflag_ub, jflag_lb, jflag_ub

! initialize flags
iflag_lb = 0
iflag_ub = 0
jflag_lb = 0
jflag_ub = 0

! determine i-index
if (ind1 .le. IndData1(1)) then
 i=1            ! ind1 less than lower bound
 iflag_lb = 1
```

```
elseif (ind1 .ge. IndData1(nRows)) then
 i=nRows          ! ind1 greater than upper bound
 iflag_ub = 1

else

 do ii=1,nRows-1
  if ((ind1 .ge. IndData1(ii)) .and. (ind1 .lt. IndData1(ii+1))) then
   i=ii          ! ind1 is between IndData1(ii) and IndData1(ii+1)
  end if
 end do

end if

! determine j-index
if (ind2 .le. IndData2(1)) then
 j=1          ! ind2 less than lower bound
 jflag_lb = 1

elseif (ind2 .ge. IndData2(nCols)) then
 j=nCols          ! ind2 greater than upper bound
 jflag_ub = 1

else

 do jj=1,nCols-1
  if ((ind2 .ge. IndData2(jj)) .and. (ind2 .lt. IndData2(jj+1))) then
   j=jj               ! ind2 is between IndData2(jj) and IndData2(jj+1)
  end if
 end do

end if

! logic trap to catch points below the lower bound of the table
if(iflag_lb .eq. 1) then     ! outside lower bound
 if( (jflag_lb .eq. 1) .or. (jflag_ub .eq. 1) ) then
  dep=DepData(i,j)          ! corner point

 else
 ! linearly interpolate along lower-bound edge
  dep=DepData(i,j)  &
     + (ind2-IndData2(j))/(IndData2(j+1)-IndData2(j))  &
        *(DepData(i,j+1)-DepData(i,j))
 end if
end if

! logic trap to catch points above the upper bound of the table
if(iflag_ub .eq. 1) then    ! outside upper bound
 if( (jflag_lb .eq. 1) .or. (jflag_ub .eq. 1) ) then
  dep=DepData(i,j)          ! corner point
 else
 ! linearly interpolate along upper edge
  dep=DepData(i,j)  &
    + (ind2-IndData2(j))/(IndData2(j+1)-IndData2(j))  &
        *(DepData(i,j+1)-DepData(i,j))
 end if
```

```
end if

! logic trap to catch points beyond the left and right bound of the table
if( (jflag_lb .eq. 1) .or. (jflag_ub .eq. 1) ) then
 ! outside right or left bound
 if( (iflag_lb .eq. 1) .or. (iflag_ub .eq. 1) ) then
  ! trap for corner points (already calculated)
 else
  ! linearly interpolate along left or right edge
  dep=DepData(i,j)  &
    + (ind1-IndData1(i))/(IndData1(i+1)-IndData1(i))  &
      *(DepData(i+1,j)-DepData(i,j))
 end if
end if

! logic trap to catch points in the table
if( (iflag_lb .eq. 0) .and. (iflag_ub .eq. 0) .and.  &
   (jflag_lb .eq. 0) .and. (jflag_ub .eq. 0) ) then

! interpolate in j-th column between the i-th and (i+1)-th row
dep1i=DepData(i,j)  &
   + (ind1-IndData1(i))/(IndData1(i+1)-IndData1(i))  &
     *(DepData(i+1,j)-DepData(i,j))

! interpolate in (j+1)-th column between the i-th and (i+1)-th row
dep2i=DepData(i,j+1)  &
   + (ind1-IndData1(i))/(IndData1(i+1)-IndData1(i))  &
     *(DepData(i+1,j+1)-DepData(i,j+1))

! interpolate the results above results between
! the j-th and (j+1)-th columns
dep=dep1i          &
 +(ind2-IndData2(j))/(IndData2(j+1)-IndData2(j))     &
  *(dep2i-dep1i)

end if

end subroutine Interp2D
!**************************************************************************************
!**************************************************************************************
```

3.3.2 Input File For 1D Interpolation Subroutine Test Case

```
4
50.0
53.1
60.0
90.0

10
50.3    -2.431  -2.428  -2.415
51.0    -1.246  -1.244  -1.231
53.1    -0.389  -0.391  -0.380
55.2    -0.164  -0.169  -0.159
```

```
60.5   0.225    0.211    0.216
65.7   0.380    0.358    0.359
71.0   0.420    0.396    0.396
76.2   0.428    0.403    0.403
81.5   0.418    0.394    0.394
85.0   0.407    0.382    0.382
  2      3        4
; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; 1st independent variable (columns) = Abstracted Period
; 2nd independent variable (rows) = relative humidity (RH)
; dependent parameter = log Cl (i.e., log of Cl concentration (molal))
```

3.3.3 Output File For 1D Interpolation Subroutine Test Case

```
50.0000000000000   -2.43100000000000
53.1000000000000   -0.389000000000000
60.0000000000000    0.188301886792453
90.0000000000000    0.407000000000000
```

3.3.4 EXCEL Spreadsheet Replicating 1D Interpolation Subroutine

1D Interpolation Subroutine				
Lookup Table			Interpolated Values	
Independent Variable	Dependent Variable		Independent Variable	Interpolated Value of Dependent Variable
50.3	-2.431		50	-2.43100
51	-1.246		53.1	-0.38900
53.1	-0.389		60	0.18830
55.2	-0.164		90	0.40700
60.5	0.225			
65.7	0.38			
71	0.42			
76.2	0.428			
81.5	0.418			
85	0.407			

3.3.5 Input File For 2D Interpolation Subroutine Test Case

```
9
0.0 20.0
0.0 80.0
1.1 20.0
1.1 80.0
```

```
0.2 20.0
0.2 80.0
0.0 65.0
1.1 65.0
45.0
```

3.3.6 2D Lookup Table

```
7   3
          25        50        75
0.0011999  7.02        7.02        7.02
0.0012  6.78        6.86        7.02
0.01        6.986       6.95        7.02
0.1     7.11        7.03        6.97
0.5     7.23        7.18        7.14
0.9     7.09        7.22        7.18
1.0     7.05        7.22        7.19
; Salts Lookup Tables
; In-Drift Precipitates/Salts AMR (ANL-EBS-MD-000045)
; Seepage Name: Abstracted THC Seepage Water
; condition: Period 4
; 1st independent variable (columns) = temperature ('C)
; dependent parameter = pH
```

3.3.7 Output File For 2D Interpolation Subroutine Test Case

```
000000000000000E+000   20.0000000000000    7.02000000000000
0.000000000000000E+000  80.0000000000000    7.02000000000000
1.10000000000000       20.0000000000000    7.05000000000000
1.10000000000000       80.0000000000000    7.19000000000000
0.200000000000000      20.0000000000000    7.14000000000000
0.200000000000000      80.0000000000000    7.01250000000000
0.000000000000000E+000  65.0000000000000    7.02000000000000
1.10000000000000       65.0000000000000    7.20200000000000
0.250000000000000      45.0000000000000    7.09999990463257
```

3.3.8 EXCEL Spreadsheet Replicating 2D Interpolation Subroutine

2D Interpolation Subroutine						
2D Lookup Table				Interpolated Value of Dependent Variable		
1st Independent Variable	2nd Independent Variable			1st Independent Variable	2nd Independent Variable	Interpolated/ Truncated Value
	25	50	75	0	20	7.02000
0.0011999	7.02	7.02	7.02	0	80	7.02000

0.0012	6.78	6.86	7.02	1.1	20	7.05000
0.01	6.986	6.95	7.02	1.1	80	7.19000
0.1	7.11	7.03	6.97	0.2	20	7.14000
0.5	7.23	7.18	7.14	0.2	80	7.01250
0.9	7.09	7.22	7.18	0	65	7.02000
1	7.05	7.22	7.19	1.1	65	7.20200
				0.25	45	7.10000
				Intermediate Values For Last Data Set		
				7.15500	7.08625	

3.3.9 Input File Used To Test PREWAP Program

line 1 test file

line 2
line 3
Time (yr), Waste Pack Temp.(C), Drip shield temp. (C), Drift wall temp.(C), Invert temp. (C), Waste pack RH, Drip shield RH, Drift wall RH, Backfill RH, Invert RH, Liquid Satr. @ Drip Shield, Liquid Satr.@Invert, Air mass Frac, Water Vapor flux at Dwall (kg/yr/m of drift), Air flux at Dwall(kg/yr/m of drift), A Drip Shield Evapo. rate (m3/yr), Backfill Evapo. Rate (m3/yr), Invert Evapo. Rate (m3/yr), Percolation Flux at 5 m (mm/yr), Vol ume flow at top dripshield (m3/yr), volume flow at invert (m3/yr), Top of the dripshield Temp (C)
The number of Rows = 21
The fraction of this history = 0.000576
line 7
line 8
line 9
line 10
line 11 wpT dsT dwT iT wpRH dsRH dwRH
dsEvapRate pf-5m

```
   0.00  0.222933E+02 -0.999000E+02  0.222797E+02  0.223071E+02  0.999137E+00 -
0.999000E+02  0.999952E+00 -0.999000E+02  0.999180E+00 -0.999000E+02  0.000000E+00 -
0.999000E+02  0.000000E+00  0.000000E+00 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.153137E+02 -0.999000E+02  0.000000E+00 -0.999000E+02
   1.00  0.846557E+02 -0.999000E+02  0.679710E+02  0.750104E+02 -0.999000E+02
0.500429E+00  0.999958E+00 -0.999000E+02  0.876529E+00 -0.999000E+02  0.196320E-01 -
0.999000E+02  0.243105E+02  0.106586E+02 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.143936E+02 -0.999000E+02 -0.116894E-01 -0.999000E+02
  50.00  0.665731E+02 -0.999000E+02  0.612045E+02  0.633398E+02  0.100000E-01 -
0.999000E+02  0.999504E+00 -0.999000E+02  0.967314E+00 -0.999000E+02  0.316090E-01 -
0.999000E+02  0.624383E+01  0.291981E+01 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.142088E+02 -0.999000E+02 -0.279873E-02 -0.999000E+02
  50.20  0.236173E+03  0.230511E+03  0.109784E+03  0.188458E+03  0.100000E-01  0.840750E-
01  0.655213E+00  0.969566E+00  0.829800E-01  0.000000E+00  0.000000E+00  0.208500E-02
0.293924E+04  0.834146E+00 -0.123300E-05  0.235282E-02 -0.821340E-04  0.141540E+02
0.000000E+00  0.000000E+00  0.231596E+03
  51.00  0.270679E+03  0.266027E+03  0.130378E+03  0.229314E+03  0.100000E-01  0.369300E-
01  0.499133E+00  0.646741E+00  0.347820E-01  0.000000E+00  0.000000E+00  0.792600E-02
0.386056E+02 -0.176730E-01  0.300000E-08 -0.700000E-08  0.170000E-06  0.144618E+02
0.000000E+00  0.000000E+00  0.266970E+03
```

53.00 0.271006E+03 0.266812E+03 0.143359E+03 0.239704E+03 0.600000E+00 0.298220E-01 0.365954E+00 0.489141E+00 0.281430E-01 0.000000E+00 0.000000E+00 0.145170E-01 0.102893E+02 0.420108E+00 -0.310800E-05 -0.550000E-07 0.522000E-06 0.150733E+02 0.000000E+00 0.000000E+00 0.267646E+03
55.00 0.261421E+03 0.257416E+03 0.144179E+03 0.240140E+03 0.600000E+00 0.308210E-01 0.359387E+00 0.480840E+00 0.278820E-01 0.000000E+00 0.000000E+00 0.148380E-01 0.103388E+02 0.472702E+00 -0.355400E-05 -0.580000E-07 0.488000E-06 0.160079E+02 0.000000E+00 0.000000E+00 0.258208E+03
60.00 0.225009E+03 0.221233E+03 0.132806E+03 0.194677E+03 0.600000E+00 0.352420E-01 0.365349E+00 0.491466E+00 0.607210E-01 0.000000E+00 0.000000E+00 0.105486E+00 0.291557E+00 -0.355520E+00 -0.700000E-08 -0.200000E-08 0.390000E-07 0.179075E+02 0.000000E+00 0.000000E+00 0.221968E+03
65.00 0.197084E+03 0.193435E+03 0.120758E+03 0.173413E+03 0.600000E+00 0.535270E-01 0.501935E+00 0.674298E+00 0.954170E-01 0.000000E+00 0.000000E+00 0.130878E+00 0.717410E+00 -0.453557E+00 -0.100000E-08 0.100000E-08 -0.500000E-08 0.216911E+02 0.000000E+00 0.000000E+00 0.194135E+03
70.00 0.144995E+03 0.141441E+03 0.975721E+02 0.128478E+03 0.100000E-01 0.866760E-01 0.748124E+00 0.990652E+00 0.290811E+00 0.000000E+00 0.000000E+00 0.189501E+00 0.265674E+03 0.349618E+02 -0.102500E-05 -0.286851E-02 -0.755000E-06 0.268478E+02 0.000000E+00 0.000000E+00 0.142113E+03
80.00 0.949581E+02 0.915515E+02 0.814937E+02 0.938274E+02 0.600000E+00 0.130910E+00 0.992015E+00 0.997802E+00 0.926671E+00 0.126481E+00 0.609780E-01 0.223147E+00 0.220814E+03 0.193291E+02 0.128079E+00 -0.525328E-02 0.281983E+00 0.275514E+02 0.000000E+00 0.000000E+00 0.921773E+02
100.00 0.900955E+02 0.869274E+02 0.771852E+02 0.899821E+02 0.100000E-01 0.158592E+00 0.994236E+00 0.999768E+00 0.981316E+00 0.161142E+00 0.110698E+00 0.325127E+00 0.128401E+03 0.167901E+02 0.993992E-01 -0.412338E-02 0.248594E+00 0.189149E+02 0.000000E+00 0.000000E+00 0.874805E+02
110.00 0.867760E+02 0.836941E+02 0.745860E+02 0.874209E+02 0.600000E+00 0.170195E+00 0.995199E+00 0.999764E+00 0.984132E+00 0.164643E+00 0.118413E+00 0.395588E+00 0.925944E+02 0.149763E+02 0.861841E-01 -0.368624E-02 0.210613E+00 0.172476E+02 0.000000E+00 0.000000E+00 0.842257E+02
120.00 0.825661E+02 0.795754E+02 0.712272E+02 0.838059E+02 0.100000E-01 0.190156E+00 0.997187E+00 0.999758E+00 0.987154E+00 0.167614E+00 0.122490E+00 0.484554E+00 0.622246E+02 0.125183E+02 0.700028E-01 -0.307191E-02 0.169845E+00 0.162730E+02 0.000000E+00 0.000000E+00 0.800842E+02
130.00 0.810327E+02 0.781357E+02 0.700483E+02 0.824621E+02 0.100000E-01 0.219832E+00 0.998197E+00 0.999755E+00 0.988637E+00 0.168528E+00 0.123351E+00 0.514527E+00 0.543765E+02 0.116858E+02 0.647288E-01 -0.262423E-02 0.156327E+00 0.155837E+02 0.000000E+00 0.000000E+00 0.786208E+02
140.00 0.776294E+02 0.748289E+02 0.675343E+02 0.794910E+02 0.600000E+00 0.247555E+00 0.999252E+00 0.999748E+00 0.991091E+00 0.170812E+00 0.125106E+00 0.576015E+00 0.410952E+02 0.998433E+01 0.538530E-01 -0.230470E-02 0.129704E+00 0.150984E+02 0.000000E+00 0.000000E+00 0.752897E+02
150.00 0.737673E+02 0.710678E+02 0.647680E+02 0.761593E+02 0.600000E+00 0.279064E+00 0.999473E+00 0.999745E+00 0.993142E+00 0.183805E+00 0.136964E+00 0.637418E+00 0.301292E+02 0.797134E+01 0.432977E-01 -0.192148E-02 0.104080E+00 0.147780E+02 0.000000E+00 0.000000E+00 0.715033E+02
190.00 0.712332E+02 0.687596E+02 0.629677E+02 0.739267E+02 0.100000E-01 0.343920E+00 0.999606E+00 0.999741E+00 0.993787E+00 0.186603E+00 0.139378E+00 0.674327E+00 0.247632E+02 0.682169E+01 0.372664E-01 -0.176730E-02 0.896966E-01 0.143423E+02 0.000000E+00 0.000000E+00 0.691465E+02
270.00 0.690627E+02 0.668984E+02 0.613302E+02 0.718319E+02 0.100000E-01 0.442273E+00 0.999772E+00 0.999737E+00 0.994472E+00 0.187777E+00 0.140144E+00 0.705799E+00 0.207220E+02 0.593611E+01 0.322745E-01 -0.153458E-02 0.776633E-01 0.139374E+02 0.118268E+00 -0.358887E-01 0.672245E+02

615.00 0.671101E+02 0.656206E+02 0.596731E+02 0.696723E+02 0.100000E-01
0.673121E+00 0.999966E+00 0.999733E+00 0.996401E+00 0.188846E+00 0.140840E+00
0.735027E+00 0.172995E+02 0.511785E+01 0.276815E-01 -0.114842E-02 0.662257E-01
0.145990E+02 0.398767E-01 -0.350144E-01 0.658302E+02
1000000.00 0.187600E+02 0.187354E+02 0.186076E+02 0.187464E+02 0.998407E+00
0.999883E+00 0.999964E+00 0.999686E+00 0.999958E+00 0.224044E+00 0.166789E+00
0.984671E+00 0.132790E-01 -0.110600E-02 0.268370E-04 -0.663300E-05 0.548690E-04
0.610027E+02 0.112866E-02 0.184060E+00 0.187314E+02
The number of Rows = 29
The fraction of this history = 0.000960
line 3

line 4
line 5
line 6
line 7 wpT dsT dwT iT wpRH dsRH dwRH
dsEvapRate pf-5m

0.00 0.223001E+02 -0.999000E+02 0.222865E+02 0.223136E+02 0.999138E+00 -
0.999000E+02 0.999952E+00 -0.999000E+02 0.999180E+00 -0.999000E+02 0.000000E+00 -
0.999000E+02 0.000000E+00 0.000000E+00 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.152617E+02 -0.999000E+02 0.000000E+00 -0.999000E+02
1.00 0.806202E+02 -0.999000E+02 0.633204E+02 0.707888E+02 0.477524E+00 -
0.999000E+02 0.999955E+00 -0.999000E+02 0.886023E+00 -0.999000E+02 0.190470E-01 -
0.999000E+02 0.224813E+02 0.119247E+02 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.143430E+02 -0.999000E+02 -0.116604E-01 -0.999000E+02
2.00 0.874782E+02 -0.999000E+02 0.717236E+02 0.784255E+02 0.527047E+00 -
0.999000E+02 0.999416E+00 -0.999000E+02 0.869311E+00 -0.999000E+02 0.182770E-01 -
0.999000E+02 0.259342E+02 0.102259E+02 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.143530E+02 -0.999000E+02 -0.725051E-02 -0.999000E+02
5.00 0.944264E+02 -0.999000E+02 0.808013E+02 0.866099E+02 0.589066E+00 -
0.999000E+02 0.996760E+00 -0.999000E+02 0.856647E+00 -0.999000E+02 0.963900E-02 -
0.999000E+02 0.304570E+02 0.102450E+02 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.144701E+02 -0.999000E+02 -0.117121E-02 -0.999000E+02
20.00 0.890934E+02 -0.999000E+02 0.797213E+02 0.834106E+02 0.688934E+00 -
0.999000E+02 0.995898E+00 -0.999000E+02 0.900721E+00 -0.999000E+02 0.282600E-02 -
0.999000E+02 0.171358E+02 0.707731E+01 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.145367E+02 -0.999000E+02 0.000000E+00 -0.999000E+02
25.00 0.852817E+02 -0.999000E+02 0.767855E+02 0.801724E+02 0.707787E+00 -
0.999000E+02 0.996314E+00 -0.999000E+02 0.912235E+00 -0.999000E+02 0.982700E-02 -
0.999000E+02 0.144370E+02 0.576231E+01 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.144728E+02 -0.999000E+02 0.000000E+00 -0.999000E+02
30.00 0.817664E+02 -0.999000E+02 0.740034E+02 0.771318E+02 0.724692E+00 -
0.999000E+02 0.996711E+00 -0.999000E+02 0.925986E+00 -0.999000E+02 0.132880E-01 -
0.999000E+02 0.127767E+02 0.525119E+01 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.144009E+02 -0.999000E+02 0.000000E+00 -0.999000E+02
40.00 0.749153E+02 -0.999000E+02 0.684373E+02 0.710976E+02 0.756514E+00 -
0.999000E+02 0.997577E+00 -0.999000E+02 0.946729E+00 -0.999000E+02 0.171170E-01 -
0.999000E+02 0.971942E+01 0.456280E+01 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.142671E+02 -0.999000E+02 0.000000E+00 -0.999000E+02
50.00 0.678115E+02 -0.999000E+02 0.625164E+02 0.647416E+02 0.788405E+00 -
0.999000E+02 0.999037E+00 -0.999000E+02 0.963607E+00 -0.999000E+02 0.284150E-01 -
0.999000E+02 0.707103E+01 0.310949E+01 -0.999000E+02 -0.999000E+02 -0.999000E+02
0.141580E+02 -0.999000E+02 -0.278996E-02 -0.999000E+02
50.20 0.234737E+03 0.229075E+03 0.109300E+03 0.187167E+03 0.762630E-01 0.100000E-
01 0.658942E+00 0.980873E+00 0.847710E-01 0.000000E+00 0.000000E+00 0.203100E-02

0.303839E+04 0.855563E+00 -0.129200E-05 0.307937E-02 -0.861920E-04 0.141030E+02
0.000000E+00 0.000000E+00 0.230161E+03
51.00 0.268555E+03 0.263902E+03 0.127610E+03 0.226167E+03 0.362760E-01 0.100000E-
01 0.527864E+00 0.680440E+00 0.370450E-01 0.000000E+00 0.000000E+00 0.643000E-02
0.128020E+03 -0.416400E-02 0.200000E-08 0.400000E-08 0.193000E-06 0.144098E+02
0.000000E+00 0.000000E+00 0.264845E+03
53.00 0.274117E+03 0.269923E+03 0.142879E+03 0.239454E+03 0.282400E-01 0.100000E-
01 0.369748E+00 0.493922E+00 0.282940E-01 0.000000E+00 0.000000E+00 0.143340E-01
0.102595E+02 0.386741E+00 -0.283100E-05 -0.520000E-07 0.542000E-06 0.150223E+02
0.000000E+00 0.000000E+00 0.270758E+03
55.00 0.265761E+03 0.261756E+03 0.144988E+03 0.240575E+03 0.283890E-01
0.600000E+00 0.352861E+00 0.472570E+00 0.276230E-01 0.000000E+00 0.000000E+00
0.151570E-01 0.102755E+02 0.521326E+00 -0.397400E-05 -0.620000E-07 0.455000E-06
0.159587E+02 0.000000E+00 0.000000E+00 0.262547E+03
60.00 0.231692E+03 0.227916E+03 0.136306E+03 0.201924E+03 0.308040E-01
0.600000E+00 0.342139E+00 0.460237E+00 0.542150E-01 0.000000E+00 0.000000E+00
0.926510E-01 0.163887E+00 -0.218317E+00 -0.400000E-08 -0.200000E-08 -0.110000E-07
0.178319E+02 0.000000E+00 0.000000E+00 0.228651E+03
65.00 0.198981E+03 0.195333E+03 0.122966E+03 0.177266E+03 0.467120E-01
0.600000E+00 0.473065E+00 0.635232E+00 0.877210E-01 0.000000E+00 0.000000E+00
0.124235E+00 0.474730E+00 -0.461679E+00 -0.100000E-08 0.400000E-08 0.890000E-07
0.215856E+02 0.000000E+00 0.000000E+00 0.196033E+03
70.00 0.139131E+03 0.135577E+03 0.976314E+02 0.128600E+03 0.781570E-01
0.600000E+00 0.746703E+00 0.989340E+00 0.289581E+00 0.000000E+00 0.000000E+00
0.190654E+00 0.265218E+03 0.348544E+02 -0.103400E-05 -0.285501E-02 -0.763000E-06
0.268695E+02 0.000000E+00 0.000000E+00 0.136249E+03
80.00 0.100158E+03 0.967514E+02 0.857046E+02 0.970909E+02 0.115084E+00 0.100000E-
01 0.985973E+00 0.995477E+00 0.884019E+00 0.650060E-01 0.264120E-01 0.146113E+00
0.397487E+03 0.303699E+02 0.153011E+00 -0.498900E-02 0.204364E+00 0.275664E+02
0.000000E+00 0.000000E+00 0.973771E+02
100.00 0.934533E+02 0.902852E+02 0.818526E+02 0.942050E+02 0.140307E+00
0.600000E+00 0.990235E+00 0.997121E+00 0.919350E+00 0.124630E+00 0.604280E-01
0.217854E+00 0.229181E+03 0.193812E+02 0.130214E+00 -0.515831E-02 0.235767E+00
0.188267E+02 0.000000E+00 0.000000E+00 0.908383E+02
110.00 0.887102E+02 0.856283E+02 0.795500E+02 0.922187E+02 0.150632E+00
0.100000E-01 0.991787E+00 0.999695E+00 0.959159E+00 0.141891E+00 0.773060E-01
0.267986E+00 0.172739E+03 0.181566E+02 0.112748E+00 -0.293494E-02 0.271712E+00
0.171724E+02 0.000000E+00 0.000000E+00 0.861599E+02
120.00 0.874543E+02 0.844636E+02 0.784762E+02 0.912332E+02 0.168459E+00
0.600000E+00 0.992456E+00 0.999765E+00 0.975882E+00 0.151229E+00 0.917010E-01
0.293625E+00 0.151039E+03 0.175141E+02 0.105458E+00 -0.453336E-02 0.266612E+00
0.162056E+02 0.000000E+00 0.000000E+00 0.849724E+02
130.00 0.840941E+02 0.811971E+02 0.756464E+02 0.885412E+02 0.194897E+00
0.100000E-01 0.993634E+00 0.999763E+00 0.980092E+00 0.162964E+00 0.115489E+00
0.368973E+00 0.104537E+03 0.155809E+02 0.912377E-01 -0.373414E-02 0.225596E+00
0.155216E+02 0.000000E+00 0.000000E+00 0.816822E+02
140.00 0.807761E+02 0.779757E+02 0.729943E+02 0.857868E+02 0.220070E+00
0.100000E-01 0.995169E+00 0.999759E+00 0.982636E+00 0.165588E+00 0.120302E+00
0.439992E+00 0.758019E+02 0.136974E+02 0.778465E-01 -0.346009E-02 0.190273E+00
0.150399E+02 0.000000E+00 0.000000E+00 0.784364E+02
150.00 0.777314E+02 0.750318E+02 0.706811E+02 0.832177E+02 0.248718E+00
0.600000E+00 0.997062E+00 0.999755E+00 0.985363E+00 0.167470E+00 0.122409E+00
0.499941E+00 0.580119E+02 0.120507E+02 0.671403E-01 -0.294301E-02 0.162715E+00
0.147219E+02 0.000000E+00 0.000000E+00 0.754674E+02
180.00 0.752735E+02 0.727402E+02 0.687718E+02 0.809819E+02 0.293681E+00
0.600000E+00 0.999266E+00 0.999751E+00 0.988900E+00 0.168870E+00 0.123639E+00

0.546981E+00 0.468024E+02 0.107262E+02 0.588192E-01 -0.261450E-02 0.142453E+00
0.143975E+02 0.000000E+00 0.000000E+00 0.731398E+02
225.00 0.729992E+02 0.706785E+02 0.668359E+02 0.786637E+02 0.355414E+00
0.100000E-01 0.998974E+00 0.999745E+00 0.989652E+00 0.171033E+00 0.125191E+00
0.593248E+00 0.378513E+02 0.950032E+01 0.507596E-01 -0.230120E-02 0.122659E+00
0.140623E+02 0.000000E+00 0.000000E+00 0.710345E+02
315.00 0.707678E+02 0.687327E+02 0.649136E+02 0.763492E+02 0.442330E+00
0.100000E-01 0.999309E+00 0.999745E+00 0.991455E+00 0.182473E+00 0.135905E+00
0.635019E+00 0.304144E+02 0.802757E+01 0.435520E-01 -0.194807E-02 0.104876E+00
0.138135E+02 0.968528E-01 -0.127453E+00 0.690353E+02
475.00 0.686313E+02 0.669335E+02 0.628589E+02 0.737972E+02 0.548132E+00
0.100000E-01 0.999531E+00 0.999740E+00 0.992464E+00 0.185740E+00 0.138739E+00
0.677026E+00 0.243129E+02 0.672385E+01 0.366556E-01 -0.170702E-02 0.881237E-01
0.137836E+02 0.574295E-01 -0.773144E-01 0.671779E+02
615.00 0.671560E+02 0.656666E+02 0.614066E+02 0.719363E+02 0.630850E+00
0.600000E+00 0.999704E+00 0.999736E+00 0.993185E+00 0.186764E+00 0.139402E+00
0.704846E+00 0.207516E+02 0.593717E+01 0.323022E-01 -0.150387E-02 0.778167E-01
0.145462E+02 0.396563E-01 -0.347207E-01 0.658761E+02
1000000.00 0.188336E+02 0.188090E+02 0.186851E+02 0.188401E+02 0.998413E+00
0.999883E+00 0.999964E+00 0.999686E+00 0.999958E+00 0.223843E+00 0.166600E+00
0.984575E+00 0.151070E-01 -0.179900E-02 0.296850E-04 -0.676300E-05 0.632210E-04
0.607919E+02 0.112650E-02 0.183561E+00 0.188050E+02
The number of Rows = 32
The fraction of this history = 0.001153
Coordinate Location:
The easting coordinate = 170256.20 m
The northing coordinate = 234314.20 m
Infiltration rate:
qinf = 60.37322 mm/yr
0 2.23E+01 -9.99E+01 2.23E+01 2.23E+01 9.99E-01 -9.99E+01 1.00E+00 -9.99E+01
9.99E-01 -9.99E+01 0.00E+00 -9.99E+01 0.00E+00 0.00E+00 -9.99E+01 -9.99E+01 -
9.99E+01 1.52E+01 -9.99E+01 0.00E+00 -9.99E+01

1 7.88E+01 -9.99E+01 6.12E+01 6.88E+01 4.67E-01 -9.99E+01 1.00E+00 -9.99E+01
8.90E-01 -9.99E+01 1.86E-02 -9.99E+01 2.15E+01 1.24E+01 -9.99E+01 -9.99E+01 -
9.99E+01 1.42E+01 -9.99E+01 -1.16E-02 -9.99E+01

40 7.56E+01 -9.99E+01 6.91E+01 7.19E+01 7.56E-01 -9.99E+01 9.97E-01 -9.99E+01
9.43E-01 -9.99E+01 1.66E-02 -9.99E+01 1.00E+01 4.62E+00 -9.99E+01 -9.99E+01 -
9.99E+01 1.42E+01 -9.99E+01 0.00E+00 -9.99E+01

50.2 2.26E+02 2.20E+02 1.06E+02 1.82E+02 4.90E-01 5.50E-01 6.78E-01 1.00E+00
9.38E-02 0.00E+00 0.00E+00 4.08E-02 2.91E+03 4.62E+00 -1.25E-06 6.81E-03 -
8.42E-05 1.40E+01 0.00E+00 0.00E+00 2.21E+02

51 2.64E+02 2.60E+02 1.23E+02 2.20E+02 5.50E-01 6.50E-01 5.56E-01 7.18E-01
4.24E-02 0.00E+00 0.00E+00 4.70E-03 5.85E+02 1.78E-01 -5.00E-09 2.50E-08
1.26E-06 1.43E+01 0.00E+00 0.00E+00 2.61E+02

52 2.74E+02 2.69E+02 1.34E+02 2.33E+02 6.50E-01 8.50E-01 4.54E-01 5.95E-01
3.23E-02 0.00E+00 0.00E+00 1.02E-02 2.39E+01 1.90E-02 0.00E+00 -1.80E-08
4.61E-07 1.46E+01 0.00E+00 0.00E+00 2.70E+02

55 2.72E+02 2.68E+02 1.45E+02 2.40E+02 8.50E-01 4.90E-01 3.55E-01 4.76E-01
2.77E-02 0.00E+00 0.00E+00 1.50E-02 1.01E+01 4.94E-01 -3.75E-06 -6.00E-08

4.68E-07 1.59E+01 0.00E+00 0.00E+00 2.69E+02

60 2.55E+02 2.51E+02 1.45E+02 2.19E+02 9.00E-01 9.50E-01 2.87E-01 3.87E-01
3.88E-02 0.00E+00 0.00E+00 6.17E-02 -1.31E-01 9.90E-02 3.00E-09 -3.00E-09 -
1.03E-07 1.96E+01 0.00E+00 0.00E+00 2.52E+02

65 2.26E+02 2.22E+02 1.35E+02 2.00E+02 9.50E-01 9.00E-01 3.48E-01 4.68E-01
5.60E-02 0.00E+00 0.00E+00 9.70E-02 1.96E-01 -2.53E-01 -4.00E-09 -2.00E-09 -
8.00E-09 2.14E+01 0.00E+00 0.00E+00 2.23E+02

1180 6.54E+01 6.44E+01 6.01E+01 7.02E+01 4.90E-01 5.50E-01 1.00E+00 1.00E+00
9.94E-01 1.86E-01 1.39E-01 7.29E-01 1.77E+01 5.21E+00 2.83E-02 -1.14E-03
6.87E-02 3.91E+01 1.35E-02 9.16E-02 6.46E+01

1420 6.34E+01 6.25E+01 5.80E+01 6.75E+01 5.50E-01 6.50E-01 1.00E+00 1.00E+00
9.98E-01 1.87E-01 1.41E-01 7.63E-01 1.42E+01 4.33E+00 2.31E-02 -9.44E-04
5.61E-02 3.93E+01 9.53E-03 1.01E-01 6.26E+01

1680 6.13E+01 6.05E+01 5.60E+01 6.48E+01 6.50E-01 8.50E-01 1.00E+00 1.00E+00
9.99E-01 1.89E-01 1.43E-01 7.92E-01 1.14E+01 3.59E+00 1.90E-02 -7.95E-04
4.71E-02 3.94E+01 7.26E-03 1.06E-01 6.06E+01

1900 5.94E+01 5.86E+01 5.41E+01 6.22E+01 8.50E-01 4.90E-01 1.00E+00 1.00E+00
1.00E+00 1.92E-01 1.44E-01 8.17E-01 9.15E+00 2.97E+00 1.55E-02 -7.74E-04
3.84E-02 3.96E+01 5.85E-03 1.10E-01 5.87E+01

1950 5.91E+01 5.84E+01 5.38E+01 6.19E+01 9.00E-01 9.50E-01 1.00E+00 1.00E+00
1.00E+00 1.92E-01 1.44E-01 8.20E-01 8.90E+00 2.89E+00 1.51E-02 -7.60E-04
3.75E-02 4.14E+01 5.80E-03 1.16E-01 5.85E+01

1975 5.90E+01 5.83E+01 5.37E+01 6.17E+01 9.50E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 1.92E-01 1.44E-01 8.21E-01 8.79E+00 2.86E+00 1.49E-02 -7.54E-04
3.71E-02 4.32E+01 5.81E-03 1.21E-01 5.84E+01

2060 5.89E+01 5.82E+01 5.36E+01 6.16E+01 4.90E-01 5.50E-01 1.00E+00 1.00E+00
1.00E+00 1.92E-01 1.44E-01 8.23E-01 8.69E+00 2.83E+00 1.48E-02 -7.48E-04
3.67E-02 4.50E+01 5.83E-03 1.26E-01 5.83E+01

2080 5.88E+01 5.81E+01 5.35E+01 6.14E+01 5.50E-01 6.50E-01 1.00E+00 1.00E+00
1.00E+00 1.93E-01 1.44E-01 8.24E-01 8.58E+00 2.80E+00 1.46E-02 -7.43E-04
3.63E-02 4.67E+01 5.84E-03 1.32E-01 5.82E+01

2100 5.87E+01 5.80E+01 5.34E+01 6.13E+01 6.50E-01 8.50E-01 1.00E+00 1.00E+00
1.00E+00 1.93E-01 1.44E-01 8.25E-01 8.48E+00 2.77E+00 1.44E-02 -7.37E-04
3.59E-02 4.85E+01 5.86E-03 1.37E-01 5.81E+01

2120 5.86E+01 5.79E+01 5.33E+01 6.12E+01 8.50E-01 4.90E-01 1.00E+00 1.00E+00
1.00E+00 1.93E-01 1.44E-01 8.26E-01 8.38E+00 2.75E+00 1.43E-02 -7.31E-04
3.56E-02 5.03E+01 5.87E-03 1.42E-01 5.80E+01

2140 2.00E+01 5.78E+01 5.32E+01 6.10E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 1.93E-01 1.44E-01 8.28E-01 8.28E+00 2.72E+00 1.00E+00 -7.26E-04
3.52E-02 1.00E+00 5.89E-03 1.48E-01 5.79E+01

2160 2.00E+01 5.77E+01 5.31E+01 6.09E+01 9.00E-01 9.00E-01 1.00E+00 1.00E+00
1.00E+00 1.93E-01 1.44E-01 8.29E-01 8.18E+00 2.69E+00 4.50E-01 -7.21E-04

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    3.48E-02   1.00E+00   5.90E-03   1.53E-01   5.78E+01

2180   2.00E+01   5.76E+01   5.30E+01   6.08E+01   9.00E-01   9.00E-01   1.00E+00   1.00E+00
    1.00E+00   1.93E-01   1.44E-01   8.30E-01   8.09E+00   2.66E+00   0.00E+00   -7.05E-04
    3.45E-02   1.00E+00   5.92E-03   1.58E-01   5.77E+01

2200   2.00E+01   5.75E+01   5.29E+01   6.06E+01   9.00E-01   9.00E-01   1.00E+00   1.00E+00
    1.00E+00   1.93E-01   1.44E-01   8.31E-01   8.01E+00   2.62E+00   -1.00E-02   -6.83E-04
    3.41E-02   1.00E+00   5.93E-03   1.64E-01   5.76E+01

2600   4.40E+01   5.57E+01   5.12E+01   5.82E+01   9.00E-01   9.00E-01   1.00E+00   1.00E+00
    1.00E+00   1.96E-01   1.46E-01   8.51E-01   6.41E+00   2.10E+00   1.00E+00   -4.56E-04
    2.76E-02   1.00E+00   4.99E-03   1.69E-01   5.58E+01

3050   5.60E+01   5.40E+01   4.95E+01   5.61E+01   9.00E-01   9.00E-01   1.00E+00   1.00E+00
    1.00E+00   1.98E-01   1.47E-01   8.67E-01   5.34E+00   1.78E+00   4.50E-01   -4.21E-04
    2.33E-02   1.00E+00   4.46E-03   1.72E-01   5.41E+01

3600   6.70E+01   5.24E+01   4.80E+01   5.40E+01   9.00E-01   9.00E-01   1.00E+00   1.00E+00
    1.00E+00   1.99E-01   1.47E-01   8.81E-01   4.45E+00   1.48E+00   0.00E+00   -3.67E-04
    1.96E-02   1.00E+00   3.96E-03   1.73E-01   5.24E+01

4300   6.70E+01   5.06E+01   4.63E+01   5.18E+01   9.00E-01   9.00E-01   1.00E+00   1.00E+00
    1.00E+00   2.00E-01   1.48E-01   8.94E-01   3.57E+00   1.22E+00   -1.00E-02   -3.94E-04
    1.61E-02   1.00E+00   3.84E-03   1.74E-01   5.07E+01

5100   9.80E+01   4.89E+01   4.48E+01   5.00E+01   9.00E-01   9.00E-01   1.00E+00   1.00E+00
    1.00E+00   2.06E-01   1.54E-01   9.04E-01   3.08E+00   9.34E-01   1.00E+00   -2.72E-04
    1.39E-02   1.00E+00   3.44E-03   1.75E-01   4.90E+01

6000   9.80E+01   4.73E+01   4.33E+01   4.81E+01   9.00E-01   9.00E-01   1.00E+00   1.00E+00
    1.00E+00   2.08E-01   1.55E-01   9.13E-01   2.61E+00   7.93E-01   4.50E-01   -2.42E-04
    1.17E-02   1.00E+00   3.02E-03   1.88E-01   4.73E+01

7000   9.80E+01   4.56E+01   4.17E+01   4.64E+01   9.00E-01   9.00E-01   1.00E+00   1.00E+00
    1.00E+00   2.09E-01   1.56E-01   9.21E-01   2.27E+00   7.00E-01   0.00E+00   -2.02E-04
    1.02E-02   1.00E+00   2.90E-03   2.05E-01   4.57E+01

8000   9.80E+01   4.42E+01   4.04E+01   4.48E+01   9.00E-01   9.00E-01   1.00E+00   1.00E+00
    1.00E+00   2.10E-01   1.56E-01   9.27E-01   2.00E+00   6.17E-01   -1.00E-02   -1.74E-04
    9.11E-03   1.00E+00   2.64E-03   2.19E-01   4.42E+01

1000000   1.89E+01   1.89E+01   1.88E+01   1.89E+01   9.00E-01   9.00E-01   1.00E+00
    1.00E+00   1.00E+00   2.24E-01   1.66E-01   9.84E-01   1.66E-02   -5.50E-03   3.20E-05   -
6.84E-06   7.01E-05   6.04E+01   1.12E-03   2.21E-01   1.89E+01
```

3.3.10 Output From PREWAP Test Case

```
! 1st comment line
! 2nd comment line
! 3rd comment line
#  3 21
#  17
```

```
# 5.760E-04
! t      wpT      wpRH      dsT      dsRH      wpPHnd      wpCLnd      wpPHd      wpCLd
dsPHnd      dsCLnd      dsPHd      dsCLd      ipkPHnd      ipkCLnd      ipkPHd      ipkCLd      barPHnd
barCLnd      barPHd      barCLd      PercFlux5m
 5.100E+01  2.707E+02  1.000E-02  2.660E+02  3.693E-02 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.446E+01
 5.300E+01  2.710E+02  6.000E-01  2.668E+02  2.982E-02 -9.990E-02  9.980E-03  9.400E+00
8.836E+01 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.507E+01
 5.500E+01  2.614E+02  6.000E-01  2.574E+02  3.082E-02 -9.990E-02  9.980E-03  9.400E+00
8.836E+01 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.601E+01
 6.000E+01  2.250E+02  6.000E-01  2.212E+02  3.524E-02 -9.990E-02  9.980E-03  9.400E+00
8.836E+01 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.791E+01
 6.500E+01  1.971E+02  6.000E-01  1.934E+02  5.353E-02 -9.990E-02  9.980E-03  9.400E+00
8.836E+01 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  2.169E+01
 7.000E+01  1.450E+02  1.000E-02  1.414E+02  8.668E-02 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  2.685E+01
 8.000E+01  9.496E+01  6.000E-01  9.155E+01  1.309E-01 -9.990E-02  9.980E-03  9.400E+00
8.836E+01 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  2.755E+01
 1.000E+02  9.010E+01  1.000E-02  8.693E+01  1.586E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.891E+01
 1.100E+02  8.678E+01  6.000E-01  8.369E+01  1.702E-01 -9.990E-02  9.980E-03  9.400E+00
8.836E+01 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.725E+01
 1.200E+02  8.257E+01  1.000E-02  7.958E+01  1.902E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.627E+01
 1.300E+02  8.103E+01  1.000E-02  7.814E+01  2.198E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.558E+01
 1.400E+02  7.763E+01  6.000E-01  7.483E+01  2.476E-01 -9.990E-02  9.980E-03  9.400E+00
8.836E+01 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.510E+01
 1.500E+02  7.377E+01  6.000E-01  7.107E+01  2.791E-01 -9.990E-02  9.980E-03  9.400E+00
8.836E+01 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.478E+01
 1.900E+02  7.123E+01  1.000E-02  6.876E+01  3.439E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.434E+01
 2.700E+02  6.906E+01  1.000E-02  6.690E+01  4.423E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.394E+01
 6.150E+02  6.711E+01  1.000E-02  6.562E+01  6.731E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03  9.400E+00  8.836E+01 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.460E+01
 1.000E+06  1.876E+01  9.984E-01  1.874E+01  9.999E-01 -9.990E-02  9.980E-03  7.188E+00
5.166E+01 -9.990E-02  9.980E-03  7.188E+00  5.166E+01 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  6.100E+01
#  19
```

```
# 9.600E-04
! t      wpT      wpRH      dsT      dsRH      wpPHnd      wpCLnd      wpPHd      wpCLd
dsPHnd    dsCLnd    dsPHd    dsCLd    ipkPHnd    ipkCLnd    ipkPHd    ipkCLd    barPHnd
barCLnd   barPHd    barCLd    PercFlux5m
 5.020E+01  2.347E+02  7.626E-02  2.291E+02  1.000E-02 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.410E+01
 5.300E+01  2.741E+02  2.824E-02  2.699E+02  1.000E-02 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.502E+01
 5.500E+01  2.658E+02  2.839E-02  2.618E+02  6.000E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03  9.400E+00  8.836E+01 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.596E+01
 6.000E+01  2.317E+02  3.080E-02  2.279E+02  6.000E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03  9.400E+00  8.836E+01 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.783E+01
 6.500E+01  1.990E+02  4.671E-02  1.953E+02  6.000E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03  9.400E+00  8.836E+01 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  2.159E+01
 7.000E+01  1.391E+02  7.816E-02  1.356E+02  6.000E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03  9.400E+00  8.836E+01 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  2.687E+01
 8.000E+01  1.002E+02  1.151E-01  9.675E+01  1.000E-02 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  2.757E+01
 1.000E+02  9.345E+01  1.403E-01  9.029E+01  6.000E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03  9.400E+00  8.836E+01 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.883E+01
 1.100E+02  8.871E+01  1.506E-01  8.563E+01  1.000E-02 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.717E+01
 1.200E+02  8.745E+01  1.685E-01  8.446E+01  6.000E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03  9.400E+00  8.836E+01 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.621E+01
 1.300E+02  8.409E+01  1.949E-01  8.120E+01  1.000E-02 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.552E+01
 1.400E+02  8.078E+01  2.201E-01  7.798E+01  1.000E-02 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.504E+01
 1.500E+02  7.773E+01  2.487E-01  7.503E+01  6.000E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03  9.400E+00  8.836E+01 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.472E+01
 1.800E+02  7.527E+01  2.937E-01  7.274E+01  6.000E-01 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03  9.400E+00  8.836E+01 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.440E+01
 2.250E+02  7.300E+01  3.554E-01  7.068E+01  1.000E-02 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.406E+01
 3.150E+02  7.077E+01  4.423E-01  6.873E+01  1.000E-02 -9.990E-02  9.980E-03 -9.990E-02
9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.381E+01
 4.750E+02  6.863E+01  5.481E-01  6.693E+01  1.000E-02 -9.990E-02  9.980E-03  9.400E+00
8.836E+01 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03 -9.990E-02  9.980E-03  9.830E+00
9.663E+01 -9.990E-02  9.663E+01  9.830E+00  9.663E+01  1.378E+01
```

```
6.150E+02 6.716E+01 6.309E-01 6.567E+01 6.000E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.455E+01
1.000E+06 1.883E+01 9.984E-01 1.881E+01 9.999E-01 -9.990E-02 9.980E-03 7.187E+00
5.166E+01 -9.990E-02 9.980E-03 7.187E+00 5.166E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 6.079E+01
# 29
# 1.153E-03
! t wpT wpRH dsT dsRH wpPHnd wpCLnd wpPHd wpCLd
dsPHnd dsCLnd dsPHd dsCLd ipkPHnd ipkCLnd ipkPHd ipkCLd barPHnd
barCLnd barPHd barCLd PercFlux5m
5.020E+01 2.260E+02 4.900E-01 2.200E+02 5.500E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.400E+01
5.100E+01 2.640E+02 5.500E-01 2.600E+02 6.500E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.430E+01
5.200E+01 2.740E+02 6.500E-01 2.690E+02 8.500E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.460E+01
5.500E+01 2.720E+02 8.500E-01 2.680E+02 4.900E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.590E+01
6.000E+01 2.550E+02 9.000E-01 2.510E+02 9.500E-01 -9.990E-02 9.980E-03 8.580E+00
7.362E+01 -9.990E-02 9.980E-03 8.580E+00 7.362E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 1.960E+01
6.500E+01 2.260E+02 9.500E-01 2.220E+02 9.000E-01 -9.990E-02 9.980E-03 8.580E+00
7.362E+01 -9.990E-02 9.980E-03 8.580E+00 7.362E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 2.140E+01
1.180E+03 6.540E+01 4.900E-01 6.440E+01 5.500E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 7.640E+00 5.837E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 3.910E+01
1.420E+03 6.340E+01 5.500E-01 6.250E+01 6.500E-01 -9.990E-02 9.980E-03 7.640E+00
5.837E+01 -9.990E-02 9.980E-03 7.640E+00 5.837E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 3.930E+01
1.680E+03 6.130E+01 6.500E-01 6.050E+01 8.500E-01 -9.990E-02 9.980E-03 7.640E+00
5.837E+01 -9.990E-02 9.980E-03 7.640E+00 5.837E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 3.940E+01
1.900E+03 5.940E+01 8.500E-01 5.860E+01 4.900E-01 -9.990E-02 9.980E-03 7.640E+00
5.837E+01 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 3.960E+01
1.950E+03 5.910E+01 9.000E-01 5.840E+01 9.500E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 4.140E+01
1.975E+03 5.900E+01 9.500E-01 5.830E+01 9.000E-01 -9.990E-02 9.980E-03 9.400E+00
8.836E+01 -9.990E-02 9.980E-03 9.400E+00 8.836E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 4.320E+01
2.060E+03 5.890E+01 4.900E-01 5.820E+01 5.500E-01 -9.990E-02 9.980E-03 -9.990E-02
9.980E-03 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 4.500E+01
2.080E+03 5.880E+01 5.500E-01 5.810E+01 6.500E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 4.670E+01
2.100E+03 5.870E+01 6.500E-01 5.800E+01 8.500E-01 -9.990E-02 9.980E-03 7.020E+00
4.928E+01 -9.990E-02 9.980E-03 7.020E+00 4.928E+01 -9.990E-02 9.980E-03 9.830E+00
9.663E+01 -9.990E-02 9.663E+01 9.830E+00 9.663E+01 4.850E+01
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2.120E+03	5.860E+01	8.500E-01	5.790E+01	4.900E-01	-9.990E-02	9.980E-03	7.020E+00
4.928E+01	-9.990E-02	9.980E-03	-9.990E-02	9.980E-03	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	5.030E+01		
2.140E+03	2.000E+01	9.000E-01	5.780E+01	9.000E-01	-9.990E-02	9.980E-03	7.020E+00
4.928E+01	-9.990E-02	9.980E-03	7.020E+00	4.928E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	1.000E+00		
2.160E+03	2.000E+01	9.000E-01	5.770E+01	9.000E-01	-9.990E-02	9.980E-03	7.020E+00
4.928E+01	-9.990E-02	9.980E-03	7.020E+00	4.928E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	1.000E+00		
2.180E+03	2.000E+01	9.000E-01	5.760E+01	9.000E-01	-9.990E-02	9.980E-03	7.190E+00
5.170E+01	-9.990E-02	9.980E-03	7.190E+00	5.170E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	1.000E+00		
2.200E+03	2.000E+01	9.000E-01	5.750E+01	9.000E-01	-9.990E-02	9.980E-03	7.020E+00
4.928E+01	-9.990E-02	9.980E-03	7.020E+00	4.928E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	1.000E+00		
2.600E+03	4.400E+01	9.000E-01	5.570E+01	9.000E-01	-9.990E-02	9.980E-03	7.020E+00
4.928E+01	-9.990E-02	9.980E-03	7.020E+00	4.928E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	1.000E+00		
3.050E+03	5.600E+01	9.000E-01	5.400E+01	9.000E-01	-9.990E-02	9.980E-03	7.020E+00
4.928E+01	-9.990E-02	9.980E-03	7.020E+00	4.928E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	1.000E+00		
3.600E+03	6.700E+01	9.000E-01	5.240E+01	9.000E-01	-9.990E-02	9.980E-03	7.190E+00
5.170E+01	-9.990E-02	9.980E-03	7.190E+00	5.170E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	1.000E+00		
4.300E+03	6.700E+01	9.000E-01	5.060E+01	9.000E-01	-9.990E-02	9.980E-03	7.020E+00
4.928E+01	-9.990E-02	9.980E-03	7.020E+00	4.928E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	1.000E+00		
5.100E+03	9.800E+01	9.000E-01	4.890E+01	9.000E-01	-9.990E-02	9.980E-03	7.020E+00
4.928E+01	-9.990E-02	9.980E-03	7.020E+00	4.928E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	1.000E+00		
6.000E+03	9.800E+01	9.000E-01	4.730E+01	9.000E-01	-9.990E-02	9.980E-03	7.020E+00
4.928E+01	-9.990E-02	9.980E-03	7.020E+00	4.928E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	1.000E+00		
7.000E+03	9.800E+01	9.000E-01	4.560E+01	9.000E-01	-9.990E-02	9.980E-03	7.190E+00
5.170E+01	-9.990E-02	9.980E-03	7.190E+00	5.170E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	1.000E+00		
8.000E+03	9.800E+01	9.000E-01	4.420E+01	9.000E-01	-9.990E-02	9.980E-03	7.020E+00
4.928E+01	-9.990E-02	9.980E-03	7.020E+00	4.928E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	1.000E+00		
1.000E+06	1.890E+01	9.000E-01	1.890E+01	9.000E-01	-9.990E-02	9.980E-03	7.187E+00
5.166E+01	-9.990E-02	9.980E-03	7.187E+00	5.166E+01	-9.990E-02	9.980E-03	9.830E+00
9.663E+01	-9.990E-02	9.663E+01	9.830E+00	9.663E+01	6.040E+01		

3.3.11 EXCEL Spreadsheet Replicating PREWAP Test Case

Time Period	Time (yr),	Waste Pack Temp.(C),	Drip shield temp. (C),		Drift wall temp.(C),	Invert temp. (C),	Waste pack RH,	RH	pH	Reason	Drip shield RH,	RH
1st Data Set Page 1												
1st	0.0	22.29	-99.90	dst<0	22.28	22.31	1.00	0.50	-0.0999	< 50 Yrs	-99.900	-100.40
1st	1.0	84.66	-99.90	dst<0	67.97	75.01	-99.90	-100.40	-0.0999	< 50 Yrs	0.500	0.00
2nd	50.0	66.57	-99.90	dst<0	61.20	63.34	0.01	-0.49	-0.0999	RH<0.5	-99.900	-100.40
2nd	50.2	236.17	230.51		109.78	188.46	0.01	-0.49	-0.0999	RH<0.5	0.084	-0.42
2nd	51.0	270.68	266.03		130.38	229.31	0.01	-0.49	-0.0999	RH<0.5	0.037	-0.46
2nd	53.0	271.01	266.81		143.36	239.70	0.60	0.10	9.4000	pH const	0.030	-0.47
2nd	55.0	261.42	257.42		144.18	240.14	0.60	0.10	9.4000	pH const	0.031	-0.47
2nd	60.0	225.01	221.23		132.81	194.68	0.60	0.10	9.4000	pH const	0.035	-0.47
2nd	65.0	197.08	193.44		120.76	173.41	0.60	0.10	9.4000	pH const	0.054	-0.45
2nd	70.0	145.00	141.44		97.57	128.48	0.01	-0.49	-0.0999	RH<0.5	0.087	-0.41
2nd	80.0	94.96	91.55		81.49	93.83	0.60	0.10	9.4000	pH const	0.131	-0.37
2nd	100.0	90.10	86.93		77.19	89.98	0.01	-0.49	-0.0999	RH<0.5	0.159	-0.34
2nd	110.0	86.78	83.69		74.59	87.42	0.60	0.10	9.4000	pH const	0.170	-0.33
2nd	120.0	82.57	79.58		71.23	83.81	0.01	-0.49	-0.0999	RH<0.5	0.190	-0.31
2nd	130.0	81.03	78.14		70.05	82.46	0.01	-0.49	-0.0999	RH<0.5	0.220	-0.28
2nd	140.0	77.63	74.83		67.53	79.49	0.60	0.10	9.4000	pH const	0.248	-0.25
2nd	150.0	73.77	71.07		64.77	76.16	0.60	0.10	9.4000	pH const	0.279	-0.22
2nd	190.0	71.23	68.76		62.97	73.93	0.01	-0.49	-0.0999	RH<0.5	0.344	-0.16
2nd	270.0	69.06	66.90		61.33	71.83	0.01	-0.49	-0.0999	RH<0.5	0.442	-0.06
2nd	615.0	67.11	65.62		59.67	69.67	0.01	-0.49	-0.0999	RH<0.5	0.673	0.17
	1000000.0	18.76	18.74		18.61	18.75	1.00	0.50		Interpolate	1.000	0.50

Skip if wp or ds Temp < 0	wpRH or dsRH > Cor Lim (.501)	wpRH I<.501 & i+1 >.501	dsRH I<.501 & i+1 >.501	wpRH I<.501 & I-1>=.501	dsRH I<.501 & I-1 >.501	Skip if wpRH I<.501 I+1<.501 , I-1<.501	Skip if dsRH I<.501 I+1<.501 , I-1<.501	SAVE LINE	Drift wall RH,	Backfill RH,	Invert RH,	Liquid Satr. @ Drip Shield,	Liquid Satr.@Invert,	Air mass Frac,
1st Data Set page 2														
TRUE	TRUE	FALSE	FALSE					cull	1.00	-99.90	1.00	-99.90	0.00	-99.90
TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.88	-99.90	0.02	-99.90
TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	TRUE	cull	1.00	-99.90	0.97	-99.90	0.03	-99.90
FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	TRUE	cull	0.66	0.97	0.08	0.00	0.00	0.00
FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	save	0.50	0.65	0.03	0.00	0.00	0.01
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	0.37	0.49	0.03	0.00	0.00	0.01
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	0.36	0.48	0.03	0.00	0.00	0.01
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	0.37	0.49	0.06	0.00	0.00	0.11
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	0.50	0.67	0.10	0.00	0.00	0.13
FALSE	FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	save	0.75	0.99	0.29	0.00	0.00	0.19
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	0.99	1.00	0.93	0.13	0.06	0.22
FALSE	FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	save	0.99	1.00	0.98	0.16	0.11	0.33
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	1.00	1.00	0.98	0.16	0.12	0.40
FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	save	1.00	1.00	0.99	0.17	0.12	0.48
FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	save	1.00	1.00	0.99	0.17	0.12	0.51
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	1.00	1.00	0.99	0.17	0.13	0.58
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	save	1.00	1.00	0.99	0.18	0.14	0.64
FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	save	1.00	1.00	0.99	0.19	0.14	0.67
FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	FALSE	save	1.00	1.00	0.99	0.19	0.14	0.71
FALSE	TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.74
NA	NA	NA	NA	NA	NA	NA	NA	SAVE	1.00	1.00	1.00	0.22	0.17	0.98

Water Vapor flux at Dwall (kg/yr/m of drift),	Air flux at Dwall(kg/ yr/m of drift),	A Drip Shield Evapo. rate (m3/yr),	Backfill Evapo. Rate (m3/yr),	Invert Evapo. Rate (m3/yr),	Percolation Flux at 5 m (mm/yr),	Volume flow at top dripshield (m3/yr),	volume flow at invert (m3/yr) ,	Top of the dripshield Temp (C)
1st Data Set Page 3								
0.00	0.00	-99.90	-99.90	-99.90	15.31	*-99.90*	0.00	-99.90
24.31	10.66	-99.90	-99.90	-99.90	14.39	*-99.90*	-0.01	-99.90
6.24	2.92	-99.90	-99.90	-99.90	14.21	*-99.90*	0.00	-99.90
2939.24	0.83	0.00	0.00	0.00	14.15	0.00	0.00	231.60
38.61	-0.02	0.00	0.00	0.00	14.46	0.00	0.00	266.97
10.29	0.42	0.00	0.00	0.00	15.07	0.00	0.00	267.65
10.34	0.47	0.00	0.00	0.00	16.01	0.00	0.00	258.21
0.29	-0.36	0.00	0.00	0.00	17.91	0.00	0.00	221.97
0.72	-0.45	0.00	0.00	0.00	21.69	0.00	0.00	194.14
265.67	34.96	0.00	0.00	0.00	26.85	0.00	0.00	142.11
220.81	19.33	0.13	-0.01	0.28	27.55	0.00	0.00	92.18
128.40	16.79	0.10	0.00	0.25	18.91	0.00	0.00	87.48
92.59	14.98	0.09	0.00	0.21	17.25	0.00	0.00	84.23
62.22	12.52	0.07	0.00	0.17	16.27	0.00	0.00	80.08
54.38	11.69	0.06	0.00	0.16	15.58	0.00	0.00	78.62
41.10	9.98	0.05	0.00	0.13	15.10	0.00	0.00	75.29
30.13	7.97	0.04	0.00	0.10	14.78	0.00	0.00	71.50
24.76	6.82	0.04	0.00	0.09	14.34	0.00	0.00	69.15
20.72	5.94	0.03	0.00	0.08	13.94	0.12	-0.04	67.22
17.30	5.12	0.03	0.00	0.07	14.60	0.04	-0.04	65.83
0.01	0.00	0.00	0.00	0.00	61.00	0.00	0.18	18.73

2nd Data Set Page 1													
1st	0.0	22.30	-99.90	dst<0	22.29	22.31	1.00	0.50	-0.0999	< 50 Yrs	-99.900	-100.40
1st	1.0	80.62	-99.90	dst<0	63.32	70.79	0.48	-0.02	-0.0999	< 50 Yrs	-99.900	-100.40
1st	2.0	87.48	-99.90	dst<0	71.72	78.43	0.53	0.03	-0.0999	< 50 Yrs	-99.900	-100.40
1st	5.0	94.43	-99.90	dst<0	80.80	86.61	0.59	0.09	-0.0999	< 50 Yrs	-99.900	-100.40
1st	20.0	89.09	-99.90	dst<0	79.72	83.41	0.69	0.19	-0.0999	< 50 Yrs	-99.900	-100.40
1st	25.0	85.28	-99.90	dst<0	76.79	80.17	0.71	0.21	-0.0999	< 50 Yrs	-99.900	-100.40
1st	30.0	81.77	-99.90	dst<0	74.00	77.13	0.72	0.22	-0.0999	< 50 Yrs	-99.900	-100.40
1st	40.0	74.92	-99.90	dst<0	68.44	71.10	0.76	0.26	-0.0999	< 50 Yrs	-99.900	-100.40
2nd	50.0	67.81	-99.90	dst<0	62.52	64.74	0.79	0.29	-0.0999	Seep< -99	-99.900	-100.40
2nd	50.2	234.74	229.08		109.30	187.17	0.08	-0.42	-0.0999	RH<0.5	0.010	-0.49
2nd	51.0	268.56	263.90		127.61	226.17	0.04	-0.46	-0.0999	RH<0.5	0.010	-0.49
2nd	53.0	274.12	269.92		142.88	239.45	0.03	-0.47	-0.0999	RH<0.5	0.010	-0.49
2nd	55.0	265.76	261.76		144.99	240.58	0.03	-0.47	-0.0999	RH<0.5	0.600	0.10
2nd	60.0	231.69	227.92		136.31	201.92	0.03	-0.47	-0.0999	RH<0.5	0.600	0.10
2nd	65.0	198.98	195.33		122.97	177.27	0.05	-0.45	-0.0999	RH<0.5	0.600	0.10
2nd	70.0	139.13	135.58		97.63	128.60	0.08	-0.42	-0.0999	RH<0.5	0.600	0.10
2nd	80.0	100.16	96.75		85.70	97.09	0.12	-0.39	-0.0999	RH<0.5	0.010	-0.49
2nd	100.0	93.45	90.29		81.85	94.21	0.14	-0.36	-0.0999	RH<0.5	0.600	0.10
2nd	110.0	88.71	85.63		79.55	92.22	0.15	-0.35	-0.0999	RH<0.5	0.010	-0.49
2nd	120.0	87.45	84.46		78.48	91.23	0.17	-0.33	-0.0999	RH<0.5	0.600	0.10
2nd	130.0	84.09	81.20		75.65	88.54	0.19	-0.31	-0.0999	RH<0.5	0.010	-0.49
2nd	140.0	80.78	77.98		72.99	85.79	0.22	-0.28	-0.0999	RH<0.5	0.010	-0.49
2nd	150.0	77.73	75.03		70.68	83.22	0.25	-0.25	-0.0999	RH<0.5	0.600	0.10
2nd	180.0	75.27	72.74		68.77	80.98	0.29	-0.21	-0.0999	RH<0.5	0.600	0.10
2nd	225.0	73.00	70.68		66.84	78.66	0.36	-0.15	-0.0999	RH<0.5	0.010	-0.49
2nd	315.0	70.77	68.73		64.91	76.35	0.44	-0.06	-0.0999	RH<0.5	0.010	-0.49
2nd	475.0	68.63	66.93		62.86	73.80	0.55	0.05	9.4000	pH const	0.010	-0.49
2nd	615.0	67.16	65.67		61.41	71.94	0.63	0.13	9.4000	pH const	0.600	0.10
5th	1000000.0	18.83	18.81		18.69	18.84	1.00	0.50		Interpolate	1.000	0.50

2nd Data Set Page 2

TRUE	TRUE	FALSE	FALSE					cull	1.00	-99.90	1.00	-99.90	0.00	-99.90
TRUE	FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.89	-99.90	0.02	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.87	-99.90	0.02	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.86	-99.90	0.01	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.90	-99.90	0.00	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.91	-99.90	0.01	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.93	-99.90	0.01	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.95	-99.90	0.02	-99.90
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.96	-99.90	0.03	-99.90
FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	save	0.66	0.98	0.08	0.00	0.00	0.00
FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	TRUE	cull	0.53	0.68	0.04	0.00	0.00	0.01
FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	FALSE	save	0.37	0.49	0.03	0.00	0.00	0.01
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	0.35	0.47	0.03	0.00	0.00	0.02
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	0.34	0.46	0.05	0.00	0.00	0.09
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	0.47	0.64	0.09	0.00	0.00	0.12
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	0.75	0.99	0.29	0.00	0.00	0.19
FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	FALSE	save	0.99	1.00	0.88	0.07	0.03	0.15
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	0.99	1.00	0.92	0.12	0.06	0.22
FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	FALSE	save	0.99	1.00	0.96	0.14	0.08	0.27
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	0.99	1.00	0.98	0.15	0.09	0.29
FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	cull	0.99	1.00	0.98	0.16	0.12	0.37
FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	TRUE	FALSE	save	1.00	1.00	0.98	0.17	0.12	0.44
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	1.00	1.00	0.99	0.17	0.12	0.50
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	save	1.00	1.00	0.99	0.17	0.12	0.55
FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	TRUE	FALSE	cull	1.00	1.00	0.99	0.17	0.13	0.59
FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE	save	1.00	1.00	0.99	0.18	0.14	0.64
FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	0.99	0.19	0.14	0.68
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	0.99	0.19	0.14	0.70
NA	NA	NA	NA	NA	NA	NA	NA	SAVE	1.00	1.00	1.00	0.22	0.17	0.98

2nd Data Set Page 3								
0.00	0.00	-99.90	-99.90	-99.90	15.26	***-99.90***	0.00	-99.90
22.48	11.92	-99.90	-99.90	-99.90	14.34	***-99.90***	-0.01	-99.90
25.93	10.23	-99.90	-99.90	-99.90	14.35	***-99.90***	-0.01	-99.90
30.46	10.25	-99.90	-99.90	-99.90	14.47	***-99.90***	0.00	-99.90
17.14	7.08	-99.90	-99.90	-99.90	14.54	***-99.90***	0.00	-99.90
14.44	5.76	-99.90	-99.90	-99.90	14.47	***-99.90***	0.00	-99.90
12.78	5.25	-99.90	-99.90	-99.90	14.40	***-99.90***	0.00	-99.90
9.72	4.56	-99.90	-99.90	-99.90	14.27	***-99.90***	0.00	-99.90
7.07	3.11	-99.90	-99.90	-99.90	14.16	***-99.90***	0.00	-99.90
3038.39	0.86	0.00	0.00	0.00	14.10	0.00	0.00	230.16
128.02	0.00	0.00	0.00	0.00	14.41	0.00	0.00	264.85
10.26	0.39	0.00	0.00	0.00	15.02	0.00	0.00	270.76
10.28	0.52	0.00	0.00	0.00	15.96	0.00	0.00	262.55
0.16	-0.22	0.00	0.00	0.00	17.83	0.00	0.00	228.65
0.47	-0.46	0.00	0.00	0.00	21.59	0.00	0.00	196.03
265.22	34.85	0.00	0.00	0.00	26.87	0.00	0.00	136.25
397.49	30.37	0.15	0.00	0.20	27.57	0.00	0.00	97.38
229.18	19.38	0.13	-0.01	0.24	18.83	0.00	0.00	90.84
172.74	18.16	0.11	0.00	0.27	17.17	0.00	0.00	86.16
151.04	17.51	0.11	0.00	0.27	16.21	0.00	0.00	84.97
104.54	15.58	0.09	0.00	0.23	15.52	0.00	0.00	81.68
75.80	13.70	0.08	0.00	0.19	15.04	0.00	0.00	78.44
58.01	12.05	0.07	0.00	0.16	14.72	0.00	0.00	75.47
46.80	10.73	0.06	0.00	0.14	14.40	0.00	0.00	73.14
37.85	9.50	0.05	0.00	0.12	14.06	0.00	0.00	71.03
30.41	8.03	0.04	0.00	0.10	13.81	0.10	-0.13	69.04
24.31	6.72	0.04	0.00	0.09	13.78	0.06	-0.08	67.18
20.75	5.94	0.03	0.00	0.08	14.55	0.04	-0.03	65.88
0.02	0.00	0.00	0.00	0.00	60.79	0.00	0.18	18.81

3rd Data Set Page 1												
1st	0.0	22.30	-99.90	dst<0	22.30	22.30	1.00	0.50	-0.0999	< 50 Yrs	-99.900	-100.40
1st	1.0	78.80	-99.90	dst<0	61.20	68.80	0.47	-0.03	-0.0999	< 50 Yrs	-99.900	-100.40
1st	40.0	75.60	-99.90	dst<0	69.10	71.90	0.76	0.26	-0.0999	< 50 Yrs	-99.900	-100.40
2nd	50.2	226.00	220.00		106.00	182.00	0.49	-0.01	-0.0999	RH<0.5	0.550	0.05
2nd	51.0	264.00	260.00		123.00	220.00	0.55	0.05	9.4000	pH const	0.650	0.15
2nd	52.0	274.00	269.00		134.00	233.00	0.65	0.15	9.4000	pH const	0.850	0.35
2nd	55.0	272.00	268.00		145.00	240.00	0.85	0.35		Interpolate	0.490	-0.01
2nd	60.0	255.00	251.00		145.00	219.00	0.90	0.40		Interpolate	0.950	0.45
2nd	65.0	226.00	222.00		135.00	200.00	0.95	0.45		Interpolate	0.900	0.40
3rd	1180.0	65.40	64.40		60.10	70.20	0.49	-0.01	-0.0999	RH<0.5	0.550	0.05
3rd	1420.0	63.40	62.50		58.00	67.50	0.55	0.05	7.6400	pH const	0.650	0.15
3rd	1680.0	61.30	60.50		56.00	64.80	0.65	0.15	7.6400	pH const	0.850	0.35
3rd	1900.0	59.40	58.60		54.10	62.20	0.85	0.35	7.6400	pH const	0.490	-0.01
3rd	1950.0	59.10	58.40		53.80	61.90	0.90	0.40		Interpolate	0.950	0.45
3rd	1975.0	59.00	58.30		53.70	61.70	0.95	0.45		Interpolate	0.900	0.40
4th	2060.0	58.90	58.20		53.60	61.60	0.49	-0.01	-0.0999	RH<0.5	0.550	0.05
4th	2080.0	58.80	58.10		53.50	61.40	0.55	0.05	7.0200	pH const	0.650	0.15
4th	2100.0	58.70	58.00		53.40	61.30	0.65	0.15	7.0200	pH const	0.850	0.35
4th	2120.0	58.60	57.90		53.30	61.20	0.85	0.35	7.0200	pH const	0.490	-0.01
4th	2140.0	20.00	57.80		53.20	61.00	0.90	0.40		Interpolate	0.900	0.40
4th	2160.0	20.00	57.70		53.10	60.90	0.90	0.40		Interpolate	0.900	0.40
4th	2180.0	20.00	57.60		53.00	60.80	0.90	0.40		Interpolate	0.900	0.40
4th	2200.0	20.00	57.50		52.90	60.60	0.90	0.40		Interpolate	0.900	0.40
4th	2600.0	44.00	55.70		51.20	58.20	0.90	0.40		Interpolate	0.900	0.40
4th	3050.0	56.00	54.00		49.50	56.10	0.90	0.40		Interpolate	0.900	0.40
4th	3600.0	67.00	52.40		48.00	54.00	0.90	0.40		Interpolate	0.900	0.40
4th	4300.0	67.00	50.60		46.30	51.80	0.90	0.40		Interpolate	0.900	0.40
4th	5100.0	98.00	48.90		44.80	50.00	0.90	0.40		Interpolate	0.900	0.40
4th	6000.0	98.00	47.30		43.30	48.10	0.90	0.40		Interpolate	0.900	0.40
4th	7000.0	98.00	45.60		41.70	46.40	0.90	0.40		Interpolate	0.900	0.40
4th	8000.0	98.00	44.20		40.40	44.80	0.90	0.40		Interpolate	0.900	0.40
5th	1000000.0	18.90	18.90		18.80	18.90	0.90	0.40		Interpolate	0.900	0.40

3rd Data Set Page 2														
TRUE	TRUE	FALSE	FALSE					cull	1.00	-99.90	1.00	-99.90	0.00	-99.90
TRUE	FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE	cull	1.00	-99.90	0.89	-99.90	0.02	-99.90
TRUE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	cull	1.00	-99.90	0.94	-99.90	0.02	-99.90
FALSE	TRUE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	save	0.68	1.00	0.09	0.00	0.00	0.04
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	0.56	0.72	0.04	0.00	0.00	0.00
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	0.45	0.60	0.03	0.00	0.00	0.01
FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	save	0.36	0.48	0.03	0.00	0.00	0.02
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	0.29	0.39	0.04	0.00	0.00	0.06
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	0.35	0.47	0.06	0.00	0.00	0.10
FALSE	TRUE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	save	1.00	1.00	0.99	0.19	0.14	0.73
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.76
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.79
FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.82
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.82
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.82
FALSE	TRUE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.82
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.82
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.83
FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.83
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.83
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.83
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.83
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.19	0.14	0.83
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.20	0.15	0.85
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.20	0.15	0.87
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.20	0.15	0.88
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.20	0.15	0.89
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.21	0.15	0.90
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.21	0.16	0.91
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.21	0.16	0.92
FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	save	1.00	1.00	1.00	0.21	0.16	0.93
NA	NA	NA	NA	NA	NA	NA	NA	SAVE	1.00	1.00	1.00	0.22	0.17	0.98

3rd Data Set Page 3								
0.00	0.00	-99.90	-99.90	-99.90	15.20	***-99.90***	0.00	-99.90
21.50	12.40	-99.90	-99.90	-99.90	14.20	***-99.90***	-0.01	-99.90
10.00	4.62	-99.90	-99.90	-99.90	14.20	***-99.90***	0.00	-99.90
2910.00	4.62	0.00	0.01	0.00	14.00	0.00	0.00	221.00
585.00	0.18	0.00	0.00	0.00	14.30	0.00	0.00	261.00
23.90	0.02	0.00	0.00	0.00	14.60	0.00	0.00	270.00
10.10	0.49	0.00	0.00	0.00	15.90	0.00	0.00	269.00
-0.13	0.10	0.00	0.00	0.00	19.60	0.00	0.00	252.00
0.20	-0.25	0.00	0.00	0.00	21.40	0.00	0.00	223.00
17.70	5.21	0.03	0.00	0.07	39.10	0.01	0.09	64.60
14.20	4.33	0.02	0.00	0.06	39.30	0.01	0.10	62.60
11.40	3.59	0.02	0.00	0.05	39.40	0.01	0.11	60.60
9.15	2.97	0.02	0.00	0.04	39.60	0.01	0.11	58.70
8.90	2.89	0.02	0.00	0.04	41.40	0.01	0.12	58.50
8.79	2.86	0.01	0.00	0.04	43.20	0.01	0.12	58.40
8.69	2.83	0.01	0.00	0.04	45.00	0.01	0.13	58.30
8.58	2.80	0.01	0.00	0.04	46.70	0.01	0.13	58.20
8.48	2.77	0.01	0.00	0.04	48.50	0.01	0.14	58.10
8.38	2.75	0.01	0.00	0.04	50.30	0.01	0.14	58.00
8.28	2.72	1.00	0.00	0.04	1.00	0.01	0.15	57.90
8.18	2.69	0.45	0.00	0.03	1.00	0.01	0.15	57.80
8.09	2.66	0.00	0.00	0.03	1.00	0.01	0.16	57.70
8.01	2.62	-0.01	0.00	0.03	1.00	0.01	0.16	57.60
6.41	2.10	1.00	0.00	0.03	1.00	0.00	0.17	55.80
5.34	1.78	0.45	0.00	0.02	1.00	0.00	0.17	54.10
4.45	1.48	0.00	0.00	0.02	1.00	0.00	0.17	52.40
3.57	1.22	-0.01	0.00	0.02	1.00	0.00	0.17	50.70
3.08	0.93	1.00	0.00	0.01	1.00	0.00	0.18	49.00
2.61	0.79	0.45	0.00	0.01	1.00	0.00	0.19	47.30
2.27	0.70	0.00	0.00	0.01	1.00	0.00	0.21	45.70
2.00	0.62	-0.01	0.00	0.01	1.00	0.00	0.22	44.20
0.02	-0.01	0.00	0.00	0.00	60.40	0.00	0.22	18.90

4. REFERENCES

CRWMS M&O 2000a. *Users' Manual for WAPDEG 4.0.* STN: 1000-4.0-00, SDN: 10000-UM-4.0-00. Las Vegas, Nevada: CRWMS M&O.

CRWMS M&O 2000k. *Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux.* ANL-EBS-HS-000003 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0644

CRWMS M&O 2000l. *In-Drift Precipitates/Salts Analysis.* ANL-EBS-MD-000045 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0623

CRWMS M&O 2000m. *In-Package Chemistry Abstraction.* ANL-EBS-MD-000037 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000418.0818.

Golder Associates 2000. *User's Guide, GoldSim, Graphical Simulation Environment.* Version 6.02. Manual Draft #4 (March 17, 2000). Redmond, Washington: Systems Simulation Group Golder Associates Inc. TIC: 247347.