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Civilian Radioactive Waste Management System
Management & Operating Contractor

Chapter 5
Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document

Waste Package Degradation Modeling and Abstraction

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August 14, 1998

Prepared for:

U.S. Department of Energy
Yucca Mountain Site Characterization Office
P.O. Box 30307
North Las Vegas, Nevada 89036-0307

Prepared by:

TRW Environmental Safety Systems Inc.
1261 Town Center Drive
Las Vegas, Nevada 89134

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Prepared by:

Joon H. Lee Performance Assessment Operations	8/14/98 Date
Kevin G. Mon Performance Assessment Operations	8/14/98 Date
Dennis E. Longsine Performance Assessment Operations	14 Aug 98 Date
Bryan E. Bullard Performance Assessment Operations	8/14/98 Date

Checked by:

Susan Anderson Performance Assessment Operations	8/14/98 Date

Approved by:

Robert W. Andrews Performance Assessment Operations	14 Aug 98 Date

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Waste Package Degradation Modeling and Abstraction

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ACRONYMS

As	arsenic
ASTM	American Standard Testing and Materials
BWR	boiling water reactor
CAM	corrosion-allowance material
CDFs	cumulative distribution functions
Cl^-	chloride ion
CRM	corrosion resistant material
CRWMS	Civilian Radioactive Waste Management System
CSH	calcium silicate hydrate
Fe^{2+}	ferrous ion
Fe^{3+}	ferric ion
HS^-	hydrogen sulfide ion
LTCTF	Long-Term Corrosion Testing Facility
M&O	management and operating contractor
MIC	microbiologically influenced corrosion
Mn	manganese
NE	northeast
NFGE	near-field geochemical environment
P	phosphorous
PAPR	Performance Assessment Peer Review
PCC	partial correlation coefficient
PRCC	Partial Rank Correlation Coefficients
PWR	pressurized water reactor

RH	relative humidity
S^{2-}	sulfide ion
SO_4^{2-}	sulfate ion
SATOOL	Sensitivity Analysis Tool
SAW	Simulated Acitified Water
Sb	antimony
SCC	stress corrosion cracking
SHE	standard hydrogen electrode
Sn	tin
SO_2	sulfur dioxide
SRRC	Standardized Rank Regression Coefficients
T/RH	temperature/relative humidity
TSPA-VA	Total System Performance Assessment—Viability Assessment
VA	Viability Assessment
WAPDEG	Waste Package Degradation
WPDEE	Waste Package Degradation Expert Elicitation

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ADDENDUM TO CHAPTER 5 – 8/22/98

Please note that the following figures were inadvertently omitted from this chapter during the reproduction process. They have been included here for technical consistency and and to facilitate the review, although they are not formally part of Revision 00.

Figure 5-56. Flow chart for CRM Pitting Corrosion Modeling

A Performance Report (PR) will be issued to correct this chapter. Revision 01 will also include these figures.

21-Aug-98

Peter S. Hastings, Deputy Manager
Performance Assessment Operations

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5. WASTE PACKAGE DEGRADATION MODELING AND ABSTRACTION

This chapter provides an assessment of the waste package degradation modeling and abstraction for the Total System Performance Assessment-Viability Assessment (TSPA-VA) analysis. The information presented in this chapter is the outcome of the work that incorporates the information generated from different management and operating (M&O) organizations (especially Performance Assessment Operations and Waste Package Operations), the recently conducted Waste Package Degradation Expert Elicitation (WPDEE), interactions with the Performance Assessment Peer Review (PAPR) panel, and other relevant activities within the M&O.

5.1 INTRODUCTION

As part of the characterization efforts for the potential repository at Yucca Mountain, Nevada, which is being studied for the disposal of the nation's high-level radioactive waste including commercial spent nuclear fuels and vitrified high-level waste, the Viability Assessment (VA) of the potential repository is being conducted (Civilian Radioactive Waste Management System [CRWMS] M&O 1997b). The current design concept for a multibarrier waste container provides the primary component of the engineered barrier system of the potential repository. Fulfillment of the requirements for substantially complete containment of the waste and subsequent controlled/gradual release of radionuclides from breached waste package into the geosphere will rely on a robust waste container design, among other engineered barrier system components.

Given that the waste package must "fail" (i.e., breached to an extent that the mobile water present in the near-field environment can enter the waste package and any dissolved radionuclides can be transported out of the waste package) before any dissolution of the waste form can occur, it is important to be able to provide reasonable estimation of waste package degradation. Waste package failure is defined as having an opening through the wall of the waste package through which advective or diffusive transport of gas or radionuclide can occur (CRWMS M&O 1997d, p. 3-64). The degradation rate of the waste container depends on (1) the waste container design including the material(s) used for the waste container, the thickness of these material(s), and the fabrication technique used; (2) the near-field thermal-chemical-hydrologic regime (driven by the repository design such as the thermal load, the presence of backfill, etc.) in the emplacement drifts adjacent to the waste container surface (in particular, the temperature, relative humidity, seepage onto the waste package and chemical and redox conditions); and (3) the degradation characteristics of the waste container materials (including the criteria for corrosion initiation and the rate of corrosion as a function of the near-field thermal-chemical-hydrologic environment and local exposure conditions on the waste package). Information from each of these topics is required as input to the waste container degradation model to predict the degradation rate of the waste packages.

The primary role of the waste package degradation modeling and abstraction, which is the subject of this chapter, is to provide information on the lifetime and overall degradation of the waste package. The degradation description is developed as a function of the exposure environment of the waste package. This model is very significant in the overall total system

performance assessment (TSPA), because it significantly contributes to determining the rate and time of release of radionuclides from the waste package. This chapter presents the waste package container material properties, their corrosion degradation models and the data on which they are based, and the model results, which provide the waste package degradation histories to be abstracted into TSPA-VA.

5.1.1 Overview

This subsection includes a brief description of the current waste package design, what the waste package degradation processes are, and how the process fits in with the other processes. Those processes that affect and are affected by the waste package degradation process include near-field thermal hydrological conditions including water dripping on waste package, near-field bulk geochemical conditions, waste form degradation, and radionuclide transport from a breached waste package.

Figure 5-1 shows three representative waste package types in an emplacement drift: waste packages for spent nuclear fuels from commercial pressurized water reactors (PWRs) and boiling water reactors (BWRs) and waste packages containing vitrified defense high-level waste and DOE-owned spent nuclear fuel.

The current reference design specifies a two-layer barrier system with a 100-mm thick corrosion-allowance material (CAM) as the outer barrier and a 20-mm thick corrosion-resistant material (CRM) as the inner barrier. The candidate materials are carbon steel (or ASTM A516) for CAM, and Alloy 22 (or UNS N06022) for the CRM (CRWMS M&O 1998a). Dimensions of the three representative waste package types are given in Table 5-1. Although failure of the waste container will most likely occur in the form of "perforations" created by localized corrosion of the corrosion-resistant inner barrier, high-performance corrosion-resistant alloys such as the candidate inner-barrier material could undergo corrosion degradation dominantly by general corrosion (CRWMS M&O 1998b). An additional small fraction of waste containers may fail prematurely due to material and manufacturing defects, damage during handling and by rockfall during emplacement, or other processes such as ground motions from earthquake and fault displacement. Even if perforated with holes and cracks, the waste container should still be able to provide a substantial barrier to radionuclide release (Lee 1997; Lee, Chambré, and Andrews 1996; Lee, Atkins, McNeish, and Vallikat 1996; Pigford 1993).

Under the near-field environmental conditions expected in the unsaturated media at Yucca Mountain, the majority of waste packages are expected to be exposed to humid air conditions during the emplacement period. Some fraction of the waste packages that are emplaced in areas where dripping occurs may be dripped on during the emplacement period. Thus, the significant contributors to the degradation of the waste package are the temperature and relative humidity in the drift and the water contact mode. Dripping rate and frequency of the seepage and its chemistry (especially, pH and chloride [Cl^-] concentration) will also significantly affect the degradation of the waste packages.

Figure 5-2 schematically shows information flow in the TSPA-VA model. Some information, such as conceptual models, assumptions, data, abstracted model results, is transferred between

the waste package degradation process and other processes that affect and are affected by the waste package degradation process. The key inputs for evaluating the waste package include:

- Layout of the repository, especially, the thermal loading and spacing between waste packages.

- Design of the waste packages including the materials and dimensions.

- Thermal hydrologic conditions in the emplacement drift (i.e., temperature, relative humidity, liquid saturation and in-drift seepage flux) as a function of time and location. The drift-scale thermal-hydrologic modeling provides the temperature, RH, and liquid saturation. A further abstraction produces the seepage rates and locations.

- Near-field geochemical environment (NFGE) conditions include pH and Cl^- concentration of dripping water and oxygen partial pressure inside the drift as a function of time and location. The NFGE modeling and abstraction provides these inputs.

The key outputs from the waste package degradation modeling and abstraction are a quantitative assessment of the waste package degradation. The output from the waste package degradation model is presented as a time to initial penetration of the waste packages—in the form of either "small" holes (pits) resulting from localized corrosion or "large" openings ("patch" perforations) resulting from general corrosion—and subsequent perforations (or openings) of the waste packages as a function of time. The time of the initial perforation is assumed to lead to the initiation of the waste form degradation inside the breached waste package. The perforated or opened area on the waste package provides the area through which radionuclides are released. The uncertainty and spatial variability of the degradation information also are provided as an output from the waste package degradation model.

5.1.2 Synopsis of Current Approach and Treatment

Degradation of the waste package is evaluated with the WAste Package DEGradation (WAPDEG) model. Three different versions of WAPDEG were used for the analyses presented in this chapter. The base case analysis (Section 5.11) was conducted with Version 3.07 (CRWMS M&O 1998c), and the sensitivity analysis (Section 5.12) was with Versions 3.09 and 3.11 (CRWMS M&O 1998h, 1998k). This was due to the continued development of the code to meet the needs for various sensitivity analyses. The WAPDEG code is based on a stochastic simulation approach and provides a description of waste package degradation, which occurs as a function of time and repository location for specific design and thermal-hydrologic modeling assumptions.

The stochastic waste package degradation model incorporates the following individual corrosion models:

- Humid-air general corrosion model for the CAM outer barrier

- Humid-air "roughness" factor (or localization factor) model for the outer barrier

- Aqueous general corrosion model for the outer barrier
- Aqueous "roughness" factor (or localization factor) model for the outer barrier
- Aqueous pitting corrosion model for the outer barrier when contacted with an alkaline solution (pH≥10)
- General corrosion model for the CRM inner barrier without drips
- General corrosion model for the CRM inner barrier in the presence of drips
- Localized corrosion (pitting and crevice corrosion) model for the CRM inner barrier.

Detailed discussion of the corrosion models is given in Sections 5.6 to 5.9. In addition, the following corrosion parameters were abstracted and implemented in the waste package degradation model:

- Temperature threshold for the initiation of corrosion of the CAM outer barrier
- Relative humidity threshold for the initiation of humid-air corrosion of the CAM outer barrier
- Relative humidity threshold for the initiation of aqueous corrosion of the CAM outer barrier
- Local exposure conditions on the CRM inner barrier (after breach of the outer barrier) and their probability to attain
- Critical temperature threshold for the initiation of localized corrosion of the CRM inner barrier.

In TSPA-VA, the waste package degradation is modeled by dividing the waste package surface into "patches" and populating the corrosion rates stochastically over the patches, depending on the local corrosion conditions. A patch size is defined as the maximum area in which relatively uniform local conditions exist, thus a uniform general corrosion rate is applied. The patches approach is an attempt to explicitly represent the variability in corrosion rates within a single waste package and to address multiple corrosion modes underway within a single waste package at a given time.

Data for corrosion and other degradation processes of the candidate materials and their process models are being developed under the comprehensive corrosion testing programs at Lawrence Livermore National Laboratory (McCright 1997). However, long-term testing data are not yet available under prototypic conditions. In addition, there has been a limited field experience for the candidate corrosion resistant alloy because of a short performance history. As a result, the models for waste package performance have large uncertainties. Consequently, a panel of six widely recognized engineers and scientists in corrosion were convened, and an expert elicitation

was conducted to develop additional information and models that are needed for waste package degradation modeling for TSPA-VA. Another major objective of the expert elicitation was to capture the uncertainties involved in assessing waste package degradation processes, including uncertainty both in the models used to represent corrosion processes and the parameter values used in those models. In the elicitation, the experts provided an overview of the processes for waste package degradation in the potential repository, taking into consideration potential evolutions of the exposure conditions in the emplacement drifts. Then, the experts developed assessments for the models of various key corrosion processes and the parameters of the corrosion models for the CAM (carbon steel) and CRM (Alloy 22) barriers. The assessments for the above models and parameters also expressed uncertainties in the respective model and parameter values.

A substantial amount of information for the individual corrosion model parameters and waste package degradation parameters, which are employed in the current waste package degradation model was derived from the recently conducted WPDEE (CRWMS M&O 1998b). A summary of the WPDEE results is given in Section 5.3. It should be noted that because of the time constraints imposed on the completion of the TSPA-VA analysis and extended elicitation processes, the interim elicitation results were provided to facilitate the analysis (Pendleton 1998), and those interim results were used in the base case analysis (see Section 5.11) and subsequent sensitivity analysis (see Section 5.12). Consequently, the elicitation results for some parameters that were presented in this report are not exactly the same as those in the final report (CRWMS M&O 1998b). As will be discussed further in the corresponding sections (Sections 5.7 to 5.9), the differences in the parameter values between those two versions are insignificant to the extent that they should not affect the analysis results.

Variability in waste package degradation across the repository because of varying exposure conditions is modeled by incorporating explicitly the spatial distribution of the exposure conditions. These exposure condition parameters to be included in the waste package degradation modeling are temperature, relative humidity, in-drift water dripping, and pH of the contacting water. In addition, variability in waste package degradation because of *uncertain variations* of corrosion processes and local exposure conditions are not readily quantifiable. These may include local (or micro-scale) electrochemical conditions of solution contacting waste package, uncertain long-term post-closure exposure conditions (such as water dripping and rockfalls), manufacturing of waste package, variation of the materials properties (especially microstructure-scale) etc. Where quantitative information for those uncertain parameters is available, the information was implemented explicitly in the waste package degradation modeling. For example, the WPDEE provided allocation of the elicited parameter values to its variability and uncertainty (see Sections 5.3 and 5.7 to 5.9). Otherwise, effects of those parameters for which quantifiable information is not available were represented by stochastically varying the corrosion rate parameters over the waste packages to be simulated and the patches in each waste package.

5.1.3 Significance of Waste Package Degradation to TSPA

In the current repository design, the waste package is one of a few most important components in the potential repository system, providing the major role in the waste containment and isolation. As defined in the Controlled Design Assumptions Document (CRWMS M&O 1997d, p. 4-26

and 4-27), the performance goals of the waste package are (1) complete containment of waste, and (2) controlled/gradual release of waste after failure. Waste package failure is defined as having an opening through the wall of the waste package through which advective or diffusive transport of gas or radionuclide can occur. The important information relevant to waste package degradation that could affect significantly the total system performance of the potential repository is:

- Waste package failure time
- Waste package failure rate
- Waste package failure mode
- Subsequent waste package degradation rate.

Once waste package is breached with an opening (by a pit penetration, a crack propagation, or gradual thinning from general corrosion as discussed in later sections), the waste form inside the breached waste package would undergo degradation and alteration, making the radionuclides available for release from the waste package. Thus, the time of waste package failure (or breach) defines the initiation time for waste form degradation and subsequent waste form mobilization. The current waste form degradation model is a function of temperature with other parameters; thus, the waste form degradation rates are affected by the waste form temperature at the time of waste package failure.

Next important information on waste package degradation is how fast the waste package failure occurs. As previously mentioned, once the waste package fails, the waste inventory inside becomes available for degradation and mobilization. The repository performance would be better if the waste package and associated engineered barrier system are designed to have the waste package failure rate at which the waste inventory becomes available for degradation and mobilization spread over a long period of time (CRWMS M&O 1995, Chapter 10). Thus, the waste package failure rate is important to the overall repository performance.

As will be discussed in Section 5.4, the current waste package degradation modeling considers two types of waste package failure, that is, "small holes" from the localized corrosion of the CRM, and "large openings" from a gradual thinning by the CRM general corrosion. The small hole penetrations, which are likely filled with the corrosion products and other mineral precipitates would provide a barrier to radionuclide transport out of the breached waste package (Lee 1997; Lee, Chambré, and Andrews 1996; Lee, Atkins, McNeish, and Vallikat 1996; Pigford 1993). However, the large openings from the CRM general corrosion may not provide any barrier roles to radionuclide transport from the failed waste package. The CRM failure (or breach) types would have a significant impact on the radionuclide release rate from the breached waste package.

Lastly, radionuclide release rates from the breached waste package would be affected by the number of perforations, which provide the area on the waste package available for radionuclide transport. Thus, the rate at which the failed waste package undergoes additional degradation beyond the first breach (or opening) is also important.

5.1.4 Roadmap of This Chapter

This section provides a roadmap for the remainder of this chapter, providing the reader with the direction for key components of the section.

- Section 5.2 discusses an overview of the exposure conditions and summarizes the corrosion modes of the candidate waste package materials, which are relevant to the expected exposure conditions at the potential repository.

- Section 5.3 presents a summary of the recently conducted WPDEE (CRWMS M&O 1998b).

- Section 5.4 summarizes the outcome of the waste package degradation abstraction and testing workshop that was conducted as part of the preparation of the TSPA-VA analysis. It also describes the conceptual model and assumptions used in the development of the waste package degradation model (WAPDEG).

- Section 5.5 describes the data, rationale, approach, and results for the development and abstraction of humid-air general corrosion and roughness factor models for the CAM outer barrier.

- Section 5.6 discusses the data, rationale, approach, and results for the development and abstraction for aqueous general corrosion and roughness factor models for the CAM outer barrier.

- Section 5.7 discusses the abstraction of general corrosion model for the CRM inner barrier without drips, which is based on the WPDEE results. Uncertainties in the abstracted model and future developments designed to reduce these uncertainties are discussed.

- Section 5.8 presents the abstraction of general corrosion model for the CRM inner barrier in the presence of drips. It discusses the local exposure condition scenarios on the CRM under dripping conditions and the probability to attain them, and presents different ranges of the general corrosion rate for the different exposure conditions. Then, it describes the abstraction for the general corrosion model, incorporating the above inputs from the WPDEE, and its uncertainties and discusses future work designed to reduce these uncertainties.

- Section 5.9 discusses the abstraction developed for the CRM localized corrosion model incorporating the pit growth law model developed by the Project's corrosion testing and modeling programs. It also describes the abstraction for the critical temperature-based criterion for CRM localized corrosion initiation, which is based on the WPDEE results.

- Section 5.10 describes implementation of the exposure conditions and abstracted corrosion models and model parameters into the waste package degradation model (WAPDEG). It discusses the representation of variability and uncertainty of waste

package degradation in WAPDEG, features and capabilities of the program, and its structure. It also describes of the input and output of the program.

- Section 5.11 presents the base-case waste package degradation model (WAPDEG) and simulation parameters, and then discusses the base case analysis results and guidance for the sensitivity analyses.

- Section 5.12 presents a suite of scenarios and cases for sensitivity analysis and discusses the analysis results. The sensitivity cases that were considered in the analyses are for (1) the parameters related to waste package and repository exposure conditions; (2) CAM and CRM corrosion parameters; and (3) waste-package and engineered-barrier-system design options including backfill, dripshield, and ceramic coating on the waste package.

- Section 5.13 summarizes the modeling and abstraction results of the individual corrosion models and waste package degradation. It discusses recommendations for the License Application to improve confidence in the waste package degradation representation.

In addition, Appendix A contains tables for the data that were used in and generated from the analyses presented in this chapter. Table A-1 lists the status of the input and output data and the data tracking number for the figures presenting the waste package degradation model abstraction analysis. Table A-2 lists the information for the software used and the status of the input and output data for the figures reporting the waste package degradation analysis results. Table A-3 lists the status of the data listed in the tables in this report and the data tracking number for the data.

5.2 GENERAL DESCRIPTION OF WASTE PACKAGE DEGRADATION PROCESSES IN THE POTENTIAL REPOSITORY

5.2.1 Introduction

This section provides a brief review of the various processes that are relevant to waste package degradation in the potential repository and, where available, summarizes analysis results. The candidate barrier materials in the current waste-package design are A516 carbon steel for the corrosion-allowance outer barrier and Alloy 22 for the corrosion-resistant inner barrier. Many factors influence the potential corrosion modes on the candidate materials. These include (1) metallurgical factors (alloy composition and microstructure); (2) physical factors (temperature, relative humidity, and water contact mode); (3) chemical factors (pH and concentration of species such as chloride, sulfate, nitrate, and carbonate ions); and (4) mechanical factors (stress) (McCright 1997).

In general, the corrosion modes can be classified into five groups: (1) general corrosion, (2) localized corrosion (pitting and crevice corrosion), (3) environmentally induced cracking (stress corrosion cracking), (4) metallurgically influenced corrosion (intergranular corrosion), and (5) mechanically assisted degradation (erosion and corrosion fatigue) (Craig and Pohlman 1987, p. 79). A recent report discussed the important degradation modes for candidate barrier materials in the potential repository near-field environment at Yucca Mountain (McCright 1997). The potentially important degradation modes identified in the report include: (1) general

corrosion, (2) pitting corrosion, (3) crevice corrosion, (4) stress corrosion cracking, (5) galvanic effects (galvanically enhanced corrosion and galvanic protection), (6) microbiologically influenced corrosion (MIC), (7) radiation induced corrosion, (8) corrosion in welded materials, and (9) low temperature long-term oxidation.

In this report, the term "humid-air corrosion" is used to refer to corrosion that takes place under a thin film of water that forms on the container surface above a certain critical humidity threshold. Such a water film is not thick enough to behave as bulk water. The term "aqueous corrosion" is used to refer to corrosion of metal in contact with bulk water or under a thick water film that behaves like bulk water.

5.2.2 Brief Overview of Exposure Conditions

For a high-thermal loading scenario (80 to 100 MTU/acre), waste packages will be heated initially to temperatures much greater than 100°C, then slowly cool down as the drying (or boiling) fronts gradually collapse back to the repository horizon. It is expected that waste packages (i.e., the carbon-steel outer barriers) initially undergo humid-air corrosion as the waste package surface temperature cools into the temperature range where significant water adsorption can occur; the temperature where this occurs is dependent on relative humidity and surface condition. Dry-oxidation of the outer barrier under low humidity conditions and at elevated temperatures does occur although the rate is insignificantly low (see summary of recent modeling results in this section).

The length of time during which active humid-air corrosion of the outer barrier occurs would depend on the relative humidity, temperature, and the physical and chemical conditions (especially contamination with salts and fine particles) of the waste package surface. It is expected that humid-air corrosion is operative at elevated temperatures and could last for an extended period of time. It is also expected that some waste packages may be exposed to episodic dripping even during the periods when the temperature inside the drift is greater than 100°C. After the in-drift temperature drops below 100°C, these and other additional waste packages may be exposed to water dripping. These dripping conditions are likely to deposit extensive salt-scales on the waste package (i.e., outer barrier) surface. The presence of hygroscopic salts can significantly lower the threshold "critical" humidity. Primary parameters that could potentially affect corrosion of outer barrier in humid-air conditions are the relative humidity, temperature, chemical and physical conditions of the outer barrier surface, and water dripping conditions (frequency and rate).

As the waste package surface cools further, and the in-drift conditions become more humid, the water film that forms on the surface of the corroding waste package could become thicker under some conditions. Aqueous corrosion may be assumed when the water film becomes thick enough to be visible and behave like bulk water (Tsuru et al. 1995). There are several factors and processes that can enhance condensation of a thick water film on the waste package surface. These are: (1) capillary condensation of water in voluminous porous corrosion products, (2) presence of hygroscopic salts, (3) water dripping, and (4) water condensation on cool waste packages. For waste packages that have undergone humid-air corrosion, aqueous corrosion may be assumed above a critical relative humidity threshold, which is likely to be a function of temperature. If a waste package has been under episodic water dripping, the waste package is

assumed to have salt-scale deposit, and the critical relative humidity threshold would be lower than the above case. If a waste package has been under dripping water, and the temperature is below boiling, then aqueous corrosion may occur on the waste package (depending on the relative humidity in the drift).

In the post-closure repository, the concrete liner in the emplacement drift is expected to degrade from various processes. These processes may include (1) carbonation of calcium-bearing hydrated cement phases, (2) crystallization of the poorly crystalline calcium silicate hydrates (CSH) to crystalline CSH phases, (3) cracking and spallation from thermal and mechanical stresses, (4) leaching by dripping water, (5) dissolution from contact with acidified water potentially generated by microbial activity, and others. With the quasi-crystalline CSH phases still existing, the concrete can potentially generate alkaline water with a pH greater than 11. After crystallization of the CSH phases and carbonation of the calcium-bearing phases, the pH of the water contacting the degrading concrete would become less alkaline (pH values probably dropping below 9 or 10) (Atkinson, Everitt, and Guppy 1989; Scheetz and Roy 1989). If the outer barrier is contacted by alkaline water with pH≥10, the outer barrier may undergo pitting corrosion.

5.2.3 Thermal Embrittlement

Fracture toughness in steels, especially in low alloy steels, is severely reduced by exposure in the temperature range of 350-575°C through isothermal aging or slow cooling. Segregation of impurities, such as Sb, P, Sn, As, along prior austenite grain boundaries is the main cause of thermal (temper) embrittlement. The most potent embrittling elements, in order of decreasing potency, are Sb, Sn, P, and As. However Sb, Sn and As are not generally present in steels. Therefore P is usually the most deleterious element to thermal embrittlement of steels (Cragnolino et al 1996, pp. 1-4 to 1-6). It was concluded that manganese (Mn) acts to enhance the effect of P on thermal embrittlement and that plain carbon steels containing less than 0.5 weight percent Mn are not susceptible to this phenomena (McMahon 1968). Not enough data exist on the long-term aging of plain C-Mn steels, particularly with high Mn contents, to disregard the possibility of thermal embrittlement.

The expected peak temperature for a waste package container is as high as 200°C for many years (CRWMS M&O 1998l, Section 3.5.5; see Figure 5-57 later in this chapter). Therefore, concerns have been raised as to whether thermal embrittlement would occur in the carbon steel outer barrier after long-term exposure to the temperatures expected in the potential repository. A bounding analysis was conducted to address the issue of P segregation in steels (the fraction of grain boundary being covered with a monolayer of P) after both a typical thermal embrittlement cycle at 350 to 575°C and a typical temperature cycle expected for a waste package in the potential repository (Huang 1997a). The analysis results showed that the total grain boundary segregation of P after the typical thermal embrittlement cycle is 0.97, while that for the expected waste package temperature cycle is 0.012. The segregation expected for the waste package is only about 1.2 percent of that for the typical thermal embrittlement cycle in steels. Therefore, it was concluded there would be no thermal embrittlement in the carbon steel outer barrier.

5.2.4 Dry Oxidation

Dry oxidation is one potential degradation mode of the CAM at the moderately elevated temperatures expected at the waste package surface in the potential repository. A model was developed based on short-term dry oxidation data for iron and low-carbon steel at temperatures from 200 to 650°C, and long-term dry oxidation of the CAM barrier in repository-relevant temperature conditions was analyzed (Henshall 1997). The model predicted the total penetration depth of the CAM barrier by dry oxidation, assuming uniform penetration is on the order of a few tenths of millimeters following 5,000 years of exposure to a repository-relevant temperature history. Under very conservative degradation assumptions with higher dry oxidation reaction rates and spalling of the oxide scales, the total penetration was predicted to be less than a few millimeters for a 5,000-year exposure time. Also, very little penetration of carbon steel by dry oxidation under repository-relevant conditions was predicted (Stahl and McCoy 1995). Based on the analysis results, it is assumed that dry oxidation is not expected to significantly degrade the performance of the thick carbon-steel outer barrier in the potential repository. A previous study concluded that the impact of oxidation of the candidate barrier materials in the potential repository condition is considered insignificant (Gdowski and Bullen 1988).

5.2.5 General Corrosion

General corrosion normally results in a relatively uniform thinning of materials without significant localized attack. The carbon steel outer barrier would be affected mostly by this corrosion mode. However, as indicated in Section 5.6, if carbon steel is exposed to alkaline water, the steel surface could be passivated and undergo localized corrosion with high-aspect ratio pitting (Marsh, Bland, and Taylor 1988).

In addition to the effect on corrosion rate caused by the presence of corrosive species, the material characteristics, and other exposure conditions, the general corrosion rate of carbon steel in water is also strongly affected by temperature, exhibiting maximum corrosion rates at temperatures around 60 to 80°C. Such corrosion behavior is commonly observed in corrosion processes governed by the reduction of dissolved oxygen. An increase in temperature enhances the diffusivity of oxygen molecules and reaction rates, but at the same time decreases the solubility of oxygen gas. The net mass transport of oxygen increases with temperature until a maximum is reached where the oxygen concentration begins to decrease approaching the boiling point. Thus, the corrosion rate attains a maximum and then decreases with further increase in temperature (Boden 1994).

The WPDEE panel experts generally agreed that alloys with a high Cr+Mo content such as Alloy 22 may not be subjected to localized corrosion in repository-relevant conditions. Consequently, degradation of these alloys would be by general corrosion (or passive dissolution). The panel concluded that under humid-air conditions and the expected environmental conditions, only very slow general corrosion of the CRM will occur (CRWMS M&O 1998b, p. 3-13). Under dripping conditions, localized corrosion of the CRM is possible, but aggressive conditions are required to initiate and sustain localized corrosion. Otherwise, only general corrosion will occur, and the general corrosion rate will be dependent on local corrosion exposure conditions (CRWMS M&O 1998b, p. 3-13 to 3-19).

5.2.6 Localized Corrosion

Localized corrosion (pitting and crevice corrosion) is induced by local variations in electrochemical potential on a micro-scale. The variations in electrochemical potential may result from local perturbations in the structure and composition of usually protective passive films on metal surfaces and also in the electrolyte composition of the solution that contacts the metal (McCright 1997). In addition, complex electrochemical processes associated with the above factors also strongly influence pit initiation and pit growth processes. In general, pitting of metals results from complicated interactions among many factors and appears to be random. As a result, stochastic approaches have been applied to represent and quantify localized corrosion processes.

In neutral pH water, localized variations of general corrosion depth of carbon steel are commonly represented with a roughness factor (or localization factor) that is defined as the ratio of the local corrosion depth to the average general corrosion depth considered over the entire sample surface at a given exposure time. Accordingly, the roughness factor has been used in modeling localized corrosion of carbon steel. However, in contact with alkaline pH water, carbon steel may undergo pitting corrosion with high-aspect ratio pits. A pit growth law was suggested to model carbon steel pitting corrosion in alkaline water (CRWMS M&O 1998b). However, the recent 6-month and 1-year data of carbon steel samples from the Long-Term Corrosion Testing Facility at Lawrence Livermore National Laboratory, which were exposed to concentrated J-13 water at pH 9.7 to 9.9, do not show such high-aspect-ratio pitting corrosion (Pasupathi 1998a). It is postulated that the presence of mixed anions in the concentrated J-13 water may prohibit such pitting corrosion.

Given a penetration of the carbon steel outer barrier, there are a number of factors that determine the probability that localized corrosion of the inner barrier will initiate. These factors include the availability of water, Cl^- content, pH, temperature, and oxidants such as oxygen (O_2) and ferric ion (Fe^{3+}). The probability of initiation is essentially the probability that an aggressive environment will exist relative to these factors. Water availability will vary with whether the waste package experiences drip and whether we consider the top, sides, or bottom of the waste package. The inner barrier surface is likely to be covered with a thick layer of the carbon steel corrosion products and other mineral precipitates. Accordingly, crevice corrosion of the inner barrier is considered a more probable corrosion process than pitting, and this process can initiate at lower temperatures than pitting. One conservative approach from the WPDEE is to initiate crevice corrosion of the CRM if the temperature is greater than or equal to 80°C when the outer barrier is breached. The probability of initiation is set to one at or above 100°C and decreases linearly to zero at 80°C. Once initiated, the crevice corrosion continues with a pit growth law (see details in Section 5.9). If the temperature is less than 80°C, no exposed sites initiate crevice corrosion, and the CRM is assumed immune to localized corrosion and degrades by general corrosion only. A recent study shows that the critical potentials for localized corrosion of Alloy 22 in concentrated chloride solutions at temperatures up to 95°C are considerably higher than those of Alloy 625 or 825 and in the range where oxygen evolution is expected to occur (Gruss et al. 1998). Similar observations were reported from the Project's corrosion testing and modeling programs (Roy et al. 1997b, 1997c).

There is potential for an enhanced susceptibility to pitting at the welds of the waste package disposal container. In particular, the pitting susceptibility could be higher at the closure welds because of potential technical difficulties associated with the stress relieving. Details of the disposal container fabrication and closure welding are discussed in TSPA-VA Summary Document (DOE 1998) (see Section 5.1.2.3 of Volume 2 and Section 3.2.2.6 of Volume 4).

5.2.7 Galvanic Coupling of Inner and Outer Barriers

Interactions of the two barriers (outer and inner barriers) could have impacts on the waste package degradation. One example of such interactions that is beneficial is galvanic coupling of the two barriers, which would galvanically protect the inner barrier and thus enhance the performance of the waste package. Another example that might be potentially unfavorable to waste package performance is the formation of crevice and gap between the two barriers, which would provide conditions in which the inner barrier is subjected to higher rates of pitting and other localized corrosion. Effects of the interactions on waste package performance were not modeled explicitly in previous TSPAs. Preliminary sensitivity studies for the benefit of the galvanic coupling were conducted in TSPA-1995 using a galvanic protection model, which is based on an expert assessment (CRWMS M&O 1995). The galvanic protection model was preliminary in nature and not based on experimental data or a systematic analysis.

The WPDEE noted (CRWMS M&O 1998b) that the potential exists for galvanic protection of the boldly exposed area of the inner barrier when the outer barrier is initially penetrated. While acknowledging that galvanic protection is possible for a limited period of time, all of the experts concluded that the period is too short to be of much significance over the time periods required for the repository. The WPDEE panel believes that the extent of galvanic protection is determined by the ionic conductivity and geometry of CAM penetration and crevice. The throwing distance or distance over which galvanic protection is effective is a function of the electrolyte conductivity and is assessed to be on the order of millimeters or, at most, a few centimeters. Therefore, for the expected CAM penetration by a general corrosion front, large areas of the CRM will be exposed at the time of CAM penetration, and thus, quickly exceeding the throwing distance. In the case of high-aspect ratio pitting of the CAM, the period of galvanic protection is expected to be longer, but still not significantly long relative to the waste package lifetime (a few hundred years, at most).

As demonstrated from a recent modeling exercise for crevice solution chemistry, galvanic coupling between the two barriers limits the pH reduction of the solution in the crevice to around 2.8 (Farmer and McCright 1998). Other factors such as mixed anions present in the solution contacting the CRM could contribute to limit the pH reduction of the crevice solution. In the TSPA-VA analysis, as discussed further for local corrosion exposure conditions on the inner barrier in Sections 5.8 and 5.9, the pH value of the crevice solution on the CRM is limited to 2.5 with a very low probability to attain such conditions in the crevice.

Potential adverse effects to long-term waste package performance, which could result from galvanic coupling between the two barriers, are enhanced corrosion of the outer barrier and hydrogen embrittlement of Alloy 22. Those two adverse effects listed above need to be addressed in future TSPA analysis.

5.2.8 Stress Corrosion Cracking

Stress corrosion cracking (SCC) is a crack propagation process that results from the combined and synergistic interaction of mechanical stress and corrosion reactions. The distribution of mechanical strain is subject to local (micro-scale) perturbations in metals because of structural inhomogeneities from one location to another on a similar scale to the electrochemical potential variations. SCC can be represented probabilistically with a nonuniform electrochemical potential distribution and a nonuniform strain distribution (McCright 1997). In many alloy systems, localized corrosion and SCC are interrelated because the sites of localized corrosion attack become the sources of initiation of stress corrosion (Farmer and McCright 1989; Farmer et al. 1988).

For SCC to occur, three factors have to exist: a source of stress, the presence of a crack, and a material-specific corrosive environment. Cracks can either preexist because of improper manufacturing practices or be initiated at locations where high stress concentration exists, such as at a groove or corrosion pit. Stress can exist because of welding residual stress, shrink-fit stress, or weight stress. Once a crack is initiated, the crack will grow by SCC when the applied stress intensity factor, K, is equal or larger than the SCC resistance parameter, K_{ISCC}. Corrosion pits can be developed at welds and base metals of the barrier materials after long exposure to the near-field environment. These act as stress risers to initiate crack fissures at the bases of the pits. SCC can be initiated from these pits when the applied stress intensity factors on these pits are equal or larger than the K_{ISCC} of the materials (Huang 1997b). Because of potential technical difficulties associated with the relieving of stresses in the closure welds of the double-walled waste container, SCC of the closure welds could be a problem, and a more complete analysis need to be conducted.

5.2.9 Microbiologically Influenced Corrosion

MIC results from the metabolic activity of microorganisms. MIC may operate throughout the life of the repository, especially after the near-field temperature of the potential repository cools down. Microbial metabolisms produce corrosive chemicals. For example, sulfate-reducing bacteria reduce sulfate (SO_4^{2-}) to sulfide (S^{2-}) which forms a hydrogen sulfide ion (HS^-), a highly corrosive species (McCright 1997; Van Konynenburg et al. 1995). Because of the localized nature of MIC and associated electrochemical perturbations, the overall effects can be modeled stochastically. In addition, the biochemical variations surrounding microbial activity are expected to introduce a further probabilistic consideration (McCright 1997). Although 300-series stainless steels are known to be susceptible to MIC, the nickel-based alloys such as Alloy 22 seem to be immune to MIC (CRWMS M&O 1998b).

Various aspects of potential microbial activity and MIC in the potential repository were discussed in the recent WPDEE (CRWMS M&O 1998b). The panel acknowledged that the potential for MIC is related to bacterial and fungal growth, which is controlled by the availability of nutrients, water, and electron acceptors. All of these conditions must be available to have the potential for MIC. Dr. B. Little (the MIC expert in the panel) noted that a mass balance inventory should be carried out for the repository, which could establish the limiting conditions in terms of a material inventory, energy-producing reactions, water availability, etc. These limiting conditions could then be used to assess the potential for MIC considering the waste

package material, environmental conditions, and MIC mechanisms. It was generally accepted that until the repository has cooled to temperatures below 100°C and the relative humidity is above 60 percent, the potential for MIC would not be present. The potential for MIC is greatly affected by the presence or absence of drips on the containers; if there are no drips, it is unlikely that there will be adequate transport of water and nutrients to support microbial activity. Possible MIC mechanisms that may potentially occur in the repository include manganese oxidation, iron oxidation, metal-reducing bacteria, sulfate-reduction, acid production by bacteria and fungi, slime production bacteria, and ennoblement. Bacteria and fungi require organic carbon and are likely to grow to a limited extent under Yucca Mountain conditions. Iron-reducing bacteria might be the most important organisms to consider in terms of corrosion within anaerobic regions of iron oxide layers. Their growth will require and be limited by organic carbon. In addition, microbial activity and growth are limited in the presence of concentrated salt solutions, which is likely to occur on the waste packages under dripping while they are at elevated temperatures.

It was generally concluded that the importance of MIC is in the probability of initiation of localized corrosion and the pit/crevice density, rather than affecting the rate once corrosion has begun. Bacterial colonies can maintain the proper conditions (e.g., low oxygen) for continued pit/crevice growth. Some experts noted that biofilms could increase the open circuit potential to +200 - 300 mV_{SCE} (saturated calomel electrode scale), thus enhancing the probability of pit/crevice initiation. The likelihood that this increase in potential will cause pit/crevice initiation is a function of the materials being considered. Some of the candidate materials (e.g., Alloy 22) have not been associated with documented cases of MIC. A recent study of the corrosion current at ambient temperature reported an increase in the corrosion current of five to six fold for inoculated carbon steel samples over sterile samples (Horn et al.1998).

5.2.10 Radiation Induced Corrosion

Radiation-induced corrosion could be another potentially important degradation process of waste package materials. Radiolysis of water under gamma radiation could form oxygen and hydrogen peroxide, which will enhance corrosion of metals. If a liquid phase is in contact with atmospheric gases and irradiated under gamma radiation, fixed nitrogen may exist in the liquid phase as nitrite and nitrate ions that could form corrosive species. The total amount of nitrite and nitrate that can be formed in a liquid phase is limited by the gamma radiation dose rate and the volume of air irradiated. If a thin film of water on the waste package container is irradiated in the contact with a relatively thicker air space, it is possible to achieve a significant concentration of nitric acid in the relatively small amount of water in the film (Van Konynenburg et al. 1995). However, in the potential repository, it may not be significant during the boiling period (i.e., high radiation dose period) because most of the air (and nitrogen) initially present in the vicinity of the waste package would be replaced by water vapor. When the waste package surface cools down to the level at which a water film thick enough to support corrosion reactions can form the radiation dose would be lowered to a level that is considered insignificant to long-term waste package performance.

5.2.11 Alloy Microstructure

Alloy microstructure, which can be thought of as the alloy composition at a very local level, may be an important parameter in many degradation modes. Because the alloy microstructure is most likely to vary in and around welds, differences in the behavior are most likely to be with the welded materials (Strum et al. 1988). One consequence of this would be enhanced SCC in the welded regions, especially the closure welds as discussed earlier. Potential for slow delayed microstructural evolution from long-term exposure at moderately elevated temperatures (such as those expected in the potential repository) was recognized particularly for corrosion resistant alloys, but the effects on the long-term waste package degradation are not well understood (McCright 1997, Section 2.9).

5.2.12 Structural Failure

After significant degradation of the concrete liners, rockfall is expected in the emplacement drift. A degrading waste package with rocks will experience a static load. The degrading waste package will experience a static load also from the weights of the waste package itself and the waste inside. After a certain degree of corrosion degradation, the waste package is expected to lose structural stability.

A recent analysis reported results for waste package component thinning and how that relates to structural failure mechanisms (CRWMS M&O 1996b). The structural analyses in the report provide a basis for determining the structural capabilities of a waste package at various levels of degradation. The analysis results under conditions of reduced thickness of the carbon steel outer barrier (A 516) and inner barrier (Alloy 625) that were structurally loaded by rockfalls concluded that the waste package maintains containment until the entire outer barrier and more than half of the inner barrier have been removed (i.e., 9.5 mm of the original 20 mm remains). The analysis assumed no support from the basket assembly inside the waste package. The above analysis results for a waste package with the Alloy 625 inner barrier could be applied to a waste package with the Alloy 22 inner barrier.

In addition, because there are potential technical difficulties in annealing the closure welds of the disposal container, an incomplete tempering of the heat-affected zone of the closure welds is possible, and it would reduce the impact strength of the heat-affected zone. Rockfall could have a significant bearing on the structural integrity if toughness is severely reduced in the heat-affected zone, and it could cause premature structural failure. The potential for this effect was not considered in the waste package degradation analysis.

5.2.13 Juvenile Failure

Considering the number of waste packages to be manufactured (about 12,000 waste packages) and a long period of design lifetime of waste packages in the potential repository, there will likely be events that could fail waste packages by processes other than anticipated corrosion degradation. These processes could include material defects, human-induced factors (manufacturing including welding, handling, and transportation), improper emplacement in the drift, potential placement on active displacement faults, potential shifts during emplacement, rockfalls, shaking of waste packages by seismic activity, etc. These processes could result in

early failure of waste packages, and such failure is collectively called in this report juvenile failure. Quantification of juvenile failure of the waste package is highly uncertain, and thus, inclined to a subjective judgement. The TSPA-VA analyses attempt to include this potential failure mode based on information gained from available sources.

In an earlier study, the probability of waste disposal containers being initially perforated was assessed based on data for simple pressure vessel components (Doubt 1984). The analogy between unfired pressure vessels and waste disposal containers may seem inappropriate because of the wide differences in mechanical complexity, but the analysis was to suggest an upper limit to the probability of early container perforation because of the existence of undetected defects, which may be present despite nondestructive examination. In the study, failure data among about 20,000 pressure vessels were examined, and of these, 17 were similar to the type of failure that would characterize early failure of waste disposal containers, i.e., external leakage or rupture in service, caused by a preexisting defect in weld or base material or by use of an incorrect material. The resulting failure rate is 8.5×10^{-4} per vessel (17 out of 20,000); that is, about 1 in 1,000 among a heterogeneous mixture of high quality pressure vessels can be expected to fail early because of an undetected critical defect. The report suggested that in a large population of geometrically simple waste disposal containers subjected to highly standardized inspection procedures, the proportion containing critical undetected defects should be much lower.

A recent report discusses the analysis results for occurrence of through-wall manufacturing defects that would essentially render the waste package breached at emplacement (CRWMS M&O 1997c). The analysis considered two manufacturing processes for the inner barrier: cylinder within a cylinder and weld clad inner barrier. They postulated that waste package defects could occur during the two welding processes to which the waste package is subject: welding of base metal sections (and bottom lids) and/or inner barrier cladding during fabrication of the disposal container, and welding of the lids onto the waste package to seal it after waste has been loaded.

Because a direct pathway to the environment is assumed to exist for either inner barrier manufacturing process, an estimation of the total through-wall breach due to manufacturing (weld) defects used the more conservative value of the weld clad inner barrier approach. Assuming independence between inner and outer barrier weld failures, a probability of 5.8×10^{-6} through-wall defects per waste package was estimated (CRWMS M&O 1997c, p. 61). Based on 10,938 total waste packages and the estimated frequency of waste-package through-wall defects, the probability that there will be one waste package with a through-wall manufacturing defect in the potential repository was estimated to be 6.3×10^{-2}. At 456 waste packages per year, the estimated frequency yielded an annual frequency of 2.6×10^{-3}, making this process an unlikely, but credible event for preclosure.

5.3 SUMMARY OF THE WASTE PACKAGE DEGRADATION EXPERT ELICITATION

This section summarizes the key results of the recent WPDEE, which was conducted as part of the TSPA-VA analysis (CRWMS M&O 1998b). As will be discussed in the following sections, the WPDEE results were incorporated to a large extent into the current waste package

degradation analysis. The elicitation results were used to develop the conceptual model of waste package degradation (Section 5.4), abstractions of individual corrosion models (Sections 5.5 to 5.9), and abstractions of other corrosion parameters (Section 5.10). As additional data are collected from the project's ongoing corrosion testing and modeling programs, the elicited assessments will be revised and replaced with the data and analysis results.

Because of the time constraints imposed on the TSPA-VA analysis, interim expert assessment results were provided for the VA analysis (Pendleton 1998). Therefore, the experts' assessments used in the current model abstraction and analysis are not identical to those in the final WPDEE report (CRWMS M&O 1998b). However, the differences are small, and the analysis results are not affected. The experts on the panel and their affiliations are:

- Peter L. Andresen (GE Corporate Research and Development)
- Joseph C. Farmer (M&O/Lawrence Livermore National Laboratory)
- Brenda J. Little (Stennis Space Center)
- R. Daniel McCright (M&O/Lawrence Livermore National Laboratory)
- John R. Scully (University of Virginia)
- David W. Shoesmith (Atomic Energy of Canada Limited)

5.3.1 The Objectives of the WPDEE

Data for corrosion and other degradation processes of the candidate materials and their process models are being developed under the comprehensive corrosion testing and modeling programs at Lawrence Livermore National Laboratory (McCright 1997). However, long-term testing data are not yet available under prototypic conditions, and, as a result, the models for waste package performance have large uncertainties. Consequently, an expert elicitation was conducted with the objective of developing additional information and models that are needed for waste package degradation modeling for TSPA-VA (CRWMS M&O 1998b).

Another major objective of the expert elicitation was to capture the uncertainties involved in assessing waste package degradation processes, including uncertainty both in the models used to represent corrosion processes and the parameter values used in those models. To ensure that the analysis included a range of perspectives, multiple individual judgements were elicited from members of an expert panel. The panel members, who were experts from within and outside the Yucca Mountain Project, represented a range of experience and expertise. A deliberate process was followed in facilitating interactions among the experts, in training them to express uncertainties, and in eliciting their interpretations. The resulting assessments and probability distributions, therefore, provide a reasonable aggregate representation of the knowledge and uncertainties about key issues regarding waste package degradation.

5.3.2 Summary of Key Assessments

In the elicitation, the experts provided an overview of the processes for waste package degradation in the potential repository, taking into consideration potential evolutions of the exposure conditions in the emplacement drifts. Then, the experts developed assessments for the models of various key corrosion processes and the parameters of the corrosion models for the CAM (carbon steel) and CRM (Alloy 22) barriers. Details of the elicitation process and a summary of the elicitations are found in the M&O report (CRWMS M&O 1998b). The corrosion models and parameters elicited by the experts have been incorporated in the waste package degradation model (WAPDEG). Those parameters for which assessments were provided include:

- Temperature threshold for the initiation of corrosion of the CAM outer barrier
- Relative humidity threshold for the initiation of humid-air corrosion of the CAM outer barrier
- Relative humidity threshold for the initiation of aqueous corrosion of the CAM outer barrier
- Humid-air "roughness" factor (or localization factor) model for the CAM outer barrier
- Aqueous "roughness" factor (or localization factor) model for the CAM outer barrier
- Aqueous pitting corrosion model for the CAM outer barrier when contacted with an alkaline solution (pH≥10)
- Pit density of CAM in alkaline conditions (pH≥10)
- Local exposure conditions on the CRM inner barrier (after breach of the outer barrier) and their probability to attain
- Critical temperature threshold for the initiation of localized corrosion of the CRM inner barrier
- General corrosion model for the CRM inner barrier without drips
- General corrosion model for the CRM inner barrier in the presence of drips
- Localized corrosion (pitting and crevice corrosion) model for the CRM inner barrier
- Pit density and pit diameter and size distributions of CRM.

The assessments for the above models and parameters also expressed uncertainties in the respective model and parameter values.

5.3.2.1 Corrosion of Carbon Steel Outer Barrier

The experts addressed the issue of corrosion of the carbon steel as a function of the temperature, relative humidity, water dripping, and chemistry of the dripping water within the repository. The first assessment is the nature of oxidation of the carbon steel CAM during the initial period where the repository is at its hottest temperatures and relative humidities are lowest. The experts generally agree that the dominant process during this period would be dry oxidation of the carbon steel and consequently very slow corrosion. There are differences of opinion regarding the nature and thickness of the oxide film that would develop on the waste package during this period and the potential for spalling of the oxide layer. Some of the experts conclude that, because the temperatures are relatively low (relative to 500°C where carbon steel oxidation has been observed), a thin oxide layer will develop that is not flaky and prone to spalling. Others believe that a thick, nonadherent, flaky, and porous oxide layer will form that will become prone to spalling.

As the temperature of the repository cools, there will be a threshold temperature below which dry oxidation of the carbon steel will be replaced by humid-air or aqueous corrosion, depending on the exposure conditions. All of the experts concluded that the threshold temperature was essentially the boiling point of water that contacts the waste package surface. Below that point, the relative humidity will be important to corrosion processes.

A persistent theme across the panel is that drips are very important to the corrosion processes and rates of corrosion of the CAM as well as the CRM. Important aspects are the spatial distribution, persistence through time, and frequency of drips. All experts noted that drips during the time that the waste packages are relatively hot will evaporate and leave behind hydrated salt deposits, whose constituents would include concentrated J-13 water and contributions from other engineered barrier system components such as the degrading concrete liner. Persistent drips onto these salt deposits could lead to saturated chemistries. Importantly, the presence or absence of drips is also judged to control to a large extent the pH of water on the package surface, which, in turn, controls the mode of corrosion of the carbon steel.

In general, the relative humidity threshold at which humid-air corrosion processes become operative is believed by the experts to be a function of the nature of the surface that will exist at the time that relative humidities rise. The experts' assessments of the relative humidity threshold range generally from about 60 to 80 percent relative humidity, depending on the nature of the surface. The relative humidity threshold for the onset of aqueous conditions is generally in the range of 85 to 100 percent relative humidity and drips or pooled water are required to achieve aqueous corrosion conditions.

Assuming the onset of corrosion, the mode of corrosion of the carbon steel CAM is judged to be governed by the pH of the water contacting the surface. The experts conclude that the expected corrosion mode of the carbon steel in the case of no drips and neutral pH is uniform or general corrosion, and in the case of high pH drips is high-aspect ratio pitting.

The panel generally concluded that the presence or absence of drips is a controlling aspect of the spatial distribution of corrosion both across multiple waste packages and on individual waste packages. Aqueous corrosion modes are assumed to be possible only in the case of dripping

water and on the top of the waste packages, defined variously by the panel as the upper 90 to 180 degrees in cross-sectional slice. Some experts also considered the bottom of the waste package to have the potential for aqueous corrosion.

In the case of general corrosion (neutral pH), the experts concluded that an average penetration rate of the propagating general corrosion front, together with some measure of the roughness of the front, would properly characterize the corrosion rate. The experts generally concluded that the average general corrosion penetration rate in an aqueous condition given in TSPA-1995 provides a reasonable average rate for carbon steel under neutral pH conditions. They concluded that the humid-air corrosion model in TSPA-95 be used for the average general corrosion rate of carbon steel in humid-air conditions. The model should be updated as additional data are generated, especially for the corrosion rate at elevated temperatures. This average rate would, in turn, be associated with a roughness or localization factor to model the propagating general corrosion front.

In the case of high-aspect ratio pitting, it is generally concluded that an appropriate way to express the corrosion rate is with a pit growth law that expresses the penetration depth as a function of time. The experts provided their assessments of the rate parameters and their uncertainties that characterize the corrosion rate of the carbon steel.

5.3.2.2 Corrosion of Alloy 22 Inner Barrier

The experts concluded that corrosion of the CRM inner barrier is tied to the manner in which it is exposed by penetration of the CAM outer barrier and the locations where those penetrations occur. Because of the temporal and spatial variations in penetrations of the CAM, the sites of initiation of inner-barrier corrosion should be modeled according to the evolution of pit penetration through the outer barrier (as is being modeled for TSPA-VA). The probability of pit or crevice initiation in the CRM is a function of the availability of water, Cl^- concentration, pH, Fe^{3+}, and oxygen. Given that the candidate CRM material is Alloy 22, under humid-air conditions and the expected environmental conditions, only very slow general corrosion of the CRM will occur. For localized corrosion to initiate and propagate, the aggressive conditions must be present, which might result from drips; otherwise only general corrosion will occur. Therefore, those waste packages subjected to drips are the locations that have a potential for localized attack of the CRM. The most likely corrosion mode for the CRM is judged to be crevice corrosion, with the possibility of high-aspect-ratio pitting and SCC. It generally was postulated that the low pH conditions and presumably high Cl^- within a crevice or pit in the CAM could lead to crevice corrosion along the crevice at the margins of the pit.

Galvanic Protection - While acknowledging that galvanic protection is possible for a limited period, all of the experts concluded that the period is too short to be of much significance over the periods related to the repository. The panel concluded that the extent of galvanic protection is determined by the ionic conductivity and geometry of CAM penetration and crevice corrosion. Given the electrolyte conductivity, the throwing power or distance is assessed to be on the order of millimeters or, at most, a few centimeters. Therefore, for the expected CAM penetration by a general corrosion front, large areas of the CRM will be exposed at close to the same time, quickly exceeding the throwing distance. In the case of high-aspect pitting of the CAM, the

period of galvanic protection is expected to be longer, but still not significantly long (a few hundred years, at most) enough to affect the performance of the waste package.

Environmental Conditions Relevant to CRM Corrosion - Based on a consideration of the bulk environmental conditions that are postulated to affect the waste package, the evolution of those conditions with time, and the potential for developing variable local exposure conditions on the waste package (e.g., saline solutions due to evaporation, alkaline solutions, mixed ion chemistry, presence of Fe^{3+}), the expert panel developed a consensus assessment of the environmental conditions that are pertinent to the potential for corrosion of the CRM. They arrived at a set of relevant "local environmental scenarios" that they believed were possible, given the bulk environmental conditions and the potential for modified local conditions from a variety of mechanisms (MIC, oxidation of Fe^{2+} to Fe^{3+}, etc.) These scenarios provided the basis for questions related to the general corrosion rate of the CRM, the probability of localized corrosion initiation, and the rate of localized corrosion. Although all of the environmental scenarios are possible, the *probability* of their occurrence differs significantly. The experts, therefore, provided an estimate of the probability of occurrence of the various environmental states.

Moisture conditions assumed were either humid-air conditions or the presence of drips. Relatively uniform local exposure conditions were assumed for humid-air conditions. For dripping conditions, local exposure conditions on the CRM were assessed for three temperatures (25, 50, and 100°C), two pH conditions (pH 2.5 and pH 3 to 10), and two oxidizing states (equivalent to corrosion potentials of 340 mV_{SHE} (standard hydrogen electrode scale) and 640 mV_{SHE}). Each of the experts assessed the probability that the three environments could occur at temperatures of 25, 50, and 100°C. Because the experts' assessments differ in the interpretation of how this probability should be expressed, they are not readily amenable to forming an aggregate assessment of the probability. The experts all agreed that the presence of water (drips) is needed to achieve the levels of oxidizing potential considered in the three environmental states.

Although given a low probability of occurrence, the low pH, high-oxidizing condition scenarios are included to represent conditions that can occur in the presence of Fe^{3+} ions. Panel members assessed that after the carbon steel CAM is penetrated, the Fe^{2+}/Fe^{3+} oxide of the CAM corrosion products in contact with the CRM could oxidize to predominantly Fe^{3+}. Under passive corrosion conditions, the Alloy 22 would require only a very low cathodic current density (Fe^{3+} reduction) to induce a high corrosion potential. However, when active crevice or pitting corrosion begins, much larger currents would be required.

General Corrosion Rate - For humid-air conditions (without drips), the general corrosion rate was assessed for three temperature states: 25, 50, and 100°C. For dripping conditions, general corrosion (passive dissolution) rates for the CRM are assessed for each of the above local exposure conditions and on two assumed ionic concentrations of concentrated J-13 water, either 1000× or fully saturated.

Probability of Localized Corrosion Initiation - Panel members developed a consensus for assessing localized corrosion of Alloy 22 that incorporates the probability that localized

corrosion will initiate *and* sustain itself on the surface of the CRM. These assessments were conditional on the three environmental dependent defined above and on temperature.

As was the case for the probability of the occurrence of the above environmental conditions, the experts differed in their interpretation of the condition being assessed; and a composite assessment was not computed. A conservative approach from the WPDEE recommended that crevice corrosion be assumed to initiate if the exposure temperature is greater than or equal to 80°C when the outer barrier is penetrated. The probability of crevice corrosion initiation is set to one at a temperature greater than or equal to 100°C and decrease linearly to zero at 80°C (uniform distribution).

Localized Corrosion Rate - The experts defined the corrosion penetration rates for localized corrosion of the CRM in terms of the power growth law. They provided assessments for the parameters of the model for the three local environmental states and for temperatures of 25, 50, and 100°C. These assessments are conditional on the initiation of localized corrosion, which the experts assessed to require dripping water.

The experts considered potential for stifling of crevice/pits, although specific criteria (i.e., environmental conditions at which stifling occurs) generally were not specified because of limited data for Alloy 22.

5.3.2.3 Microbiologically Influenced Corrosion

The potential for MIC is related to the formation of a biofilm, which is controlled by the availability of nutrients, water, and electron acceptors. All of these conditions must be met in order to have the potential for MIC. The potential for MIC is greatly affected by the presence or absence of drips on the containers; if there are no drips, there will not be adequate water or, likely, nutrients available to support the microorganisms. The importance of MIC is in the probability of initiation of localized corrosion and the pit/crevice density, rather than affecting the rate once corrosion has begun. Drs. J. Scully and B. Little note that MIC can increase the open circuit potential to +200 - 300 mV_{SCE} (saturated calomel electrode scale), and thus enhance the probability of pit/crevice initiation. The likelihood that this increase in potential will cause pit/crevice initiation is a function of the materials being considered, and the experts note that some of the candidate materials (e.g., Alloy 22) have not been associated with documented cases of MIC.

5.4 DEVELOPMENT OF WASTE PACKAGE DEGRADATION CONCEPTUAL MODEL

This section provides a brief summary of the Waste Package Degradation Abstraction and Testing Workshop held in January 1997. The workshop provided support for the development of the waste package degradation model and analysis of waste package degradation for the TSPA-VA analysis. In addition, this section discusses the conceptual model developed to model waste package degradation in the potential repository. A detailed description of the base case conceptual model and the logic flow that were implemented into the waste package degradation model are presented in this section.

5.4.1 Summary of Waste Package Degradation Abstraction and Testing Workshop

The Waste Package Degradation Abstraction and Testing Workshop for development of plans and implementation of waste package degradation into TSPA-VA was held in January 1997 (CRWMS M&O 1997a). This workshop was part of a series of ten workshops intended to provide support to the TSPA-VA (CRWMS M&O 1996a).

The Waste Package Degradation Workshop attempted to bring together the key project personnel working on waste package degradation including data collectors, process level modelers, and TSPA modelers. At the workshop, various key issues regarding waste package degradation were discussed. The TSPA modelers had an opportunity to present the issues, which they expect will be important in the repository, and to discuss how these issues can be incorporated into total system performance assessment models. The process level modelers presented their current level of knowledge. The data collectors presented their current understanding of the various phenomenon and discussed their schedules for gaining additional information.

Objectives of Workshop - The primary goals of the workshop were to (1) identify and prioritize issues important to waste package degradation, and (2) develop plans for developing and testing appropriate model abstractions to address the important issues in the waste package degradation model. Issues of waste package degradation (e.g., processes and parameters) were identified based on their importance to long-term performance of waste packages. Prioritization of the issues was based on the criteria that affect long-term performance of waste packages. The two major performance goals of waste packages are (1) complete containment of waste for an initial time period and then (2) gradual release of waste over a long period of time after failure of complete containment (CRWMS M&O 1997d p. 4-26 and 4-27).

Approach for Prioritization of Issues - The workshop participants generated subissues for each of prescribed five major issues. Because only a limited amount of time and resources are available for TSPA-VA, it would not be possible to address all of the subissues identified by the participants. Thus, it was necessary to prioritize the subissues to select only the key subissues that are most important to waste package performance. For TSPA-VA, efforts would only be made to develop models to address the key subissues.

The criteria for screening and prioritization of issues were developed based on the performance goals of waste packages, i.e., (1) complete containment of waste for an initial time period and then (2) controlled/gradual release of waste after failure (CRWMS M&O 1997d p. 4-26 and 4-27). Waste package failure is defined as having an opening through the wall of the waste package through which advective or diffusive transport of gas or radionuclide can occur. Once a waste package is breached with an opening, the waste form inside the breached waste package would undergo degradation and alteration, making the radionuclides available for release from the waste package. However, the failed waste package would still perform as a barrier to radionuclide release to a degree defined by the extent of subsequent perforations which provide the area on the waste container available for radionuclide transport. Thus, the rate at which the failed waste package undergoes additional degradation beyond the first breach (or opening) is also important.

Based on the above reasoning, three criteria were developed for use in prioritizing the subissues: (1) how significantly the issue affects the time of the first perforation of the first breached waste package (*initiation of waste package failure*); (2) how significantly the issue affects the rate of first perforation of subsequent waste packages (*waste package failure rate*), and (3) how significantly the issue affects the rate of subsequent perforations of failed waste packages (*waste package degradation rate*).

Development of Final Topics and Abstraction and Testing Plans - At the workshop, the participants generated a total of 94 subissues for the prescribed five major issues, which the participants thought should be considered in waste package degradation modeling. However, because of the constraints on *time* and *resources* that are available for TSPA-VA, it would not be possible to address all of the subissues. Thus it, was necessary to prioritize the subissues to select only the key issues that are most important to waste package performance. The selected key issues were combined into four major topics as follows:

- Carbon-steel outer-barrier corrosion
- Corrosion-resistant inner-barrier corrosion
- Microbiologically influenced corrosion
- Effects of variability in near-field conditions, manufacturing, and materials on waste package degradation.

Detailed discussions of the abstraction/testing plans developed for the four major topics are given in the workshop report (CRWMS M&O 1997a).

5.4.2 Conceptual Model for Waste Package Degradation Modeling

Figure 5-3 presents drawings showing various aspects of a waste package undergoing corrosion degradation. In particular, the profile view of the degrading waste package attempts to demonstrate variable corrosion processes underway in a waste package, depending on the exposure conditions. A portion of the waste package that does not experience drips would undergo corrosion in humid-air environments, and the CRM would degrade by general corrosion at extremely low rates. For a portion of the waste package that is dripped on, local concentration of salts is possible, and this, compared to the no-drip condition, could cause an earlier breach of the CAM and provide local exposure conditions that the CRM degrades at higher general corrosion rates and is subject to localized corrosion. This could lead to an earlier CRM breach than no-drip conditions. Also shown in the figure are typical morphology for a pit-opening and a patch-opening on the CRM.

In TSPA-VA, the waste package degradation will be modeled by dividing the waste package surface into "patches" and populating the corrosion rates stochastically over the patches, depending on the local exposure conditions on the waste package. A schematic for this approach is shown in Figure 5-4. The schematic shown in the figure intends to show a representative waste package placed in an emplacement drift. In the TSPA-VA analysis, a patch size is defined as the maximum area in which relatively uniform local conditions exist, thus a uniform general

corrosion rate is applied. In the base case model, a uniform size was assumed for the patches, with a single patch size of 310-cm^2, which is based on the American Standard Testing and Materials (ASTM) standard test coupon size (ASTM 1992). The "patches" approach is an attempt to explicitly represent the variability in corrosion rates within a single waste package and to potentially represent the occurrence of multiple corrosion modes within a single waste package at a given time (Lee et al. 1997). For example, the patches that are dripped on would have potential for the formation of salt deposits while the waste package surface temperature is above boiling temperature. In this condition, highly concentrated salt solutions could form locally on those patches. As the waste package temperature decreases and the relative humidity in the vicinity of the waste package increases, the salts on these patches absorb moisture resulting in the formation of concentrated salt solutions. Under those conditions, significantly increased corrosion rates were observed for carbon steel (Gdowski 1998). As will be discussed later, the susceptibility of the CRM to localized corrosion is higher in the presence of increased salt (especially chloride) concentrations. As discussed in Section 5.11.1, the waste package degradation model does not consider the effect of potential run-off of salt solutions from the waste package surface under sustained dripping and high humidity conditions as the repository slowly cools to below boiling temperature. This would lead to less corrosive conditions on the waste package.

Variability in waste package degradation across the repository due to varying exposure conditions will be modeled by incorporating explicitly the spatial distribution of the exposure conditions. The exposure conditions that were included in the TSPA-VA waste-package degradation modeling are temperature and relative humidity at the waste package surface, in-drift water dripping, and pH of the water contacting waste package.

5.4.3 Base Case Conceptual Model

The base case model for waste package degradation was developed using the information developed from the WPDEE and literature data. A logic diagram for the base case model is shown in Figure 5-5. In the conceptual model, the waste package surface temperature that is provided from the thermal-hydrologic model abstraction (see Chapter 3) is tested against the temperature threshold (T_{th}) for corrosion initiation of the CAM. When the surface temperature becomes less than the threshold temperature, the waste package undergoes different corrosion degradation modes depending on whether it is dripped on or not.

For waste packages that are not dripped on, the CAM outer barrier undergoes either humid-air or aqueous corrosion dependent on the relative humidity at the waste package surface. When a CAM patch is breached, moist conditions are assumed at the surface of the CRM patch that is underneath the CAM patch that was penetrated. This conceptual reasoning is based on the shrink-fit manufacturing approach, in which there will be isolated gaps between the two barriers and moisture could permeate through the isolated gaps. The assumption of moist conditions on the CRM patch is based on observations of the occurrence of capillary condensation of moisture by gel-like porous corrosion products of the outer barrier covering the inner barrier surface (Vernon 1933) and the hygroscopic nature of corrosion products (Fyfe 1994; Haynie et al. 1978), which would provide an aqueous corrosion condition at the surface of the CRM patch. The assumption is also based on a potential for crevice formation between the uncorroded CAM and CRM barriers, in which moisture could condense and an aqueous condition could exist. In the

absence of drips, the CRM inner barrier patch undergoes general corrosion all the time and fails eventually by a gradual thinning of the inner barrier patch. As will be discussed in Sections 5.7 and 5.8, CRM general corrosion rates in the absence of drips are much lower than those with drips.

For a waste package that is dripped on, the CAM undergoes either humid-air or aqueous corrosion, depending on the relative humidity at the waste package surface. Even with drips, if the relative humidity is low, the water will evaporate, and the waste package surface would experience humid-air-like exposure conditions. Persistence of this exposure condition will be affected by the drip rate and frequency. However, because information on this is not available for the TSPA-VA analysis, the CAM of a dripped-on patch is assumed to undergo humid-air corrosion until the relative humidity of the waste package surface increases above the threshold relative humidity for the initiation of aqueous corrosion. This assumption will, at elevated temperatures, provide higher corrosion rates for the affected CAM patches than assuming aqueous conditions under dripping without considering the relative humidity conditions (see Sections 5.5 and 5.6). Drips could leave salt deposits on the CAM patches, and this could cause the affected CAM patches to corrode at higher rates. These effects are not modeled explicitly in the waste package degradation model, but this should not cause any significant impacts on the results. As discussed in Section 5.6.5, the aqueous CAM general corrosion model is conservative such that the general corrosion depths predicted by the model are greater by a factor of five to ten compared to the 1-year data of carbon steel coupons tested in concentrated solutions of the site groundwater (see Figure 5-19 later in this chapter). When a CAM patch is breached, the CRM patch underneath the breached CAM patch is assumed to undergo aqueous corrosion under dripping conditions, and the corrosion mode—either general corrosion or localized corrosion—is dependent on the local exposure corrosion environment on the CRM patch as discussed later.

For a waste package that is dripped on, if the relative humidity at the waste package surface is greater than the threshold relative humidity for aqueous corrosion initiation, the corrosion mode of the affected CAM patches is dependent on the pH of the dripping water. If the pH of the dripping water is greater than or equal to 10, pitting corrosion with high-aspect ratios is assumed to occur; if it is in a neutral pH range (i.e., the pH is greater than 4 and less than 10), general corrosion with a low "roughness factor" (commonly called a "localization factor") is assumed. When the CAM is penetrated, crevice is assumed to form on the CRM patch underneath the breached CAM patch. Underneath the breached CAM patch, crevice could form between the uncorroded CAM and CRM barriers and under CAM corrosion products and other mineral precipitate deposits. If the local corrosion exposure conditions inside the crevice are more aggressive than the crevice corrosion initiation threshold, the CRM undergoes crevice corrosion and general corrosion; if they are less than the threshold, the CRM degrades by general corrosion only.

Because the evolution of the crevice solution chemistry and local exposure condition under dripping conditions is not well understood, and the current waste-package degradation model is not yet capable of adequately representing the crevice solution chemistry, an approximate—and necessarily conservative—approach is taken in the base case by using the information developed from the recent WPDEE. As described in detail in Section 5.8, the expert panel developed the local corrosion exposure condition scenarios in terms of pH, corrosion potential of the CRM, and

temperature, assuming the ionic concentration of the contacting solution is equivalent to saturated J-13 water. The panel also developed the probability of the conditions to occur. The CRM general corrosion rates used in the base case for dripping conditions were developed based on the local corrosion exposure condition scenarios, the probability of the occurrence of the local exposure conditions, and general corrosion rates corresponding to the different local exposure conditions. For CRM localized (pitting and crevice) corrosion, the experts provided an initiation probability that is conditional on the local exposure conditions and the probability to attain them. The base case model has adopted an approach based on the critical temperature threshold for localized corrosion initiation, which is simple to implement and also most conservative compared to other assessments. Thus, in the base case, localized corrosion for a CRM patch is assumed to initiate if the exposure temperature is greater than 80°C when the CAM patch is penetrated. The probability of localized corrosion initiation is set to one at T greater than or equal to 100°C and decreases linearly to zero at 80°C (uniform distribution). Once initiated, pits will continue to grow. If T less than 80°C when a CAM patch is penetrated, the CRM patch does not initiate localized corrosion and can be assumed immune to localized corrosion (general corrosion would still occur).

In the base case waste package degradation model, localized corrosion (pitting and crevice corrosion) in the inner barrier is assumed to initiate only under dripping conditions. This assumption is supported by the WPDEE (CRWMS M&O 1998b) and various experimental observations on the necessary presence of aggressive ions (such as chloride, etc.) in order to sustain pit growth (Fontana 1986, pp. 51-73; Lillard and Scully 1994; McCafferty et al. 1997; Sridhar and Dunn 1997). The only mechanism for these ions to gain ingress to the drift is through drips. The output of the waste package degradation model for waste packages not seeing drips is a time history of patch perforations (no inner barrier localized corrosion), and for waste packages that are dripped on are time histories for pit perforations and patch perforations.

5.5 ABSTRACTION FOR HUMID-AIR CORROSION MODELS FOR CAM

Carbon steel, the candidate corrosion allowance barrier material, undergoes active corrosion both in humid-air and aqueous environments. In the potential repository, it is expected that the waste container will be exposed to humid-air and aqueous conditions at elevated temperatures for extended periods of time. In this report, the term "humid-air corrosion" is used to refer to corrosion, which takes place under a thin film of water that forms on the container surface above a certain critical humidity threshold. Such a water film is not thick enough to behave as bulk water. The term "aqueous corrosion," which is the topic for the next section, is used to refer to corrosion of metal in contact with bulk water or under a thick water film that behaves as bulk water.

This section outlines the development and abstraction of the general and localized corrosion models of the candidate corrosion allowance barrier materials in humid-air and presents the results of these models.

5.5.1 Abstraction Approach

The humid-air corrosion data used in development of the current model were obtained from atmospheric corrosion tests in which the exposure conditions could fluctuate over short time

periods. The data are collected in the form of average corrosion depth considered over the entire sample surface versus total exposure time. The average corrosion depth is calculated from weight loss measurements of the samples. In such atmospheric exposure conditions, humid-air corrosion normally does not occur during the entire exposure time because for some fraction of the exposure time dry conditions exist, and a water film of sufficient thickness required to support corrosion reactions can not exist on the sample surface. Thus, it is necessary to estimate the fraction of the total exposure time during which humid-air corrosion is active. Experimental studies have revealed that the relative humidity must exceed about 70 percent before active humid-air corrosion will occur. Subsequently, generalized environmental relationships were derived that allow the average relative humidity and temperature during the total exposure time to determine (1) the fraction of the total exposure time during which humid-air corrosion was active and (2) the average exposure conditions (temperature and relative humidity) during that time fraction. The collected data points are then transformed using these relationships to determine the average temperature, relative humidity, and time relevant to the exposure conditions during that fraction of time when humid-air corrosion was actively occurring.

Functional dependencies of the humid-air corrosion rate on exposure parameters such as exposure temperature, relative humidity, time, and pollutant concentrations are obtained from the literature and combined into a humid-air corrosion model. Using the collected (atmospheric) humid-air corrosion data, the model parameters are evaluated through multiple linear regression techniques.

Because the local corrosion depth profile resulting from humid-air corrosion is observed to vary about the average general corrosion depth, a roughness factor is used to represent local variations from the calculated average general corrosion depth. The roughness factor is defined as the ratio of the local general corrosion depth to the average general corrosion depth considered over the entire sample surface. Literature data and guidance from expert elicitation are used to abstract a roughness factor model.

5.5.2 Humid-Air General Corrosion Data Compilation

A considerable amount of data for humid-air (atmospheric) general and pitting corrosion of commercial iron and steel has been accumulated by numerous testing programs over the past few decades in the U.S. and other countries. An average general corrosion depth at a given exposure time is determined from a weight loss measurement (after removing the corrosion products) on a test specimen. The pit (or local corrosion) depths are determined directly by measuring the depth of each pit with a device equipped with a microscope and a fine measuring needle. A literature survey was conducted to collect data for atmospheric general and pitting corrosion for a suite of cast iron and carbon steel that are known to exhibit corrosion behavior similar to the candidate carbon steel. The atmospheric corrosion data include the effects of pollutants such as sulfur dioxide (SO_2) and other chemicals in the atmosphere, which interact with test specimens. The data also embed any effects of salts that may form on the surface of the corroding specimen because of cyclic wetting and drying. Data from marine sites were excluded because marine environments are much more corrosive (due mostly to the presence of chloride salts in a marine atmosphere) than humid-air conditions expected in the potential repository. Future TSPA analyses may incorporate the effects of such corrosive environments for different conceptual

models of near-field water chemistry, such as those that may result from salt precipitation in a moisture refluxing condition at elevated temperatures.

Important testing parameters that were considered in the data compilation included test duration, average exposure temperature and relative humidity, and average sulfur dioxide content in the test atmosphere. From the general corrosion data collected, a total of 186 data points (see Table 5-2) were included in the model abstraction. The test environments included rural, urban, and industrial sites. The following is the list of the data sources used in the model development.

- Knotková, Holler, and Vlčková (1981)
- Knotková-Čermáková, Vlčková, and Honzák (1982)
- Tri, Huy, Cuong, and San (1993)
- Wei (1991)
- Southwell and Bultman (1982)
- Townsend and Zoccola (1982)
- Komp (1987)
- Haynie and Upham (1971).

The longest-term data were from the 16-year corrosion test program conducted by the Naval Research Laboratory in a tropical environment in Panama (Southwell et al. 1976; Southwell and Bultman 1982). The exposure conditions for the entire set of data range from 5 to 27°C average temperature, 63 to 84 percent average relative humidity, and an average SO_2 level of 2 to 406 μg SO_2/m^3.

There does exist limited short-term humid-air corrosion data from the project's corrosion testing and modeling programs. However, most of it is qualitative in nature and not suitable for long-term corrosion prediction (Gdowski 1998; McCright 1997).

5.5.3 Exposure Parameter

Atmospheric exposure conditions can fluctuate over periods as short as a day. Therefore, it was necessary to transform the corrosion data (time of exposure, corrosion rate, etc.) to reflect the fact that humid-air corrosion does not actively occur during the entire exposure time. Humid-air corrosion data manipulations such as this are common in the corrosion literature (Guttman and Sereda 1968; Knotková-Črmáková et al. 1982).

In the data transformation, three generalized relationships were needed to transform the exposure conditions and corrosion data: (1) a relationship to estimate the fraction of the exposure time during which corrosion was active, (2) a relationship to estimate the average relative humidity during that fraction of the time, and (3) a relationship to estimate the average temperature during that fraction of the time. In an effort to develop generalized relationships, hourly weather data for a 10-year period from 9 geographical areas were received from the Western Climatic Center in Reno, Nevada (Prowell 1994). The areas were selected to cover a wide range of weather conditions from hot and dry (Las Vegas, Nevada; Albuquerque, New Mexico; and Tucson, Arizona) to warm and humid (Honolulu, Hawaii and Arcata, California) to cold and humid (Great Falls, Montana; Denver, Colorado; Cheyenne, Wyoming; and Anchorage, Alaska). The

hourly weather data and regression calculations discussed below have been previously submitted in electronic format (MI: 30048-M04-001) in association with the WAPDEG software routine reports (CRWMS M&O 1998c).

5.5.3.1 Time Fraction for Relative Humidity Greater than 70 Percent

Numerous experimental results of iron specimens exposed to controlled humidity conditions have shown that at around 70 percent relative humidity their surfaces become covered with a thin water film and active corrosion initiates (Vernon 1933; Phipps and Rice 1979). Accordingly, 70 percent relative humidity was chosen as the threshold level at which active humid-air corrosion initiates. Using the weather data, a relationship for estimating the fraction of time during which relative humidity is greater than or equal to 70 percent (RH ≥ 70 percent) was developed as a function of the average relative humidity and average temperature considered over 720-hour (30-day) months. There were a total of 121 such months obtained from each of the nine cities considered. For each month's hourly weather data, the time fraction during which RH ≥ 70 percent was calculated and fit to a sigmoidal function of the monthly average relative humidity and temperature. The resulting functional form is expressed as

$$f_{70} = \frac{1}{1 + exp\left[0.92781 + \frac{28.01246(56.44258 - RH_{avg})}{(T_{avg} + 273.15)}\right]} \tag{5-1}$$

where f_{70} is the fraction of time during which RH ≥ 70 %, RH_{avg} is the monthly average relative humidity (%), and T_{avg} is the monthly average temperature (°C). The eighth column of Table 5-2 contains the values of f_{70} calculated from T_{avg} and RH_{avg} using Equation (5-1). Details of the calculations are described in CRWMS M&O (1998h, Appendix A). Estimates made with Equation (5-1) are compared to the weather data in Figure 5-6. The ninth column of Table 5-2 contains the new exposure times ($t_{new} = f_{70}\, t$, where t is the reported exposure time reported in the source literature) for each data point (CRWMS M&O 1998h, Appendix A). This is meant to represent the time fraction during which humid-air corrosion was actively occurring.

5.5.3.2 Reduction of Relative Humidity and Temperature

It was also necessary to estimate a new average relative humidity and new average temperature of each corrosion data point for that period of time during which RH ≥ 70 percent (i.e., corrosion was active). The weather data were used to develop relationships for estimating the new average relative humidity and new average temperature as follows: for each geographical location, the average monthly (30 day) relative humidity and temperature were calculated for the periods with RH ≥ 70 percent, and fit to a function of RH_{avg} and T_{avg}. The relationship developed for the new average relative humidity is:

$$RH_{new} = 83.24 - 0.1422\ RH_{avg} - 0.1054\ T_{avg} + 0.002377\ RH_{avg}^2 \tag{5-2}$$

where RH_{new} is the new average relative humidity (%). Similarly, the new average temperature was fit to the following equation:

$$T_{new} = -13.33 + 0.1512\ RH_{avg} + 1.017 T_{avg} \tag{5-3}$$

where T_{new} is the new average temperature (°C). The new average relative humidity and temperature are used in the humid-air corrosion model development as the average relative humidity and temperature during the period when corrosion was active. The new average relative humidity, temperature, and exposure time are assumed to be the representative exposure conditions for the formulation of the humid-air corrosion model. Detailed descriptions for the calculations for Equations (5-2) and (5-3) are given in CRWMS M&O (1998h, Appendix A).

5.5.4 Roughness Factor for Humid-Air Corrosion

The corrosion depth profile resulting from humid-air corrosion is not spatially uniform; rather it is observed to vary locally about some average general corrosion depth. These spatial variations in corrosion depth are usually represented through use of a roughness factor that is defined as the ratio of the local general corrosion depth to the average general corrosion depth (from weight loss measurement) considered over the entire sample surface. The results from the extensive corrosion testing programs in inland tropical environments in Panama (Southwell and Bultman 1982; Southwell et al. 1976) indicate that the roughness factor for carbon steels and cast irons exposed to "normal" atmospheric conditions (i.e., in the absence of highly aggressive conditions such as in acidic or concentrated salt conditions) decreases markedly with exposure time and ranged from about 2 to 6 after 16 years of exposure. Table 5-3 is derived from data presented in Southwell and Bultman (1982). These investigators reported not only the deepest pit measured on each sample but also the average depth of the 20 deepest pits observed after 16 years of exposure. It is reasonable to assume that the roughness factor will continue to decrease with longer exposure times (or with depth). Reduction of the maximum pit penetration rate (or deepest pit penetration rate) by more than a factor of 10 over a 100-year exposure period was reported for underground water mains (Wakelin and Gummow 1991). The maximum pitting rate reduction manifests as a roughness factor reduction with time (or depth). The recently completed WPDEE (CRWMS M&O 1998b) indicated that the regions of increased localized corrosion depth are generally hemispherical in shape and coalesce with time into a more uniform corrosion front with smaller local roughness perturbations. Three of the five experts recommended using the general corrosion rate only (i.e., a roughness factor of one). One expert, Peter Andresen, elicited that the roughness factor appropriate for long time periods should be normally distributed with a mean of 1.1 and a standard deviation of 0.1. The complete elicitation resulting from the WPDEE, not including the three expects who elicited a value of one, is shown in Figure 5-7. McCright based his assessment for the roughness factor on the 16-year data from the Panama Canal,, and noted that the factor would reduce with increasing general corrosion depth (or time).

5.5.5 Development of Humid-Air Corrosion Model

This section describes the development of the conceptual model for humid-air general corrosion of the CAM, the model fitting procedures, and the model fitting results. It will also discuss the conceptual model for the roughness factor and its abstraction including incorporation of information from the WPDEE (CRWMS M&O 1998b).

5.5.5.1 The Humid Air General Corrosion Model

The following dependencies of general corrosion on exposure conditions in humid-air are based on the current conceptual understanding of humid-air corrosion (Guttman and Sereda 1968; Haynie and Upham 1974; Knotková, et al. 1981; Tri, et al. 1993) and were incorporated into the model.

$$D_g \propto t^A \tag{5-4}$$

$$\frac{dD_g}{dt} \propto e^{\frac{B}{RH}} \tag{5-5}$$

$$\frac{dD_g}{dt} \propto e^{\frac{C}{T}} \tag{5-6}$$

$$\frac{dD_g}{dt} \propto e^{D[SO_2]} \tag{5-7}$$

where D_g is general corrosion depth (μm), dD_g/dt is general corrosion rate (μm/yr), t is exposure time (years), RH is relative humidity (%), T is temperature (K), and $[SO_2]$ is sulfur dioxide content in the testing atmosphere (μg/m^3). A, B, C, and D are constants. Although no significant SO_2-level is expected in the potential repository, SO_2-content has a significant effect on humid-air corrosion making it necessary to include SO_2-content in the model formulation.

By combining Equations (5-4) through (5-7), the humid-air general corrosion model can be expressed as follows:

$$\ln D_g = a_o + \frac{a_1}{T_{new}} + \frac{a_2}{RH_{new}} + a_3 \ln t_{new} + a_4 [SO_2] + \varepsilon \tag{5-8}$$

where a_o, a_1, a_2, a_3, and a_4 are constants determined from fitting Equation (5-8) to the collected corrosion data (Table 5-2). T_{new}, RH_{new}, and t_{new} used in Equation (5-8) are the adjusted (as described in Section 5.5.3) temperature, relative humidity, and exposure time reflecting the exposure conditions during the time periods in which humid-air corrosion actively occurs. ε is a term representing uncertainties not explained by the model and has a normal distribution with a

mean of zero. Linear regression gives the following estimates for the parameters in Equation (5-8): $a_o = 17.185$, $a_1 = -623.46$, $a_2 = -974.46$, and $a_3 = 0.62270$. Because there is not expected to be any sulfur dioxide in the repository, a_4 is not used in WAPDEG. The covariance matrix was determined to be:

$$V = \begin{bmatrix} 6.9934 & -231.79 & -523.80 & -2.4608 \cdot 10^{-2} \\ -231.79 & 104703 & -10892 & 2.5731 \\ -523.80 & -10892 & 47470 & 1.3009 \\ -2.4608 \cdot 10^{-2} & 2.5731 & 1.3009 & 6.9319 \cdot 10^{-4} \end{bmatrix} \tag{5-9}$$

and the variance of ε determined from the linear regression is *0.12757* (CRWMS M&O 1998h, p. 10). This covariance structure was used in WAPDEG to incorporate variability in the general corrosion rate between waste packages and across individual waste packages in humid-air environments: Carbon steel corrosion rate could be enhanced under frequent wet and dry cycle conditions (Stratmann 1990; Tsuru, Nishikata and Wang 1995). The above humid-air corrosion model, which is based on atmospheric corrosion data and may have embedded the effect of frequent wet and dry cycles, could represent higher corrosion rates in the exposure conditions without frequent wet and dry cycles.

The corrosion data used and the model estimate with its uncertainties (± 2 standard deviations) are shown in Figure 5-8. The input parameters (15°C, 84% RH, and 89 μg SO_2/m^3) for the estimate in the figure are the averages of the data set. The atmospheric pollution level of 70 μg SO_2/m^3 was chosen arbitrarily to differentiate corrosion behaviors in heavily polluted areas from that in relatively clean atmospheric environments.

The humid-air general corrosion model (and the aqueous general corrosion model discussed in Section 5.6.4.1) is applicable to constant exposure conditions. The "corrosion-time" concept was developed to use the model for time-dependent exposure conditions such as in the potential repository (Lee, Atkin, and Dunlap 1997) (see Section 5.10.2 for detailed discussions). Initiation of humid-air general corrosion was not modeled. For simplicity, it was conservatively assumed that humid-air corrosion would occur whenever the relative humidity was above some threshold value (RH_{thresh}). One option within WAPDEG requires that the temperature must also be below some threshold (T_{thresh}) for the CAM barrier general corrosion to occur.

5.5.5.2 The Humid-Air Roughness Factor Model

As discussed earlier, the roughness factor of the CAM decreases with the general corrosion depth. Three of the five experts of the WPDEE panel, who elicited the roughness factor recommended using of the general corrosion depth only (i.e., a roughness factor of one) for long-term corrosion of the 10-centimeter thick CAM (CRWMS M&O 1998b). However, the roughness factor is used in the TSPA-VA analysis to model conservatively the CAM corrosion degradation.

In localized corrosion models, pit initiation and pit growth rate are two major parameters that need to be quantified. However, these parameters are influenced by many local factors including material characteristics, exposure conditions, and aggressive species present. In addition, complex electrochemical processes associated with these factors also strongly influence pit initiation and pit growth processes. In general, localized corrosion of metal results from complicated interactions among many factors and appears to be random. As a result, stochastic approaches have been applied to represent and quantify localized corrosion processes.

Humid-air local variations of corrosion of CAMs are commonly represented by a roughness factor defined as the ratio of the local general corrosion depth to the average general corrosion depth considered over the entire sample surface at a given exposure time. Accordingly, the roughness factor has been used in developing a stochastic localized corrosion model for the corrosion allowance barrier in a humid-air condition.

The roughness factor concept discussed in Section 5.5.4 is introduced into WAPDEG in the following manner. It is assumed that there exists a "pit" density of 10 pits/cm^2 (Marsh and Taylor 1988; Marsh, Bland, and Taylor 1988; Marsh, Bland, and Sooi 1988) and associated with each pit is a roughness factor. The term "pit" is used in the CAM humid-air corrosion model to refer to a local spot where the roughness factor is applied, and it does not refer to a cylindrical, high-aspect ratio pit that is observed typically in CRMs. The roughness factor is constrained to be greater than or equal to 1 (i.e., the local general corrosion depth is never less than the average general corrosion depth). The roughness factor is different for each pit, but for a given pit it is assumed constant through time.

The roughness factor is sampled randomly and used as a multiplier to the general corrosion depth. For the base case, the distribution for the roughness factor that one expert suggested for long-term periods was used except that the mean and standard deviation were increased to be equivalent to those for the aqueous conditions; that is, normal distribution with a mean of 1.5 and a standard deviation of 0.25 (Section 5.6). This was to be conservative in modeling the local corrosion depths. In fact, the comparison of the roughness factors in humid-air conditions in Table 5-3 with those in aqueous conditions presented in Table 5-5 indicates that the roughness factor in these conditions are comparable at least for up to a 16-year exposure period. Thus, the localized corrosion model of the CAM in humid-air used in the base case is expressed as follows:

$$D_p = f_p D_g = \begin{cases} normal(1.5,\ 0.25)\, D_g & \text{if } normal(1.5,\ 0.25) \geq 1 \\ resampled & \text{if } normal(1.5,\ 0.25) < 1 \end{cases} \tag{5-10}$$

where D_p is the total penetration depth and f_p is the roughness factor. In the stochastic localized corrosion modeling, pit initiation was not explicitly considered. Instead, all the pits that can form on the CAM are conservatively assumed to start growing at the same time as when general corrosion initiates. Because of a large number of sampling sites for local corrosion depths, the above equation assures that some sites will always be substantially deeper than the average corrosion depth.

WAPDEG has the capability to use roughness factors that are uniformly, normally, loguniformly, or lognormally distributed as well as fixed values or values read from a cumulative distribution function supplied as an input file.

5.5.6 Humid-Air Corrosion Model Results

Model predictions of the general corrosion rate as a function of exposure time at different humidities (80, 90, and 95 percent relative humidity) are shown in Figures 5-9 and 5-10 for exposure temperatures of 60°C and 90°C, respectively. The figures show that the general corrosion rate decreases rapidly with the exposure time. The rate reduction is due primarily to corrosion products formed on the bare metal, which act as a barrier to the transport of reacting species.

The model predictions for the effects of relative humidity on the general corrosion rate for different exposure times are shown in Figure 5-11 for an exposure temperature of 75°C. The general corrosion rate of CAM is negligible at relative humidity values less than about 65 percent. The general corrosion rate starts to increase with humidity at about 70 percent relative humidity, and the rate of increase becomes greater with increasing relative humidity. However, the relative humidity effects on the general corrosion rate decrease with exposure time. The model predictions are consistent with the literature data discussed in Section 5.5.2.

Similar model predictions at different exposure temperatures showing the effects of relative humidity on the general corrosion rate are shown in Figure 5-12 for an exposure time of 1 year. The figure shows that relative humidity has a greater effect on general corrosion than temperature. This conclusion is lent further credence by Figure 5-13 in which the variation of the humid-air general corrosion rate with temperature at various exposure times is presented. The humid-air corrosion rate is shown to be relatively insensitive to temperature particularly at later exposure times. The corrosion behavior predicted with the current model is consistent with numerous observations from the literature (Duncan and Spedding 1973; Guttman 1968; Guttman and Sereda 1968; Haynie and Upham 1974; Kucera and Mattson 1974).

5.5.7 Inputs to and Outputs from the Model

The primary inputs to the humid-air CAM corrosion model are the roughness factor distribution and the temperature and relative humidity histories. In the TSPA-VA base case, the same roughness factor distribution is used for the humid-air and aqueous CAM corrosion models, a bounded normal distribution with a mean of 1.5, a standard deviation of 0.25, a lower bound of 1, and effectively no upper bound. This is the roughness factor distribution recommended for the aqueous CAM corrosion model and is a conservative choice for the humid-air CAM corrosion model (see Sections 5.5.4 and 5.5.5.2). The humid-air CAM corrosion model depends on the exposure conditions (temperature, relative humidity, and exposure time) through Equation (5-8). The covariance matrix shown in Equation (5-9) is hard-wired into the WAPDEG code. The user may specify the fraction of the total model variance is allocated to waste package-to-waste package variability with the remainder allocated among the patches (subregions of the waste package surface—see Section 5.4). It is possible to use only the mean values of the corrosion model parameters through use of flags supplied in the WAPDEG input file.

5.6 ABSTRACTION FOR AQUEOUS CORROSION MODELS FOR CAM

The aqueous corrosion rate of carbon steel is affected by the chemistry of the corrosive environment material characteristics and other exposure conditions. Corrosion rates of CAMs in water are strongly affected by temperature, exhibiting maximum corrosion rates at temperatures around 60 to 80°C. This behavior has been explained by temperature-induced variations in the dissolved oxygen reduction kinetics within solution (Boden 1994). High temperatures increase the mobility of dissolved oxygen molecules tending to increase the reaction rate; however, the oxygen solution solubility is decreased at higher temperatures, decreasing the reaction rate. The net mass transport of oxygen in solution increases with temperature until a maximum is reached where the oxygen concentration begins to decrease approaching the boiling point. Thus, the corrosion rate attains a maximum and then decreases with further increase in temperature.

This section outlines the development and abstraction of general and localized corrosion models of the candidate corrosion allowance barrier materials in aqueous environments and presents results of these models.

5.6.1 Abstraction Approach

The aqueous corrosion data are collected in the form of average corrosion depth (considered over the entire sample surface) versus total exposure time and temperature. The average corrosion depth is calculated from weight loss measurements of the samples. Functional dependencies of the aqueous corrosion rate on exposure parameters such as exposure temperature and time are obtained from the literature and combined into an aqueous corrosion model. Using the collected aqueous corrosion data, the model parameters are evaluated through multiple linear regression techniques. The data used to formulate the aqueous corrosion model were collected in a variety of environments (lake water, polluted rivers, and distilled water), and the data are considered to represent a reasonable range of exposure conditions and potential water chemistries, and the potential effects of microbial activity on the corrosion rate of carbon steels.

Because the local corrosion depth profile resulting from aqueous corrosion is observed to vary about the average general corrosion depth, a "roughness factor" is used to represent local variations from the calculated average general corrosion depth. The roughness factor is defined as the ratio of the local general corrosion depth to the average general corrosion depth considered over the entire sample surface. Literature data as well as guidance from expert elicitation is used to abstract a roughness factor model.

5.6.2 Aqueous General Corrosion Data Compilation

Aqueous corrosion data (Table 5-4 with 70 observations) was gathered from a number of sources. Long-term corrosion data (up to 16 years) in polluted river water (Coburn 1978) and in tropical lake water (Southwell and Alexander 1970) were used to estimate the time dependence of aqueous corrosion. These data were also used as a baseline because they include the potential effects of microbial activity and various chemical species dissolved in the waters. A set of short-term (100 days) corrosion data of mild steel in distilled water at temperatures from 5 to 90°C (Brasher and Mercer 1968; Mercer et al. 1968) was used to develop the temperature dependence of aqueous corrosion. This dependence was incorporated into the aqueous corrosion models, but

was scaled to be consistent with the lake and river water because distilled water provides a much less hostile environment. Important testing parameters that were considered in the data compilation included test duration, average exposure temperature, and type of exposure environment.

5.6.3 Roughness Factor for Aqueous Corrosion

As in humid-air corrosion of the CAM, discussed in Section 5.5, the corrosion depth profile resulting from aqueous corrosion is not spatially uniform, rather it is observed to vary locally about some average general corrosion depth. These spatial variations in corrosion depth are usually represented through use of a roughness factor that is defined as the ratio of the local general corrosion depth to the average general corrosion depth over the entire sample surface. Table 5-5 is derived from data presented in Southwell, Bultman and Alexander (1976). These investigators reported not only the deepest pit measured on each sample but also the average depth of the 20 deepest pits observed after 16 years of exposure. The reported roughness factors are similar to those presented in Table 5-3 for the case of humid-air corrosion. Literature observations (Marsh and Taylor 1988; Marsh et al. 1988; Strutt et al. 1985) indicate that the aqueous roughness factor is roughly normally distributed with a mean of 1.5. Although values greater than seven have been observed, a majority of the experts who participated in the WPDEE Project (CRWMS M&O 1998b) stated that such high roughness factors were possible only during the early stages of corrosive attack. With the passage of time (or increasing depth), the roughness factor decreases resulting in a more uniform corrosion front. The localized regions of enhanced corrosive attack were hemispherical and would coalesce into a more uniform corrosion front. Indeed, three of the five experts recommended using the general corrosion rate only (i.e., a roughness factor of 1). One expert, Andresen, elicited the aqueous roughness factor as normally distributed with a mean of 1.5 and a standard deviation of 0.25. Another expert, McCright, elicited a pit factor distribution varying between 2.5 and 13, a full order of magnitude above any other elicited value (CRWMS M&O 1997e). The composite graph of the roughness factor for aqueous corrosion provided in the WPDEE report, not including the elicitations from the three experts who felt the roughness factor should be equal to one, is shown in Figure 5-14. The high roughness factors elicited by Dr. McCright are based on observations of samples tested in sea water. He stated that the roughness factor would decrease with time (or increasing depth) (CRWMS M&O 1997e). Reduction of the maximum pit penetration rate (or deepest pit penetration rate) by more than a factor of 10 over a 100-year exposure period was reported for underground water mains made of different classes of irons and steels (Wakelin and Gummow 1991). The maximum pitting rate reduction manifests as a roughness factor reduction with time (or depth).

5.6.4 Development of Aqueous Corrosion Model

This section will describe the development of the conceptual model for aqueous general corrosion of the CAM, the model fitting procedures, and the model fitting results. It will also discuss the conceptual model for the roughness factor and its abstraction including incorporation of information from the WPDEE (CRWMS M&O 1998b).

5.6.4.1 The Aqueous General Corrosion Model

The following aqueous general corrosion dependencies on exposure conditions were obtained from the literature (Boden 1994; Protter and Mann 1962) and incorporated into the model development:

$$D_g \propto t^E \tag{5-11}$$

$$\frac{\partial D_g}{\partial t} \propto e^{\left(\frac{F_1}{T}+F_2T^2\right)} \tag{5-12}$$

where E, F_1, and F_2 are constants, and other symbols were defined for Equations (5-4) to (5-7). By combining Equations (5-11) and (5-12), the aqueous general corrosion model is expressed as follows:

$$ln D_g = b_0 + b_1 ln t + \frac{b_2}{T} + b_3 T^2 + \varepsilon \tag{5-13}$$

where b_o, b_1, b_2 and b_3 are constants to be determined by fitting Equation (5-13) to the aqueous general corrosion data. ε is a term representing uncertainties not accounted for in the model and has a normal distribution with a mean of zero. The estimates of the parameter values are: b_o = 111.53, b_1 = 0.53199, b_2 = -23291, and b_3 = -3.1918 × 10^{-4}. The covariance matrix for these estimates is:

$$V = \begin{bmatrix} 116.63 & -9.4226\cdot 10^{-4} & -24761 & -3.7926\cdot 10^{-4} \\ -9.4226\cdot 10^{-4} & 7.4149\cdot 10^{-4} & 1.7704\cdot 10^{-11} & 2.7491\cdot 10^{-19} \\ -24761 & 1.1689\cdot 10^{-11} & 5.2627\cdot 10^{6} & 8.0311\cdot 10^{-2} \\ -3.7926\cdot 10^{-4} & 1.8355\cdot 10^{-19} & 8.0311\cdot 10^{-2} & 1.2410\cdot 10^{-9} \end{bmatrix} \tag{5-14}$$

and the variance of ε determined from the linear regression is *0.0362* (CRWMS M&O 1998h, p. 11). This covariance structure was used in WAPDEG to incorporate variability between waste packages and across individual waste packages in the general corrosion rate in aqueous environments. One should note that this covariance matrix is not fully symmetric (the parameters in row 2 column 3 and row 3 column 2 are not equal; this is the same for the parameters in row 2 column 4 and row 4 column 2). The small magnitude of these parameters indicates that time and temperature terms are not strongly correlated, and the asymmetry is due to computational round-off effects. The aqueous general corrosion model is applicable to constant exposure conditions. The "corrosion-time" concept was developed to use the model for time-dependent exposure conditions such as in the potential repository (Lee, Atkin, and Dunlap 1997) (see Section 5.10.2 for detailed discussions).

5.6.4.2 The Aqueous Roughness Factor Model

As discussed earlier, the roughness factor of the CAM decreases with the general corrosion depth. Three of the five experts on the WPDEE panel, who elicited the roughness factor, recommended using of the general corrosion depth only (i.e., a roughness factor of one) for long-term corrosion of the 10-centimeter thick CAM (CRWMS M&O 1998b). However, the roughness factor is used in the TSPA-VA analysis to model conservatively the CAM corrosion degradation.

As in humid-air corrosion, aqueous localized corrosion is influenced by many factors including material characteristics, exposure conditions, and aggressive species present. Complex electrochemical processes associated with these factors strongly influence pit initiation and pit growth. As a result of the apparently random nature of pit initiation and propagation, stochastic approaches have been applied to represent and quantify pitting processes.

Aqueous localized corrosion of CAMs is commonly represented by a roughness factor defined as the ratio of the local general corrosion depth to the average general corrosion depth over the entire sample surface at a given exposure time. Accordingly, the roughness factor has been used here in developing a stochastic localized corrosion model for the corrosion allowance barrier in an aqueous condition.

The roughness factor concept discussed in Section 5.6.2 is introduced into WAPDEG in much the same way as for humid-air corrosion. It is assumed that there exists a "pit density" of 10 pits/cm^2 (Marsh and Taylor 1988; Marsh, Bland, and Taylor 1988; Marsh, Bland, and Sooi 1988) and that associated with each pit is a roughness factor. The term "pit" is used in the CAM humid-air corrosion model to refer to a local spot where the roughness factor is applied. It does not refer to a cylindrical, high-aspect ratio pit that is observed typically in CRMs. The roughness factor is constrained to be greater than or equal to 1, (i.e. the pit depth is never less than the general corrosion depth). The roughness factor is different for each pit, but for a given pit it is assumed constant through time.

The roughness factor is sampled randomly and used as a multiplier to the general corrosion depth. For the base case, the distribution for the roughness factor that one expert suggested for long-term periods (normal distribution with a mean of 1.5 and a standard deviation of 0.25) was used. Thus, the localized corrosion model of the CAM in aqueous condition used in the base case is expressed as follows:

$$D_p = f_p D_g = \begin{cases} normal(1.5, 0.25)\, D_g & \text{if } normal(1.5, 0.25) \geq 1 \\ resampled & \text{if } normal(1.5, 0.25) < 1 \end{cases} \tag{5-15}$$

where D_p is the total penetration depth and f_p is the roughness factor. In the stochastic pitting modeling, pit initiation was not explicitly considered. Instead, all the pits that can form on the CAM are conservatively assumed to start growing at the same time as when corrosion initiates. Because of a large number of sampling sites for local corrosion depths, the above equation assures that some sites will always be substantially deeper than the average corrosion depth.

WAPDEG has the capability to use aqueous roughness factors that are uniformly, normally, loguniformly, or lognormally distributed as well as fixed values or values read from a cumulative distribution function supplied as an input file.

5.6.5 Aqueous Corrosion Model Results

All of the graphs presented in this section do not make use of the roughness factor. Shown in Figure 5-15 are the long-term aqueous general corrosion data in lake water and (polluted) river water that were used for the model development and the model estimate with its uncertainty envelope of two standard deviations. The temperature-dependent general corrosion data of mild steel in distilled water are shown in Figure 5-16 along with the model estimate with its uncertainty envelope of two standard deviations. The aqueous general corrosion rate of CAM is shown to reach a maximum at approximately 60°C. The aqueous general corrosion rate as a function of temperature at various exposure times is shown in Figure 5-17. As in Figure 5-16, the corrosion rate increases with temperature until about 60°C, after which the general corrosion rate decreases. As was explained in the introduction, the kinetics of corrosion processes governed by the reduction of dissolved oxygen have a complex temperature dependence. The temperature dependence is affected by the diffusivity of oxygen molecules in solution, which increases with increasing temperature and thus increases corrosion reaction rates, and by the solubility of oxygen in the liquid phase, which decreases with increasing temperature and thus decreases corrosion reaction kinetics (Boden 1994).

Predictions of the aqueous general corrosion rate of CAM as a function of exposure time are shown in Figure 5-18 at four exposure temperatures (40, 60, 80 and 90°C). The calculations were made using the expected values of the model parameters. As shown in Figure 5-18, the general corrosion rates are about the same at 40 and 80°C, higher at 60°C, and lower at 90°C. The reasons for this temperature dependence have been discussed in relation to Figures 5-16 and 5-17. Predictions of the temperature dependence of general corrosion rates at various exposure times shown in Figure 5-17 indicate the temperature dependence decreases with increasing exposure time. This is due to the increased thickness of the corrosion products forming on the bare metal over time limiting oxygen access to the underlying uncorroded metal.

The current model estimate is compared in Figure 5-19 with the 0.5 and 1.0 year general corrosion data of A516 carbon steel obtained from the Long-Term Corrosion Testing Facility (LTCTF) at Lawrence Livermore National Laboratory, which were tested in 10× and 1000× simulated J-13 water (CRWMS M&O 1998d). The model estimate is seen to be more conservative than the LTCTF data. In the corrosion of carbon steel in distilled water, dissolved oxygen (O_{2aq}) and, to a lesser extent, hydrogen ions (H^+_{aq}) in the water may have been the major species that participated in the corrosion reduction reactions (Mercer et al. 1968). For corrosion in simulated concentrated J-13 water, oxygen solubility is decreased because of the presence of other dissolved species leading to reduced corrosion rates. In addition, the presence of nitrate ions, which is known to inhibit localized corrosion may also have contributed to the lower corrosion rates observed.

5.6.6 CAM Pit Growth Law Corrosion Model

The experts participating in the WPDEE (CRWMS M&O 1998b) stated that the pH of the water contacting the outer barrier surface was a dominant parameter in determining the corrosion mode and corrosion rate of the CAM. The experts endorsed the aqueous corrosion model discussed above for use when dripping water had a neutral pH (pH 4 to 10). However, water that passes through the degrading concrete drift-wall liner will likely surpass that pH. After the concrete liner fully degrades, the contacting water pH would return to neutral ambient levels. The experts concluded that in the case of high pH water drips, the expected corrosion mode of carbon steel would be high-aspect ratio pitting. Shoesmith elicited that unless the drips were frequent and persistent, pit stifling would occur, likely before penetration of the 10-cm CAM. McCright suggested that elevated chloride ion (Cl^-) concentrations were necessary to develop high-aspect-ratio pits under alkaline conditions, as would be the case if salts were deposited from evaporating drips.

In assessing the localized corrosion rate associated with high-aspect ratio pits, the experts recommended the use of a pit growth law having the following form:

$$D_{LC} = Bt^n \tag{5-16}$$

where D_{LC} is the localized corrosion depth (mm) at time t (years), n is the pit growth law time exponent and B is a rate constant (mm/yr^n). B and n are sampled from the aggregate distributions of the expert elicited cumulative distribution functions (CDFs) shown in Figures 5-20 and 5-21, respectively. One can see that the upper percentiles of the rate constant distribution correspond to values such that the 100-mm thick CAM is penetrated within a few years. Figure 5-22 shows the localized corrosion depth variation with time during the first one year of exposure. The dark solid line corresponds to the 100-mm CAM thickness. One can see that even with the optimistic choice of n = 0.3, sampling a corrosion rate constant corresponding to a high percentile results in almost instantaneous CAM failure. As discussed earlier, the corrosion data from the LTCTF, collected at a solution pH between 9.8 and 9.9, do not support the current pit growth law model from the WPDEE. The model is unrealistically conservative and needs to be reevaluated for its parameter values and applicability. It seems that the corrosion mode of carbon steel and the rate may be dependent not only on the pH of the contacting solution, but also concentrations of other ions present in the solution.

5.6.7 Inputs to and Outputs from the Model

The primary inputs to the aqueous CAM general corrosion model are the roughness factor distribution and the temperature and relative humidity histories. In the TSPA-VA base case, the same roughness factor distribution is used for the humid-air and aqueous CAM corrosion models—a bounded normal distribution with a mean of 1.5, a standard deviation of 0.25, a lower bound of 1, and effectively no upper bound. This is the roughness factor distribution recommended for aqueous CAM corrosion for long exposure time periods. The aqueous CAM corrosion model depends on the exposure conditions (temperature and exposure time) through Equation (5-13). The covariance matrix [Equation (5-14)] is hard-wired into the WAPDEG code. The user may specify the fraction of the total model variance is allocated to waste

package-to-waste package variability with the remainder allocated among the patches (subregions of the waste package surface). It is possible to use only the mean values of the corrosion model parameters through use of flags supplied in the WAPDEG input file.

The CAM Pit Growth Law corrosion model depends only on the exposure time and the values sampled for its parameters B and n.

5.7 ABSTRACTION FOR GENERAL CORROSION MODEL FOR CRM WITHOUT DRIPS

5.7.1 Abstraction Approach

General corrosion of the corrosion-resistant inner barrier was not included in previous PA waste package degradation modeling endeavors. However, the recently conducted WPDEE (CRWMS M&O 1998b) has indicated that CRM general corrosion could be a dominant long-term waste package degradation mode in the potential repository. As was discussed in Section 5.4 in the current conceptual model for waste package degradation, the waste package surface is divided into patches, and waste package corrosion is modeled for the individual patches (see Figure 5-4). It is assumed that as soon as a patch of the outer barrier is penetrated, moist conditions exist at the interface under that patch, and the inner barrier patch surface is subject to corrosion. This assumption is based on observations of the occurrence of capillary condensation of moisture by gel-like porous corrosion products of the outer barrier (Vernon 1933) that cover the inner barrier surface and the hygroscopic nature of corrosion products (Fyfe 1994), which would provide moist conditions at the surface of the inner barrier. The assumption is also based on a potential for crevice formation between the outer and inner barriers, in which moisture could condense and an aqueous condition could exist. Thus, in the current model, once it is exposed from the outer barrier penetration, the inner barrier surface under the outer barrier patch that was penetrated is assumed to undergo general corrosion in humid-air conditions. As there is no localized corrosion in the absence of drips, the failure mode of the CRM inner barrier is solely through thinning of the container wall through general corrosion. This results in the failure of entire patches (310 cm^2 in area for the base case simulations) of the inner barrier. As will be discussed in detail in Sections 5.8 and 5.9, if an inner barrier patch is dripped on, it undergoes localized corrosion (pitting and crevice corrosion) in addition to general corrosion.

The general corrosion (or passive dissolution) rate of highly corrosion resistant materials such as Alloy 22 in humid-air exposure conditions (i.e., without dripping on waste package) is extremely low, and no long-term data for Alloy 22 general corrosion rates in prototypic conditions are available. Because waste package performance analysis in the repository deals with tens (or hundreds for some cases) of thousands of years for the repository lifetime, assessment of such low corrosion rates are needed to assess long-term waste package degradation. Consequently, as part of the recently conducted WPDEE, experts were elicited to provide assessments for the general corrosion rate, including uncertainty, of Alloy 22 in humid-air exposure conditions. The WPDEE has provided assessments of general corrosion rates in the form of distributions for the alloy at three different temperatures (25, 50, and 100°C). For each exposure temperature, an aggregate distribution for the Alloy 22 general corrosion rate was developed by combining the individual expert's assessments. The variability and uncertainty portions of the total variance of the aggregate distributions were then separated using a technique referred to as Gaussian

Variance Partitioning. CDFs representing the variability and uncertainty of the general corrosion rate at the three temperatures were used in the waste package degradation model (WAPDEG). More details of the abstraction processes are described in the following sections.

Because of the time constraints imposed on the TSPA-VA analysis, interim expert assessment results were provided for the VA analysis (Pendleton 1998). Therefore, the experts' assessments used in the current model abstraction are not identical to those in the final WPDEE report (CRWMS M&O 1998b). However, the differences are small and the analysis results are not affected.

5.7.2 No-Drip CRM General Corrosion Model Development

This section describes the abstraction process of the CRM general corrosion model in the absence of dripping from the WPDEE results, in particular (1) development of aggregate distributions from individual expert's assessments, (2) allocation of the variability and uncertainty variances, and (3) development of partitioned CDFs for use in the waste package degradation model.

5.7.2.1 General Corrosion Rates from the WPDEE

As indicated previously, in the recently conducted WPDEE, general corrosion rates of Alloy 22 in humid-air exposure conditions (without drips) were elicited at three different temperatures (i.e., 25, 50, and 100°C). Details of the elicitation process are presented in the WPDEE report (CRWMS M&O 1998b). The CDFs of the individual expert assessments and the aggregate assessment are shown in Figures 5-23 through 5-25 at 100, 50, and 25°C, respectively. Mechanical (or analytical) aggregation (Kotra et al. 1996) giving equal weight to each expert's assessment, was used in obtaining the aggregate CRM general corrosion rate distributions. The aggregate probability was obtained by averaging the probabilities provided by the experts at each value of the CRM general corrosion rate. The method of mechanical aggregation is discussed further in several reports and publications (Hora and Iman 1989; Kotra et al. 1996). Details specific to this application of mechanical aggregation of the CRM general corrosion rate have been presented elsewhere (CRWMS M&O 1998f). As can be seen in Figures 5-23 through 5-25, the expert elicitations span four to five orders of magnitude, and thus, so do the aggregate general corrosion rate distributions.

The no-drip CRM general corrosion model makes direct use of up to three CDF inputs each associated with an exposure temperature at which they are to be applied. Semi-logarithmic interpolation (extrapolation, where necessary) is used to determine CRM general corrosion rates at temperatures differing from those at which input CDFs have been supplied. As the CRM general corrosion rate, R, is directly sampled, the CRM general corrosion depth is determined from the simple equation:

$$D = Rt \tag{5-17}$$

For the 100°C assessments (Figure 5-23), the 50th percentile rate of the aggregate distribution is about 3.4×10^{-6} mm/yr (0.0034 μm/yr), the upper end of the distribution is 2.0×10^{-4} mm/yr, and

the lower end of the distribution goes to 2.0×10^{-8} mm/yr (2.0×10^{-5} μm/yr). The lower end distribution value would be regarded as no corrosion. For the 50°C general corrosion rate, shown in Figure 5-24, the corresponding values (50th percentile rate, upper end of the distribution rate, and lower end of the distribution rate) are about 8.9×10^{-7} mm/yr, 5.0×10^{-5} mm/yr, and 2.4×10^{-9} mm/yr, respectively. Those values for 25°C, shown in Figure 5-25, are respectively 6.0×10^{-7} mm/yr, 3×10^{-5} mm/yr, and 5.6×10^{-10} mm/yr.

5.7.2.2 Allocation of Variability and Uncertainty - Gaussian Variance Partitioning

As discussed earlier, the experts participating in the WPDEE agreed that the variance (spread in general corrosion rate values) in their assessments included both uncertainty and variability. In order to assess waste package failure distribution over time in the repository, it was desired to use only the fraction of the total variance because of variability in the waste package degradation simulations. A methodology (referred to as Gaussian Variance Partitioning) was applied to separate the contributions of uncertainty from their elicited distributions.

To understand Gaussian Variance Partitioning, assume a model in which a random variable (i.e., a model parameter), Y, is normally distributed,

$$Y \sim N(\mu, \sigma^2) \tag{5-18}$$

where $N(\mu, \sigma^2)$ represents a normal distribution with parameters given by the mean, μ and variance, σ^2. The tilde is read as "is distributed as." The variation in the model parameter value is considered to be due to both uncertainty and variability. Assuming independence of uncertainty and variability, the total variance can be represented as the sum of two variances.

$$Y \sim N(\mu, \sigma_u^2 + \sigma_v^2) \tag{5-19}$$

Thus Y is a random variable, normally distributed around a mean, μ, with a total variance given by the sum of the variances due to uncertainty, σ_u^2, and variability, σ_v^2. If uncertainty is defined as uncertainty in the mean value and variability as the variance about that mean, then Y may be alternatively parameterized as

$$Y \sim N(m, \sigma_v^2), \text{ where } m \sim N(\mu, \sigma_u^2) \tag{5-20}$$

The uncertain mean is represented by the random variable, m, which is normally distributed with mean, μ, and variance, σ_u^2. The random variable, Y, is then the convolution of the distributions of the random variable given by m and a random variable, v (corresponding to a mean zero variability distribution), that is normally distributed with mean zero and variance, σ_v^2. This convolution of distributions is also represented by the addition of two normal random variables.

$$Y = m + v, \quad \text{where } m \sim N(\mu, \sigma_u^2) \text{ and } v \sim N(0, \sigma_v^2) \tag{5-21}$$

Thus, given the distributions for m and v, to realize a variability distribution, a value (m) is sampled from the parameter uncertainty distribution and added to the mean zero variability distribution.

Given a normal distribution with a total variance, σ^2, due to both uncertainty and variability and a fraction of the total variance due to either uncertainty or variability (assuming independence) there exists a unique solution for σ_u^2 and σ_v^2.

This partitioning method may be extended to nonnormal parameter distributions by means of a normal score transform (Deutsch and Journel 1992, p. 138) mapping the percentiles (cumulative probability values) of the nonnormal parameter CDF to those of the standard normal by a lookup table. The normal score transform works best if the nonnormal CDF is as symmetric as possible (like the normal distribution). Thus, steps should be taken to symmetrize the nonnormal distribution. For example, symmetrization could be accomplished by taking natural logarithms of the parameter values (as was done to the expert elicited CRM general corrosion CDFs). To accomplish uncertainty/variability partitioning of nonnormal parameter distributions (such as the expert elicited CRM general corrosion CDFs), one should:

- Symmetrize the input non-normal distribution as much as possible
- Perform the normal score transformation
- Partition the total variance (using Equation (5-21)) between uncertainty and variability
- Perform the normal score transformation in reverse to obtain non-normal distributions for uncertainty and variability which can be used in simulation endeavors.

As mentioned before, the average uncertainty/variability partition ratio elicited by the experts participating in the WPDEE was 75%/25% uncertainty/variability. While this partition ratio was accepted as the expected value the allocation of the total variance between uncertainty and variability was also an uncertain process, and thus, partition ratios of 25%/75% and 50%/50% were also investigated.

5.7.2.3 Development of Partitioned CDFs

Following the procedures outlined in the previous section, the aggregate CRM general corrosion rate distributions shown in Figures 5-23 through 5-25 were partitioned with uncertainty/ variability ratios of 75%/25%, 50%/50%, and 25%/75%. The resulting uncertainty distributions were sampled at the 5th, 50th, and 95th percentiles to obtain the median values (not mean values as the distributions are nonnormal), m in Equation (5-21), and used for the resulting variability distributions. Thus, a total of 27 CRM general corrosion rate CDFs with no drips were generated ([3 different temperatures] × [3 uncertainty/variability partitioning ratios] × [3 samples of uncertainty percentiles]). The number of uncertainty/variability partitioning ratios and samples of uncertainty quantiles was limited to three each to allow for preparation and execution of waste package degradation simulations in the time allotted and still reasonably sample the range over which these parameters vary.

5.7.3 Analysis of Model Behavior

Figure 5-26 shows the no drip CRM general corrosion rate variability CDFs at 25, 50, and 100°C, generated using the expected value 75%/25% uncertainty/variability partition ratio and the 50th percentile of the uncertainty distribution. The variances (span in values) of the variability CDFs are not as great as those of the aggregate (uncertainty+variability) distributions (shown in Figures 5-23 through 5-25). This is expected as the fraction of the variance because of uncertainty has been removed. However, the Gaussian Variance Partitioning technique results in distributions that span the same range of values as the input distributions, but decreases the probabilities associated with the tails (upper and lower ranges) of the output distributions.

Figure 5-27 shows no drip CRM general corrosion rate variability CDFs at 100°C generated using the 25%/75%, 50%/50%, and 75%/25% uncertainty/variability partition ratios and the 50th uncertainty percentile. These three CDFs and the aggregate (uncertainty+variability) CDF (Figure 5-23) share the same median (0.5 cumulative probability) value. As the fraction of the total variance allocated to variability decreases, so does the variance of the variability CDF.

Figure 5-28 shows the no drip CRM general corrosion rate variability CDFs at 100°C generated using the expected value 75%/25% uncertainty/variability partition ratio and the 5th, 50th, and 95th uncertainty percentiles. The uncertainty percentile (median variability CRM general corrosion rate) used has a large effect on the magnitude of the CRM general corrosion rates used in a waste package degradation simulation.

Figure 5-29 shows the Alloy 22 CRM general corrosion depth variation with time at 100°C in the absence of dripping using the expected value 75%/25% uncertainty/variability partition ratio, the 50th uncertainty percentile, and the 0th, 50th, and 100th variability percentile corrosion rates. The bold black line on the graph indicates a depth of 20 mm (the thickness of the CRM). The figure shows that even at 100°C and using the 100th variability percentile corrosion rate, about 100,000 years of exposure is necessary to fail the 20-mm-thick CRM. Thus, one should expect very few failures of the CRM from general corrosion processes in the absence of dripping.

5.7.4 Inputs to and Outputs from the Model

The primary inputs to this model are the expert elicited CRM general corrosion rate CDFs from the WPDEE. During a waste package simulation, the model requires the exposure temperature, exposure time, and percentile of the corrosion rate CDF to determine the CRM general corrosion rate for no-drip conditions. If the exposure temperature is equal to a temperature in which one of the user-supplied CRM general corrosion rate CDFs is applicable, then the corrosion rate corresponding to the input CDF percentile is used. If the exposure temperature lies between two temperatures in which corrosion rate CDFs have been supplied, then the corrosion rate corresponding to the input CDF percentile is determined for each of the bounding CDFs. The corrosion rate applicable to the input exposure temperature is determined through linear interpolation between the natural logs of the bounding corrosion rates (i.e., semi-log interpolation) relative to the exposure temperature. Similarly, if the exposure temperature lies below the smallest temperature (or above the highest temperature) in which a CDF has been supplied, semi-log extrapolation on the two CDFs applicable at the two temperatures nearest the exposure temperature would be carried out. Using the CRM general corrosion rate thus obtained

and the exposure time, simple application of Equation (5-17) yields the CRM general corrosion depth.

5.8 ABSTRACTION FOR GENERAL CORROSION MODEL FOR CRM WITH DRIPS

5.8.1 Abstraction Approach

Waste packages subjected to dripping can fail in one of two ways: either by localized corrosion processes that typically lead to small pit penetrations, or by thinning of the CRM container wall through a process of general corrosion that results in the failure of entire patches (310 cm^2 in area for the base case simulations) of the inner barrier. Previous performance assessment waste package degradation modeling did not consider general corrosion of the corrosion-resistant inner barrier. However, the recently conducted WPDEE (CRWMS M&O 1998b) indicated that CRM general corrosion could be a dominant long-term waste package degradation mode in the potential repository. As was discussed in Section 5.4, in the current conceptual model for waste package degradation, the waste package surface is divided into patches, and waste package corrosion is modeled on the individual patches (see Figure 5-4). It is assumed that as soon as a patch of the outer barrier is penetrated under dripping conditions, aqueous conditions exist at the interface under that patch, and the inner barrier patch surface is subject to corrosion. This assumption is based on observations of the occurrence of capillary condensation of moisture by gel-like porous corrosion products of the outer barrier (Vernon 1933) the inner barrier and the hygroscopic nature of corrosion products and other mineral precipitates (Fyfe 1994; Haynie et al. 1978), which would provide an aqueous corrosion condition at the surface of the inner barrier. The assumption is also based on a potential for crevice formation between the outer and inner barriers, in which moisture could condense and an aqueous condition could exist. Thus, in the current model, once it is exposed from the outer barrier penetration under drips, the inner barrier surface under the outer barrier patch that was penetrated is assumed to undergo general corrosion in aqueous conditions, in which the general corrosion rate is determined by the exposure temperature and local corrosion environment on the inner barrier as discussed in detail in the following sections. As will be discussed in detail in Section 5.9, if an inner barrier patch is dripped on, it may undergo localized corrosion (pitting and crevice corrosion) in addition to general corrosion.

Because general corrosion (or passive dissolution) rate of Alloy 22 is extremely low, measurement of the corrosion rate in repository-relevant conditions with confidence normally takes long testing periods. Currently, limited data for general corrosion of the alloy, from relatively short exposure times (up to one year), are available from the project's long-term corrosion testing facility (Pasupathi 1997 and 1998a; Pendleton 1988; CRWMS M&O 1998d) and from a short-term electrochemical polarization measurements (Stahl 1997). However, because of the potentially significant uncertainties associated with the corrosion rate measurements during the early testing periods, these short-term data are not sufficient for use in a long-term waste package degradation assessment of the repository, which deals with tens (or hundreds in some cases) of thousands of years of the repository lifetime. Consequently, as part of the recently conducted WPDEE, experts were elicited to provide assessments for the general corrosion rate, including uncertainty, of Alloy 22 in dripping conditions. The WPDEE has provided assessments of different local corrosion environment scenarios on the CRM and their

probability to attain the conditions and general corrosion rates in a form of distribution for each of the local corrosion environment at three different exposure temperatures (25, 50, and 100°C). For each local corrosion environment and at each exposure temperature, an aggregate distribution for the Alloy 22 general corrosion rate was developed by combining individual expert's assessments; then, for each exposure temperature, a "composite" distribution was developed by averaging the aggregate distributions for the different local corrosion environments over their probability of occurrence. The variability and uncertainty portions of the total variance of the composite distributions were then separated using a technique referred to as Gaussian Variance Partitioning. CDFs representing the variability and uncertainty variances of the general corrosion rate at the three exposure temperatures were used in the waste package degradation model (WAPDEG). More details of the abstraction processes are described in the following sections.

Because of the time constraints imposed on the TSPA-VA analysis, interim expert assessment results were provided for the VA analysis (Pendleton 1998). Therefore, the experts' assessments used in the current model abstraction are not identical to those in the final WPDEE report (CRWMS M&O 1998b). However, the differences are small, and the analysis results are not affected. As additional data are collected from the project's corrosion testing and modeling programs, the elicited assessments will be revised and/or replaced with the data.

5.8.2 Dripping CRM General Corrosion Model Development

This section describes the abstraction process of the CRM general corrosion model in the presence of dripping from the WPDEE results: in particular, (1) development of aggregate distributions for the general corrosion rate from individual expert assessments, (2) development of composite distributions from the aggregate distributions, (3) allocation of the variability and uncertainty variances, and (4) development of partitioned CDFs for use in the WAPDEG.

5.8.2.1 General Corrosion Rates from the WPDEE

As indicated previously, in the recently conducted WPDEE, general corrosion rates of Alloy 22 in the presence of dripping were elicited at three different temperatures, (i.e., 25, 50, and 100°C). Details of the elicitation process are presented in the WPDEE report (CRWMS M&O 1998b). Because the presence of drips on the waste packages could lead to a wide range of local corrosion environments on the CRM, the experts agreed that defining local corrosion environment scenarios on the CRM and their likelihood of occurrence is very important to the development of a reasonably consistent set of elicitations. As a result, the experts developed three different local corrosion environment scenarios on the CRM, as discussed below. Potential crevice formation between the outer and inner barriers at the CAM patch failure sites were considered in developing the local corrosion environment scenarios. The experts were asked to elicit CRM general corrosion rate distributions in three different local corrosion environments:

- pH in the range of 3 to 10 in an oxidizing condition that is equivalent to an electrochemical potential (driving force for corrosion) of 340 mV relative to the Standard Hydrogen Electrode (SHE)

- pH = 2.5 at 340 mV SHE

- pH = 2.5 at 640 mV SHE.

and at three exposure temperatures (25, 50, and 100°C). Detailed discussion of the effects of the electrochemical potential on metal corrosion can be found in Uhlig (1971, pp. 21-22). The CDFs of the individual expert assessments and the aggregate assessment at 100°C are shown in Figures 5-30 through 5-32. The CDFs for the other two temperatures are not shown here. As in the case of no dripping, mechanical (or analytical) aggregation (Kotra et al. 1996), giving equal weight to each expert's assessment, was used in obtaining the aggregate CRM general corrosion rate distributions. The aggregate probability was obtained by averaging the probabilities provided by the experts at each value of the CRM general corrosion rate. Details specific to this application of mechanical aggregation of the CRM general corrosion rate have been presented elsewhere (CRWMS M&O 1998g). As can be seen in Figures 5-30 through 5-32, the expert elicitations span three to five orders of magnitude, and thus, so do the aggregate general corrosion rate distributions.

The experts participating in the WPDEE were also asked to provide their assessment of the probability of occurrence of each local corrosion environment. These assessments are summarized in Table 5-6. Also in the table, the overall average occurrence probability for each local corrosion environment is presented (84 percent pH = 3 to 10 at 340 mV SHE, 13 percent pH = 2.5 at 340 mV SHE, and 3 percent pH = 2.5 at 640 mV SHE). At each exposure temperature (25, 50, and 100°C), the aggregate CRM general corrosion rate distributions (one for each of the three local corrosion environments) were mechanically aggregated, using the local corrosion environment occurrence probabilities as weighting factors, to produce the composite CRM general corrosion rate distribution applicable at each exposure temperature. The results of this second weighted mechanical aggregation are shown in Figures 5-33 through 5-35 for exposure temperatures of 100, 50, and 25°C, respectively. As the composite CRM general corrosion rate distribution is weighted 84 percent to the pH = 3 to 10 at 340 mV SHE local corrosion environment, its shape and magnitude closely mirrors the CRM general corrosion rate distribution of the pH = 3 to 10 at 340 mV SHE local corrosion environment. As discussed in Section 5.11.1, in the waste package degradation model the above composite corrosion rate distribution, which has incorporated the effect of the local corrosion exposure conditions, was applied to the entire simulation period for the waste packages that are under dripping conditions. This is conservative because, as the repository cools down slowly below boiling point and the near-field condition in the emplacement drifts returns to high humidity conditions, the salt solutions on the waste packages, which would be derived from the salt deposits formed during the earlier hot and dry periods, could be washed away under sustained dripping conditions. Subsequently, this could lead to potentially less corrosive local exposure conditions on the CRM with time. This conservative approach was taken in the TSPA-VA analysis because of a lack of information on the evolution of the local chemistry on the waste package.

For the 100°C assessments (Figure 5-33), the 50th percentile rate of the composite distribution is about 4.0×10^{-5} mm/yr (0.04 μm/yr), the upper end of the distribution is 2.0×10^{-2} mm/yr, and the lower end of the distribution goes to 1.0×10^{-7} mm/yr (1.0×10^{-4} μm/yr). The lower end distribution value would be regarded as no corrosion. For the 50°C composite general corrosion rate distribution, shown in Figure 5-34, the corresponding values (50th percentile rate, upper end of the distribution rate, and lower end of the distribution rate) are about 9.7×10^{-6} mm/yr, 1.2 ×

10^{-2} mm/yr and 1.0×10^{-7} mm/yr, respectively. Those values for 25°C, shown in Figure 5-35, are respectively 3.5×10^{-6} mm/yr, 9×10^{-3} mm/yr and 2.0×10^{-8} mm/yr.

Figure 5-36 shows the 0th, 50th, and 100th CRM corrosion rate percentiles of the WPDEE composite distributions plotted versus exposure temperature. Overlaid on the plot are Alloy 22 corrosion rate data points from the project's LTCTF six-month (Pasupathi 1997) and one-year (Pendleton 1998) data sets and short-term electrochemical polarization measurement data (Stahl 1997) as well as from literature sources (Haynes 1997b; Agarwal et al. 1993). Figure 5-36 indicates that the LTCTF data sets display corrosion rates about one order of magnitude higher than the median of the WPDEE results (but still well within the over five orders of magnitude encompassed by the WPDEE results). The LTCTF data sets are from samples exposed to Simulated Acidified Water (SAW) at a pH of 2.7, which would be considered as corresponding to the acidic exposure conditions that the expert panel proposed. The Haynes data were collected in 10 weight percent $FeCl_3$ solutions reported to have a pH of 0.7 (Pendleton 1998) and high concentrations of Fe^{3+} (strong oxidizer) and Cl^- (destabilizes passive films) ions. The data sets presented in Pasupathi (1997) and Agarwal, Heubner, and Herda (1993) were collected under similarly harsh chemical conditions. Thus, Figure 5-36 indicates that the WPDEE CRM general corrosion rates are consistent with Alloy 22 samples subjected to harsh exposure conditions (pH < 3, high Fe^{3+} and Cl^- concentrations) even though all but one expert elicited a less than 6 percent probability (Table 5-6) of any local corrosion environment other than moderately acidic (pH 3 to 10) and moderately oxidizing (340 mV SHE). In this respect, the WPDEE results (especially the right-hand tails of the CDF distributions) are considered conservative. That conservative assessment, although represented with a low probability, is a direct outcome of a poor characterization of local corrosion environments on the CRM. If the local corrosion environments on the CRM were better defined, the right-hand tails of the distributions that correspond to highly oxidizing conditions may have been eliminated. Another reason for the experts' conservatism may be the limited availability of experimental data for the relatively new alloy in such harsh exposure conditions. The large uncertainty embedded in the assessments and the accompanying conservatism will be reduced with an improved characterization of the local exposure environment and a better understanding of the alloy behavior.

The dripping CRM general corrosion model makes direct use of up to three CDF inputs each associated with an exposure temperature at which they are to be applied. Semi-logarithmic interpolation (extrapolation, where necessary) is used to determine CRM general corrosion rates at temperatures differing from those in which input CDFs have been supplied. As the CRM general corrosion rate, R, is directly sampled, the CRM general corrosion depth is determined from the simple equation:

$$D = Rt \tag{5-22}$$

5.8.2.2 Allocation of Variability and Uncertainty

As discussed earlier, the experts participating in the WPDEE agreed that the variance (spread in general corrosion rate values) in their assessments included both uncertainty and variability. In order to assess the waste package failure distribution over time and space in the repository, only the fraction of the total variance due to variability in the waste package degradation simulations

was used. The Gaussian Variance Partitioning methodology (see Section 5.7.2) was again applied to separate the contributions of uncertainty from their elicited distributions.

As mentioned before, the average uncertainty/variability partition ratio elicited by the experts participating in the WPDEE was 50%/50% uncertainty/variability. While this partition ratio was accepted as the expected value, it was felt that allocation of the total variance between uncertainty and variability was also an uncertain process, and thus, partition ratios of 25%/75% and 75%/25% were also investigated.

5.8.2.3 Development of Partitioned CDFs

The composite CRM general corrosion rate distributions shown in Figures 5-33 through 5-35 were partitioned with uncertainty/variability ratios of 75%/25%, 50%/50%, and 25%/75%. The resulting uncertainty distributions were sampled at the 5th, 50th, and 95th percentiles to obtain the median values, m in Equation (5-21), to be used for the resulting variability distributions. Thus, a total of 27 CRM general corrosion rate CDFs for dripping conditions were generated [(3 different temperatures) × (3 uncertainty/variability partitioning ratios) × (3 samples of uncertainty quantiles)]. The number of uncertainty/variability partitioning ratios and samples of uncertainty percentiles was limited to three each to allow for preparation and execution of waste package degradation simulations in the time allotted and still reasonably sample the range over which these parameters vary.

5.8.3 Analysis of Model Behavior

Figure 5-37 shows the dripping CRM general corrosion rate variability CDFs at 25, 50, and 100°C, generated using the expected value 50%/50% uncertainty/variability partition ratio and the 50th percentile of the uncertainty distribution. The variances of the variability CDFs are not as great as those of the composite (uncertainty+variability) distributions (shown in Figures 5-33 through 5-35) from which they were derived. This is expected as the fraction of variance due to uncertainty has been removed. However, one should realize that the Gaussian Variance Partitioning technique results in distributions that span the same range of values as the input distributions, but decreases the probabilities associated with the tails (upper and lower ranges) of the output distributions.

Figure 5-38 shows the dripping CRM general corrosion rate variability CDFs at 100°C generated using the 25%/75%, 50%/50%, and 75%/25% uncertainty/variability partition ratios and the 50th uncertainty percentile. These three CDFs as well as the composite (uncertainty+variability) CDF (Figure 5-33) share the same median (0.5 cumulative probability) value. As the fraction of the total variance allocated to variability decreases, so does the variance of the variability CDF.

Figure 5-39 shows the dripping CRM general corrosion rate variability CDFs at 100°C generated using the expected value 50%/50% uncertainty/variability partition ratio and the 5th, 50th, and 95th uncertainty percentiles. One can see that the uncertainty percentile (median variability CRM general corrosion rate) used has a large effect on the magnitude of the CRM general corrosion rates used in a waste package degradation simulation.

Figures 5-40 and 5-41 show the Alloy 22 CRM general corrosion depth variation with time at 100°C in the presence of dripping by using the expected value 50%/50% uncertainty/variability partition ratio, the 50th uncertainty percentile, and the 0th, 50th, and 100th variability percentile corrosion rates. The bold black line on the graph indicates a depth of 20-mm (the thickness of the CRM). Figure 5-41 shows that at 100°C and using the 50th variability percentile corrosion rate, about 500,000 years of exposure is necessary to fail the 20 mm thick CRM. However, as shown in Figure 5-40, using the 100th variability percentile, the failure time decreases to about 1,000 years. Thus, if exposed continuously at 100°C, one should expect a fair number of failures from general corrosion processes in the presence of dripping.

5.8.4 Inputs to and Outputs from the Model

The primary inputs to this model are the expert elicited CRM general corrosion CDFs from the WPDEE. During a waste package simulation, the model requires the exposure temperature, exposure time, and variability percentile to determine the CRM general corrosion rate. If the exposure temperature is equal to a temperature at which one of the user-supplied CRM general corrosion rate CDFs is applicable, then the corrosion rate corresponding to the input variability percentile is used. If the exposure temperature lies between two temperatures in which corrosion rate CDFs have been supplied, then the corrosion rate corresponding to the input variability percentile is determined for each of the bounding CDFs, and the corrosion rate applicable to the input exposure temperature is determined through linear interpolation between the natural logs of the bounding corrosion rates (i.e., semi-log interpolation) relative to the exposure temperature. Similarly, if the exposure temperature lies below the smallest temperature (or above the highest temperature) in which a CDF has been supplied, semi-log extrapolation on the two CDFs applicable at the two temperatures nearest the exposure temperature would be carried out. Using the CRM general corrosion rate thus obtained and the exposure time, simple application of Equation (5-22) yields the CRM general corrosion depth.

5.9 ABSTRACTION FOR LOCALIZED CORROSION MODEL FOR CRM

5.9.1 Abstraction Approach

In the current conceptual model for waste package degradation, the waste package surface is divided into patches, and waste package corrosion is modeled for the individual patches (see Section 5.4 for details and Figure 5-4). As discussed in Section 5.8, when the outer barrier is breached under dripping conditions, aqueous conditions are assumed at the interface between the outer and inner barriers. In the current conceptual model, localized corrosion (pitting and/or crevice corrosion) is assumed to initiate in the inner barrier only under dripping conditions. This assumption is supported by the WPDEE (CRWMS M&O 1998b) and various experimental observations on the necessary presence of aggressive ions (such as chloride) in order to initiate pitting and sustain the pit growth (Fontana 1986, pp. 51-73; Lillard and Scully 1994; McCaffery et al. 1997; Sridhar and Dunn 1997). The only mechanism for these ions to gain ingress to the drift in the potential repository is through drips. It is assumed conservatively that as soon as a patch of the outer barrier has breached, the entire surface of the inner barrier patch directly underneath the breached CAM patch is subject to general and localized corrosion. While some delay may be possible, this initiation time is not considered in the current conceptual model.

The CRM localized corrosion model used for the TSPA-VA analysis was abstracted from the Alloy 22 localized corrosion model developed by the project's corrosion testing and modeling programs (Pasupathi 1997 and 1998). The Alloy 22 localized corrosion model is a parametric correlation developed by fitting the available Alloy 22 crevice corrosion data to an elicited model. The data were from the LTCTF (6-month old) (Pasupathi 1997 CRWMS M&O 1998d), from short-term electrochemical polarization measurements (Stahl 1997) and literature data (Gdowski 1991). The resulting parametric correlation model is expressed as a function of temperature and solution chemistry (i.e., pH, equivalent NaCl concentration and $FeCl_3$ concentration) with an applicable range for each of the solution chemistry parameters. Because the local exposure environment on the CRM is poorly defined and the current (stochastic) WAPDEG is not yet capable of modeling the specific chemistry of the CRM localized corrosion environment, the parametric correlation model was abstracted into a form that is suitable for use in the waste package degradation model.

The abstraction was developed by "mapping" the exposure chemistry parameters within the suggested ranges into the corresponding localized corrosion rates. The resulting abstracted model is expressed as a function of temperature only with an uncertainty, which represents the effect of the exposure chemistry parameters and their suggested applicable range. The model uncertainty is used in the waste package degradation model to represent the effect of the uncertain and potentially variable local exposure chemistry on the CRM. The parametric correlation model, with a time-dependent term added, was endorsed by the majority of the expert panel. Localized corrosion initiation of the CRM was represented with a critical temperature threshold approach, proposed by one of the experts participating the WPDEE. The critical temperature approach is the most conservative among the assessments from the WPDEE. Details of the abstraction processes are described in the following sections. The conceptual and process models for CRM localized corrosion will be further improved for future analysis as additional data are developed from the project's corrosion testing and modeling programs.

5.9.2 CRM Localized Corrosion Model Development

This section describes the abstraction processes for the CRM localized corrosion model used in the TSPA-VA analysis. This model is based on the data from the LTCTF at Lawrence Livermore National Laboratory (Pendleton 1998) and published literature data (Haynes International 1997b), which is also summarized in Gdowski's Degradation Mode Survey (Gdowski 1991), and on the corrosion currents determined from electrochemical polarization data (Roy et al. 1997a and 1997b; Roy et al. 1996). The corrosion data and model development approach are presented in recent M&O correspondence (Pasupathi 1997; McCoy 1997; Stahl 1997 CRWMS M&O 1998d). In the following sections, the contents of these memos are summarized. Some parameter values presented here differ slightly from those in the memos as the data fitting was redone in order to evaluate the covariance-variance matrix, C (Equation [5-26]), which was necessary to abstract the model for use in the WAPDEG.

5.9.2.1 Corrosion Data

The LTCTF at Lawrence Livermore National Laboratory appears to be the most complete source of data on the corrosion of Alloy 22 in environments relevant to the potential repository. The corrosion data for Alloy 22 from the long-term corrosion tests used in the model development

are those collected during the first six months of testing, and they are summarized in the CRWMS M&O memo (Pasupathi 1997). These data have been combined with the rates calculated from the corrosion currents determined from electrochemical polarization measurements as well as the rates published by (Haynes 1997b). These additional data sets are summarized in another CRWMS M&O memo (Stahl 1997). The combined data set (Table 5-7) consisting of 38 measurements has been used as the basis of an overall correlation of penetration rates with temperature, pH, equivalent NaCl concentration, and $FeCl_3$ concentration. Solutions of $FeCl_3$ are used to simulate the environment expected in a typical crevice. In such cases, the pH depends on the $FeCl_3$ concentration and is determined by interpolation as indicated by Pasupathi (1997).

5.9.2.2 Development of Correlation for Localized Corrosion Rate

The following correlation (Pasupathi 1997 and 1998a; Stahl 1997; CRWMS M&O 1998d) is a reasonably good representation of all available experimental data for the general and localized corrosion of Alloy 22:

$$\ln\left(\frac{\Delta p}{\Delta t}\right) = b_0 + b_1\left(\frac{1000}{T}\right) + b_2(pH) + b_3(C_{NaCl}) + b_4(C_{FeCl_3}) \tag{5-23}$$

where $\Delta p/\Delta t$ is the apparent penetration rate in μm/year; T is the temperature in Kelvin; C_{NaCl} is the equivalent concentration of NaCl in weight percent; and C_{FeCl_3} is the concentration of ferric chloride also in weight percent. Within the bounds of 38 known experimental observations for Alloy 22 (Table 5-7), the coefficients are determined through multiple linear regression as follows:

$$\begin{aligned} b_0 &= +13.410 \\ b_1 &= -5.5615 \\ b_2 &= -0.8740 \\ b_3 &= +0.5696 \\ b_4 &= +0.6080 \end{aligned} \tag{5-24}$$

The values of the standard error of estimate and the coefficient of multiple determination of the above are 1.2285 and 0.65628 respectively. The coefficient of multiple determination (0.65628) indicates a reasonably good fit to the data set. In summary, the mean correlation rate is as follows:

$$\ln\left(\frac{\Delta p}{\Delta t}\right) = 13.410 - \left(\frac{5561.5}{T}\right) - 0.8740(pH) + 0.5696(C_{NaCl}) + 0.6080(C_{FeCl_3}) \tag{5-25}$$

The predictions appear to be reasonable for combinations of input parameters representative of the data used and the conditions predicted by a recently developed crevice transport model (Farmer and McCright 1998; Farmer 1997). For localized corrosion in contact with solutions with high carbonate concentrations, the applicable ranges of the solution chemistry parameters

that are to be used for the correlation are: $C_{FeCl_3} = 0.01$ weight percent, $C_{NaCl} = 0.01$ to 1 weight percent, and $pH = 5$ to 6. For a case in contacting with solutions with no carbonate, the applicable ranges are: $C_{FeCl_3} = 4$ weight percent, $C_{NaCl} = 10$ weight percent, and $pH = 1.63$. The worst case within the bounds of the regression analysis is the simulated crevice conditions used by Asphahani (1980) (10 weight percent $FeCl_3$).

5.9.2.3 Uncertainty in the Model

The uncertainty on model parameters can be determined by using the estimated variance-covariance matrix of coefficients.

$$C_{i,j} = \begin{bmatrix} 22.2988 & -7.5910 & -0.3841 & 0.2280 & 0.1300 \\ -7.5910 & 2.6318 & 0.1053 & -0.0889 & -0.0584 \\ -0.3841 & 0.1053 & 0.0507 & -0.0180 & 0.0021 \\ 0.2280 & -0.0889 & -0.0180 & 0.0204 & 0.0068 \\ 0.1300 & -0.0584 & 0.0021 & 0.0068 & 0.0101 \end{bmatrix} \tag{5-26}$$

Off-diagonal elements are estimated covariance between estimated coefficients. With normal distribution assumptions the $[100\times(1 - \alpha)]$ percent confidence interval for the population coefficient β_j is

$$b_j \pm t(\alpha/2, n-k) \times \sqrt{C_{j,j}} \tag{5-27}$$

Where $C_{j,j}$ are the diagonal elements of the estimated variance-covariance matrix of coefficients. The number of data points, n, is 38, and k, the number of coefficients estimated ($b_0, \ldots b_4$), is five, and t is the value from the student's t-distribution with given probability $\alpha/2$ lying above it and n-k degrees of freedom. For $\alpha = 0.05$, a 95 percent confidence interval for the uncertainty in the estimated coefficients are given by

$$\begin{aligned} b_0 &= +13.410 \pm 9.6073 \\ b_1 &= -5.5615 \pm 3.3005 \\ b_2 &= -0.8740 \pm 0.4582 \\ b_3 &= +0.5696 \pm 0.2908 \\ b_4 &= +0.6080 \pm 0.2040 \end{aligned} \tag{5-28}$$

5.9.2.4 Abstraction of the Model

The correlation (Equation [5-25]) is an equation that is to be applied within the range of observations for Alloy 22 corrosion data (Table 5-7). As discussed earlier, the local chemistry parameters of the correlation should be used within the suggested ranges for localized corrosion rate prediction. Estimated penetration rates falling outside of the range given in the table are considered to be unrealistic and should not be used.

The local exposure environment on the CRM and its evolution with time and the bulk condition are poorly defined, and the current (stochastic) waste package degradation model (WAPDEG) is not yet capable of modeling the specific chemistry of the CRM localized corrosion. Because of these, the parametric correlation model (Equation [5-25]), the model correlation matrix (Equation [5-26]), and the associated uncertainties, (Equation [5-27]) were reduced to a form that is suitable for use in WAPDEG. As discussed earlier in Section 5.9.2.1, the suggested applicable exposure chemistry ranges are to simulate those in a typical crevice. Accordingly, the abstraction was developed by mapping the local exposure chemistry parameters within the suggested ranges into the corresponding localized corrosion rates. This was done by substituting a range of the suggested values for the following parameters, C_{NaCl} C_{NaCl}, and pH. The range of those parameter values that were used in the model abstraction was based on the suggested applicable range for localized corrosion as follows: for pH uniform distribution from 1.63 to 6; for NaCl concentration log-uniform distribution from 0.01 to 10 weight percent; and for $FeCl_3$ concentration log-uniform distribution from 0.01 to 4 weight percent. Those parameter values were randomly sampled within the value range, then the corresponding rates were calculated. The resulting abstracted model is expressed as a function of temperature only with an uncertainty, which was to capture the effect of the local exposure chemistry in crevice. The model uncertainty is used in the waste package degradation model (WAPDEG) to represent the effect of uncertain and potentially variable local exposure chemistry on the CRM. The resulting equation takes an Arrhenius Law equation form as given below.

$$ln\left(\frac{\Delta p}{\Delta t}\right) = ln\left(R_{LC}\right) = C_{LC} + \frac{Q_{LC}}{T} + \varepsilon_{LC} \tag{5-29}$$

where R_{LC} is the localized corrosion rate, Q_{LC} is a constant equal to *5549.4 /K*, and ε_{LC} is a normally distributed term with a mean of zero representing uncertainties not accounted for in the model. The term C_{LC}, equal to *11.274*, includes all the terms, except the temperature term, of Equation (5-25) fixed at their appropriate parameter values as given above. The combined standard deviation of the intercept term, ε_{LC}, reduced by fixing all the other variables, is equal to *2.4495*.

5.9.2.5 Time Dependence of CRM Localized Corrosion Model

In the crevice, the penetration rate is expected to be diffusion limited (Pasupathi 1997). Therefore, the penetration rate should be inversely proportional to the penetration depth. Specifically:

$$\frac{dp}{dt} = \frac{k}{p} \approx \frac{\Delta p}{\Delta t} = f(T, pH, NaCl, FeCl_3) = R_{LC}(T) \tag{5-30}$$

where k is a constant, independent of time. This will result in a square-root dependence of the penetration depth on time:

$$p = \sqrt{2\,k\,t} \tag{5-31}$$

Most of the data set used in the model development is from 6 months of testing, thus the constant k is evaluated by setting

$$f \times \Delta t = \sqrt{2k \times \Delta t} \tag{5-32}$$

and

$$k = f^2 \times \frac{\Delta t}{2} \tag{5-33}$$

where $\Delta t = 0.5$. Thus, the equation for the penetration depth by localized corrosion is

$$p = f\sqrt{\Delta t}\ t^{1/2} = 0.707\, R_{LC}(T)\ t^{1/2} \tag{5-34}$$

The factor 0.707 is an approximation for a constant of the time-dependence of localized corrosion penetration. The approximation was needed because the data used to develop the localized corrosion model are for the six-month exposure time only (i.e., single time-point). In the implementation of the localized corrosion model into the waste package degradation model (WAPDEG), the factor was assumed to be one, which is the maximum value for the constant. The final equation for the Alloy 22 localized corrosion model that was implemented in WAPDEG is

$$D_{LC} = exp\left(C_{LC} + \frac{Q_{LC}}{T} + \varepsilon_{LC}\right) \cdot t^{1/2} \tag{5-35}$$

where D_{LC} is the penetration depth by localized corrosion, t is the exposure time in years. Other symbols were defined previously. In WAPDEG, the total penetration depth is the sum of the general and localized corrosion depths.

5.9.2.6 Temperature Threshold for Localized Corrosion Initiation

Given a penetration of the carbon steel outer barrier (CAM), there are a number of factors that may determine the probability that localized corrosion of the inner barrier will initiate. These factors include the availability of water, pH, temperature, and Fe^{3+}, Cl^-, and O_2 concentrations. The inner barrier surface is likely to be covered with a thick layer of the carbon steel corrosion products and other mineral precipitates at the time of CAM penetration. In addition, there is potential to form crevice between uncorroded CAM and CRM. Accordingly, crevice corrosion of the inner barrier is considered a more probable corrosion process than pitting, and this process can initiate at lower temperatures than pitting. Experts participating in the WPDEE (Pendleton 1998) expressed very low probabilities of crevice corrosion initiation. Typically, this requires

the most extreme local exposure conditions of high temperatures (~100°C), low pH (~2.5), and high corrosion potential (~640 mV SHE) for crevice corrosion initiation to occur. Dr. D. Shoesmith recommended that crevice corrosion be assumed to initiate if the exposure temperature is greater than 80°C when the outer barrier is penetrated. The probability of crevice corrosion initiation could be set to 1 at $T \geq 100$°C and decrease linearly to zero at 80°C (uniform distribution). Once initiated, a crevice will grow at a rate depicted by Equation (5-35). If $T \leq$ 80°C when the outer barrier is penetrated, no exposed site on the inner barrier would initiate a crevice, and the inner barrier can be assumed immune to localized corrosion (general corrosion would still occur).

The site-relevant corrosion testing and model development programs underway in this program (Farmer 1997; McCright 1998) should enable incorporation of detailed electrochemical and other physicochemical processes associated with waste package corrosion into future analysis, particularly for the localized corrosion initiation and rate and the stifling of pits in a thick Alloy 22 layer.

5.9.3 Abstracted Model Results

The CRM localized corrosion model results at 1,000- and 100,000-year exposure times with the expected values of the parameters and the uncertainties set at 2 and 3 standard deviations, as a function of temperature, are shown in Figures 5-42 and 5-43. One can see that the localized corrosion rate decreases about 1 order of magnitude on going from a 1,000-year to a 100,000-year exposure time.

Figures 5-44 through 5-46 show the CRM penetration depth by localized corrosion only as a function of exposure time at exposure temperatures of 90, 60 and 30°C, respectively. The solid dark line on these graphs represents the 20-mm CRM thickness. The dash-dot and dash lines are two and three standard deviations from the mean localized corrosion depth. One can see that the localized corrosion depth at a given time decreases slightly over 1 order of magnitude in going from 90 to 30°C. As shown in Figure 5-44, if the CRM is exposed continuously at 90°C, there would be a small probability that it is penetrated by localized corrosion by 1,000,000 years.

As discussed earlier, in the waste package degradation model, localized corrosion of a CRM patch initiates if the waste package temperature is greater than 80°C when the outer barrier patch is penetrated. Once localized corrosion has inititated, the total penetration depth at a given time is the sum of the penetrations by both the general corrosion and localized corrosion. As seen in the base case waste package degradation analysis results (see Figures 5-59 and 5-60), only a small fraction of waste packages fail by localized corrosion.

5.9.4 Inputs to and Outputs from the CRM Localized Corrosion Model

The inputs to the CRM localized corrosion model [Equation (5-35)] are values for Q_{LC}, C_{LC}, ε_{LC}, and n. $Q_{LC}=5549.4/K$ is a constant. The inputs for C_{LC} and ε_{LC} are combined, i.e. $C_{LC} = 11.274$ is considered to be the mean of the normally distributed ε_{LC} distribution, which has a standard deviation of 2.4495. The n is the time exponent in Equation (5-35) and is fixed at one-half.

In WAPDEG, the total penetration depth is the sum of the general [Equation (5-22)] and localized corrosion depths [Equation (5-35)]. The temperature threshold for initiation of localized corrosion is an indirect input to the model in that if the exposure temperature at the time of outer barrier penetration is less than a stochastically sampled value (uniformly distributed between 80 and 100°C), then no localized corrosion is allowed to occur (general corrosion can still occur).

5.10 IMPLEMENTATION OF WASTE PACKAGE CORROSION DEGRADATION MODEL

This section presents description for the waste package degradation model, WAPDEG, developed for TSPA-VA analyses. The major issues to be discussed in this section are:

- Implementation of the near-field exposure conditions
- Implementation of individual abstracted-corrosion models and their parameters
- Representation of the variability and uncertainty of waste package degradation in WAPDEG
- Features and capabilities of WAPDEG
- Structure of WAPDEG program
- Description of the WAPDEG input
- Description of the WAPDEG output and post-processing for the result abstraction.

5.10.1 Implementation of In-Drift Exposure Conditions

The areal distribution of the emplaced waste packages is sufficiently broad to warrant the assumption that in-drift conditions will be spatially variable across the site. Because of the heat generated by radioactive decay, both temperature and humidity will vary with time. Thus, conditions governing the waste package corrosion mechanisms are both spatially and temporally variable.

Conditions are assumed to be similar within small groups of waste packages. Results from site-wide, thermal-hydrological models can be partitioned into subareas having similar in-drift conditions. For the base case TSPA-VA model, the repository was divided into six subareas based on the different thermal-hydrological response between regions of the repository. The waste packages within each subarea were divided into waste package groups not only by the different waste forms they contain (defense high-level waste, spent nuclear fuel, etc.) but also by a criterion based on the time at which the relative humidity at the waste package surface dropped below 85 percent. Thus, a given WAPDEG simulation for a given subarea of the repository could require several different temperature/relative humidity histories. Details of the criteria used in defining the six subareas and waste package groups used in WAPDEG simulations are described in the thermal-hydrology modeling and abstraction (see Chapter 3).

At the group scale, the important parameters affecting corrosion of the CAM are the temperature and relative humidity. Because these may differ from waste package to waste package within a group, we also capture this uncertainty. A mean temperature/relative humidity history is provided for each waste package group as well as a standard deviation for temperature and one for humidity. For each waste package, a normal (mean zero, standard deviation as given) value is sampled and applied as a constant (with time) offset from the mean waste package group history. In the TSPA-VA base case analysis, the standard deviations for temperature and relative humidity were chosen to be zero.

The horizontal length of an emplaced waste package is long enough (~6m) that corrosion conditions can differ along its length. To account for differences in temperature and humidity along the waste package length and other potential effects, WAPDEG partitions the waste package surface into sections called patches. Then, the variances inherent in the general corrosion models for the CAM and CRM are shared. A portion is applied to waste package-to-waste package variability (within a group), and the remaining portion is applied to patch-to-patch variability (on a waste package). This is discussed further in Section 5.10.4. For the TSPA-VA base case, the variance allocated to waste package-to-waste package variation is 50 percent for the nondripping condition and 35 percent for the dripping condition, with the remainder allocated to patch-to-patch variation. These variance partitions were recommended by the experts participating in the WPDEE (Pendleton 1998).

A second in-drift hydrologic issue is the presence or absence of dripping water. For the TSPA-VA base case, it is assumed that either 100 percent or 0 percent of the waste package surface contacts dripping or pooled water. The TSPA-VA base case then requires two WAPDEG simulations; one where none of the waste packages are dripped on and one where all of the waste packages are dripped on all the time. The simulation results are then weighted according to the percentage of waste packages that contact dripping water.

As part of the evaluation, we also need to define top and bottom of a waste package. For the base case, the top is defined by the arc subtended by an angle of 180 degrees, and the bottom is defined by an angle of 180 degrees. With each waste package divided into two semicircles, there are no patches defined as side patches for the TSPA-VA base case.

Corrosion, especially localized corrosion, may be affected by geochemical conditions. For the TSPA-VA base case, it is assumed that dripping water has neither elevated pH nor chloride ions, and thus, no high aspect ratio pitting corrosion of the CAM is expected. Possible mechanisms that could alter the geochemistry of the drips, such as degradation of the concrete drift wall liner, and the resulting impacts on corrosion are left to the sensitivity analyses of Section 5.12.

5.10.2 Implementation of Abstracted Corrosion Models and Parameters

This section discusses the implementation of the individual abstracted-corrosion models and the model parameters described in Sections 5.5 to 5.9.

Temperature Threshold for CAM Corrosion - In addition to the direct influence of temperature on corrosion rates, there is a threshold temperature above which there will be no corrosion of the CAM. This results from the fact that the presence of a water film is a necessary

prerequisite for corrosion processes to occur at any appreciable rate (Tsuru et al. 1995). Above the boiling point of water, no such film can form. However, the critical temperature at which a water film can form on the waste package surface can differ from the boiling point of pure water because of the influence of chemical impurities in the water and modifications of the waste package surface itself, such as salt/mineral deposits. Figure 5-47 shows a cumulative probability distribution for this threshold as recommended by the WPDEE (CRWMS M&O 1997e). A numerical representation of this curve is cast as a lookup table (CRWMS M&O 1998i) for WAPDEG to be used to obtain a temperature threshold for each waste package. For the TSPA-VA base case, the same threshold applies whether or not dripping water contacts a waste package.

Relative Humidity for Initiation of CAM Humid-Air Corrosion - In addition to the direct influence of relative humidity on the rate for humid-air corrosion of the CAM, there is a threshold humidity below which there will be no corrosion of the CAM. Again, this results from literature observations that a water film of a critical thickness must be present in order for corrosion to occur (Tsuru et al. 1995; Vernon 1933; Phipps and Rice 1979). Figures 5-48 and 5-49 show cumulative probability distributions for this threshold as interpolated from the WPDEE both for the cases with and without salt films on the waste package surface. Numerical representations of these curves can be cast as lookup tables (CRWMS M&O 1998j) for WAPDEG to be used to obtain a corrosion initiation threshold for each waste package. For the TSPA-VA base case, the curve representing the no salt condition is used both for waste packages subject to dripping and those not subject to dripping.

Roughness Factors for CAM Humid-Air Corrosion - Corrosion of the CAM does not occur in a uniform fashion across the entire surface of the waste package. In the TSPA-VA analysis, the natural roughness of the corrosion front is accounted for in WAPDEG through the use of the roughness factors (discussed in Section 5.5) applied to a user specified number of pits per patch (3,100 pits/patch or a pit density of 10 pits/cm^2) (Marsh and Taylor 1988; Marsh et al. 1988; Strutt et al. 1985). WAPDEG simulations typically use a distribution of roughness factors to model a corroded surface. For the base case, the roughness factors are considered to be normally distributed with a mean of 1.5 and a standard deviation of 0.25. These values are appropriate given the results of the WPDEE (see Figure 5-7). As discussed in Section 5.5, the results provided in the WPDEE report neglected to include the elicitations of three of the experts who felt that a roughness factor of one was appropriate. One expert (Andresen) elicited that the roughness factor should be normally distributed with a mean of 1.1 and a standard deviation of 0.1. Only one expert, McCright, elicited a roughness factor distribution higher than the (normally distributed with a mean of 1.5 and a standard deviation of 0.25) implementation being used. McCright stated that the roughness factor should decrease with time (or increasing depth). Viewed from this perspective, the choice of a roughness factor normally distributed with a mean of 1.5 and a standard deviation of 0.25 is actually a conservative choice for humid-air corrosion modeling.

Relative Humidity for Initiation of CAM Aqueous Corrosion - At higher humidities corrosion of the CAM will occur under aqueous conditions. There is a threshold humidity above which corrosion of the CAM will change from humid-air to aqueous corrosion. Figures 5-50 and 5-51 show cumulative probability distributions for this threshold as interpolated from the WPDEE for the cases with and without the presence of salt on the waste package surface.

Numerical representations of these curves can be cast as lookup tables (CRWMS M&O 1998j) for WAPDEG to be used to obtain an aqueous corrosion initiation threshold for each waste package. For the TSPA-VA base case, the curve representing the no salt condition is used both for waste packages subject to dripping and those not subject to dripping.

Roughness Factors for CAM Aqueous Corrosion - As for the case of humid-air corrosion, aqueous corrosion of the CAM does not occur in a uniform fashion across the entire surface of the waste package. The natural roughness of the corrosion front is accounted for in WAPDEG through the use of the roughness factors, discussed in Section 5.6, applied to a user specified number of pits per patch (3,100 pits/patch or a pit density of 10 pits/cm^2 in the TSPA-VA base case). WAPDEG simulations typically use a distribution of roughness factors to model a corroded surface. For the base case, the roughness factors for aqueous CAM corrosion are considered to be normally distributed with a mean of 1.5 and a standard deviation of 0.25. These are the same parameters for the normal distribution as were selected for humid-air corrosion. They were selected for the same reasons discussed above for the case of humid-air corrosion roughness factors.

Description of the "Corrosion Time" Concept - The humid-air corrosion model for the CAM presented in Section 5.5, specifically Equation (5-8), and the aqueous corrosion model for the CAM discussed in Section 5.6, specifically Equation (5-13), are valid only for constant temperature and relative humidity. Because these change with time, WAPDEG adopts the use of the corrosion time concept. This concept was documented in earlier reports (CRWMS M&O 1998; Lee et al. 1997). It is described here in terms of its implementation into WAPDEG, which assumes that temperature and relative humidity are constant only over a time step. In this section, we will discuss the concept of corrosion time, which can incorporate changes in the relative humidity and the temperature between time steps.

As general corrosion of the carbon steel outer barrier progresses, corrosion products accumulate on the surface of the waste package. This corrosion-product layer restricts the movement of the reacting species and the corrosion reaction products, which causes a decrease in corrosion rate with time. In both of the carbon steel general corrosion models, the decreasing corrosion rate with time (due mostly to the accumulation of corrosion products) was reflected with a time term raised to a power that has a value between 0.0 and 1.0. This may be expressed as

$$D_g = f_{NFE}\, t^d \tag{5-36}$$

where D_g is general corrosion depth, f_{NFE} includes the constant term and the near-field exposure parameters (i.e., temperature and, for humid-air corrosion, relative humidity) in the model, t is the (real) time elapsed after the initiation of corrosion, and d is a constant having a value between 0.0 and 1.0. Equation (5-36) is just a restatement of Equations (5-8) and (5-13) in schematic form. The rate of general corrosion is given as

$$\frac{\partial D_g}{\partial t} = f_{NFE}\, d\, t^{d-1} \tag{5-37}$$

Equations (5-36) and (5-37) are both applicable to a constant exposure condition. In constant exposure environments, the dependence of the general corrosion rate on time is merely a proxy for the actual dependence of the rate on the corrosion product depth. In dynamically changing exposure environments, as are expected in the potential repository, Equations (5-36) and (5-37) can be generalized to give the corrosion in terms of the corrosion product depth. Substituting $(D_g/f_{NFE})^{1/d}$ from Equation (5-36) for t in Equation (5-37) gives

$$\frac{\partial D_g}{\partial t} = f_{NFE}\, d \left[\left(\frac{D_g}{f_{NFE}} \right)^{1/d} \right]^{d-1} = f_{NFE}^{1/d}\, d\, D_g^{1-1/d} \tag{5-38}$$

Equation (5-38) expresses the general corrosion rate in terms of the general corrosion depth. After the first time step, the general corrosion rate in Equation (5-38) is bounded. Because the general corrosion depth is known at the beginning of each time step, there will be a unique solution to Equation (5-38) for any time step after the first time step (Nagle and Saff 1993, p. 617). Thus, Equation (5-36) can be used for the first time step, and it will suffice to find a solution to Equation (5-38) with the correct corrosion depth at the beginning of the time step for each time step after the first time step.

Implementation of the "Corrosion Time" Concept - Because the near-field environment inside the emplacement drift of the potential repository changes dynamically with time, f_{NFE} will also change with time. Therefore, a direct use of Equation (5-36) does not properly capture the effects of the changing exposure conditions. One possible way to represent the effects of changing exposure conditions is to use the concept of corrosion time (t^c) and use the corrosion time to account for different exposure conditions in each time step. This entails adjusting the value of t [the real time term in Equation (5-36)] for changing exposure conditions.

The corrosion time concept and its implementation are described in detail as follows. At the beginning of each time step in which the exposure conditions are relatively constant, the corrosion time for the current time step is determined based on the corrosion depth at the end of the previous time step and the exposure conditions in the current time step. This may be expressed as

$$t_i^{\,c} = \left(\frac{D_{g,i-1}}{f_{NFE,i}} \right)^{1/b} \tag{5-37}$$

where t_i^c is the corrosion time at the beginning of the current time step i, $D_{g,i-1}$ is the general corrosion depth at the end of the previous time step i-1, $f_{NFE,i}$ embodies the exposure conditions for the current time step i, and b is a constant. In simple terms, Equation (5-39) determines the time (t_i^c) that would be required for corrosion to reach the corrosion depth ($D_{g,i-1}$) if the exposure conditions ($f_{NFE,i}$) of the current time step were applicable for all times following the onset of corrosion. The real time (t) in Equation (5-36) is replaced with the estimated corrosion time (t_i^c)

to calculate the corrosion during the current time step. Using t_i^c in Equation (5-36) will give the correct corrosion depth at the beginning of the new interval. Because Equation (5-36) satisfies Equation (5-38), using Equation (5-36) and starting the interval at t_i^c will give the correct corrosion depth, provided the duration of the time step is preserved.

5.10.2.1 Initiation Time for CRM Corrosion

An important difference between earlier versions of WAPDEG and the current version is that the current version includes general corrosion of the CRM, rather than pitting corrosion only. WAPDEG uses general corrosion as the only corrosion mechanism if there is no water dripping on or pooled under the patch. In earlier WAPDEG versions, when a pit penetrated the CAM, it initiated a pit in the CRM at the CAM penetration site, which immediately began to grow. Thus, pits were initiated on a patch of the CRM over a range of times. In the current WAPDEG version, however, any penetration of the CAM patch initiates general corrosion over the entire surface of the patch in the CRM. If pits are to be modeled on the CRM, they also initiate at that time, unless the temperature threshold for localized corrosion of the CRM (next section) is not satisfied. Inherent in this treatment is the assumption that water can permeate through isolated gaps between the two barriers, which might be present from the shrink-fitting of the barriers. So whenever the *first* penetration of the patch on the CAM occurs, WAPDEG now proceeds directly to modeling the corrosion of the entire CRM patch underneath the breached CAM patch.

5.10.2.2 Initiation Temperature for CRM Localized Corrosion

As mentioned above in the discussion of dripped-on patches, WAPDEG has the capability to allow initiation of CRM localized corrosion if the waste package temperature is above a user-defined temperature threshold when the CAM is breached. The use of such a threshold was based on a conservative approach from the WPDEE, which recommends that crevice corrosion of the CRM be assumed to initiate if the exposure temperature is greater than 80°C when the outer barrier is penetrated. The probability of crevice corrosion initiation is set to one at a temperature greater than or equal to 100°C and decrease linearly to zero at 80°C (uniform distribution). If the temperature is less than 80°C when the outer barrier is penetrated, no exposed sites on the inner barrier would initiate crevice corrosion, and the inner barrier is assumed immune to localized corrosion (general corrosion would still occur). This is the CRM localized corrosion initiation criterion used in WAPDEG.

5.10.2.3 Localized (Pitting and Crevice) Corrosion of the CRM

WAPDEG assumes that total pit depth at time t is the sum of the general corrosion depth at time t and the pit depth at time t, and that the localized corrosion model of Section 5.9 describes the latter. So the pitting model determines an incremental depth that is added independently for each pit to the general corrosion depth.

Because the incremental pit depth depends on both time and temperature, WAPDEG uses the corrosion time concept here. In particular, assume we know the incremental pit depth (d_j) at time t_j and are interested in finding the incremental pit depth (d_{j+1}) at time t_{j+1}. The corrosion time concept means:

A. Find the time that would have been required for corrosion to reach the incremental depth d_j if the temperature for the time interval (t_j, t_{j+1}) would have persisted since time zero. Do this by solving Equation (5-36) for t with d_j substituted for depth, and call the corrosion time t_j^c.

B. Find the end of the time interval also in terms of corrosion time. That is

$$t^c{}_{j+1} = t_j{}^c + (t_{j+1} - t_j) \tag{5-40}$$

C. Find incremental depth at time $t^c{}_{j+1}$ (and equivalently at t_{j+1}) by substituting the ending corrosion time into Equation (5-36)

After step C, the incremental pit depth is added to the general corrosion depth at time t_{j+1} to find total pit depth at time t_{j+1}.

5.10.3 Representation of Uncertainty and Variability in Waste Package Degradation Modeling

Uncertainty and variability are easy to define yet often difficult to treat, particularly for a stochastic code such as WAPDEG, which uses many models and model parameters. Uncertainty represents a lack of knowledge about a process being modeled; both with the model used and the parameters used within that model. A parameter or process that varies over space and time possesses the property of variability. For example, the temperature and relative humidity histories used in WAPDEG are obviously variable as are general corrosion rate distributions across the surface of the waste packages. However, within the obviously variable temperature and relative humidity histories, one could assume that there is some uncertainty from the model and model parameters used to generate them. Similarly, the uncertain infiltration flux and drip chemistry result in uncertainties in the local exposure chemistry, which could also be variable across the repository and likely across the length of a waste package as well. Therein lies the difficulty in treating variability and uncertainty; they are often found to be mixed together within the same input or output parameter distribution.

Variability is generally treated in a manner similar to that used in WAPDEG. A region of the potential repository has 400 representative waste packages and these waste packages are grouped according to which temperature/relative humidity history they would be exposed to. The waste package surface is subdivided into patches to allow for introduction of spatial variability in model parameters within a waste package. The patch is subdivided into modeling entities called pits, which for the CAM general corrosion model, are used to represent local variability in general corrosion depth through their characteristic roughness factors. Focusing on the treatment of variance-covariance of CAM corrosion model parameters, which will be discussed later in this section, the total variance is allocated, through the method of Gaussian Variance Partitioning (Section 5.7.3), so that the distribution of general corrosion rates on different patches on the same waste package have less variability than the distribution of general corrosion rates on patches on different waste packages. The CAM roughness factors are similarly distributed so that the amount of variability in surface roughness on the same patch is smaller than the amount of surface roughness variability on different patches of the same waste package. This in turn is

smaller than the amount of variability in surface roughness between patches on different waste packages. This is to capture effects of varying exposure conditions on waste package corrosion degradation. That is, the waste packages that are exposed to more corrosive conditions would corrode faster than the waste packages that are exposed to less corrosive conditions.

One approach that may be employed to characterize and quantify the effects of the uncertainty in a model would be conducting an uncertainty analysis in which multiple realizations are performed. In each realization, values for the model parameters are sampled randomly over their ranges. For example, if the CRM general corrosion rate distribution represents the true uncertainty of the passive dissolution behavior of the material in the given exposure condition, then the impact of the uncertain general corrosion rates on the waste package degradation could be analyzed as

A. For each realization (or each waste package degradation calculation), sample the CRM general corrosion rate randomly over the given range.

B. Calculate the waste package degradation with the sampled CRM general corrosion rate.

C. Repeat the above procedure for a sufficient number of realizations.

Thus, if the distribution in the CRM general corrosion rates were all (100%) because of uncertainty, then a CRM corrosion rate for a particular simulation (or realization) would be sampled randomly from the distribution given. In this case, there will be no variability in the CRM corrosion rate among the waste packages simulated and the patches within each waste package. That is, the CRM general corrosion rate of all the waste packages and all the patches would be equal to the value sampled, and all waste packages and patches on each waste package would fail at the exact same time.

Variability in Waste Package Degradation Modeling – Because the waste packages will be spread over the repository area, the different waste packages will be exposed to different local environments. The different waste packages, and even different locations on the same waste package, will also have different material characteristics and exposure conditions. These will cause variability in the corrosion rates and model parameters, both between different waste packages and on the same waste package. Because the environment and even the material would vary more between waste packages than within a waste package, more variability will be expected between locations on different waste packages than between locations on the same waste package.

Corrosion results from complicated interactions of many factors (including those listed above and others not mentioned) making it difficult to model mechanistically. Thus, in order to incorporate variability, WAPDEG models corrosion stochastically. WAPDEG uses distributions (as discussed in previous sections) for the parameters in the various corrosion models to represent the variability between different locations on different waste packages.

Repository Level Variability - There are several sources of repository-level variability in waste package degradation. Temperature and relative humidity depend on thermal load and near-field hydrologic properties causing them to vary spatially (and temporally) throughout the repository.

Discrete fractures in the host rock may yield dripping water in some regions of the repository (on some waste packages) and not in others.

Results from site-wide, thermal-hydrological models can be partitioned into subareas having similar in-drift conditions. For the base case TSPA-VA model, the repository was divided into six subareas based on the differing thermal-hydrological response between different regions of the repository. The waste packages within each subarea were divided into waste package groups not only by the differing waste forms they contain (defense high level waste, spent nuclear fuel, and other waste types) but also by a criterion based on the time at which the relative humidity at the waste package surface dropped below 85 percent. Thus, a given WAPDEG simulation for a given subarea of the repository could use several different temperature/relative humidity histories.

At the waste package group scale, the important parameters affecting corrosion of the CAM are the temperature and relative humidity. Because these may differ from waste package-to-waste package within a group to some extent, we can also capture this variability. A mean temperature/relative humidity history is provided for each waste package group as well as a standard deviation for temperature and one for humidity. For each waste package, a normal (mean zero, standard deviation as given) value is sampled and applied as a constant (with time) offset from the mean waste package group history. In the TSPA-VA base case, the standard deviations for temperature and relative humidity were chosen to be zero.

WAPDEG allows weighing of the waste package groups via user input. In particular, the user specifies the number of waste packages in each group, so the group contributes to waste package failure results in proportion to the ratio of group size to the total number of waste packages.

Waste Package Level Variability: Patches Approach - Both the material characteristics and the environment are expected to vary more between locations on the same waste package, which are far apart on a waste package, than between neighboring locations on the same waste package. Thus, the corrosion depth can also be expected to vary more between locations on the same waste package, which are far apart, than between neighboring locations on the same waste package. This can be modeled by imposing a correlation structure on the general corrosion depth at different locations on a waste package. The strength of this correlation should increase toward 1 as the distance between the two locations decreases toward 0.

This conceptual model, with a correlation structure that varies gradually between 1 and some smaller (though still strictly positive) number as the distance between two locations increases is difficult to simulate. To make things tractable, the waste package was divided into patches. Locations on the same patch would have the same general corrosion depth, while the general corrosion depth at locations on different patches would have some constant correlation because they are on the same waste package.

Literature data, which was used to develop the general corrosion models, provided the general corrosion depth of sample coupons as a function of exposure time (Lee, Atkins, and Andrews 1996). This general corrosion depth was derived from the weight loss measurements of the sample coupons. Thus the general corrosion depth at a given exposure time is an average over the entire exposed surface of the sample coupons. Most of the sample coupons were prepared

and tested following the ASTM standard procedures (ASTM 1992). The testing standards recommends a sample coupon size of 10.16 × 15.24-cm, which gives the surface area of the sample coupon of about 310 cm^2 (counting both sides). In order to use the variability of the general corrosion observed in the experiments for the variability of the general corrosion depth of a patch, the patches were taken to be the same size as the ASTM standard test coupon. Thus, the waste package surface area (about 30 m^2, or 300,000 cm^2) was divided by the sample coupon surface area of 310 cm^2. This process results in a total of 964 patches over the waste container surface.

Allocation of Variability among Patches and Pits - There is expected to be variability in the corrosion models between locations on different waste packages. Locations on different patches of the same waste package can be expected to have less variability, and locations on the same patch of the same waste package are expected to have even less variability.

The variability allocation in WAPDEG is based on user defined input parameters. The user specifies the fraction of the total variability to assign to waste package-to-waste package variations, and the remainder is assigned to patch to patch variability. For both of the CAM general corrosion models, humid-air and aqueous, the variability in the parameters is divided in the following manner. The covariance matrix, V, [see Equations (5-9) and (5-14)] is multiplied by the waste package variability fraction to obtain a new covariance matrix, V_H. Then, V_H is used to select average values of the corrosion parameters for each waste package. To select corrosion parameters for each patch on that waste package, the covariance matrix, V, is multiplied by (1 – the waste package variability fraction) to obtain a new covariance matrix, and this matrix is used to select the patch parameters. For example, 20.221 might be selected as the average value of a_o for one waste package. The waste package variability fraction is input as 0.5. In this case, the value of a_o for each patch on this waste package would be chosen from a normal distribution with a mean of 20.221 and a variance of 3.4967 (half of 6.9934, the total variance). Similarly, for each waste package, average values would be chosen for each of the parameters in the humid-air and aqueous general corrosion models for the carbon steel outer barrier. These average values would be subsequently used to choose values for these parameters for each patch.

Using the above correlation structure for the general corrosion depth gives a constant general corrosion depth within each patch. Because the outer (CAM) barrier local general corrosion depth is the general corrosion depth multiplied by the roughness factor, the pit depths will reflect the correlation structure of the general corrosion. Based on this, WAPDEG samples every roughness factor independently. This will make the amounts of variability between pit depths on the same patch smaller than the amount of variability between pit depths on different patches of the same waste package, which is smaller than the amount of variability between pit depths on different waste packages. WAPDEG also takes advantage of the patches approach for inner (CRM) barrier localized corrosion. This allows the inner barrier corrosion rate to also vary more between patches or pits on different waste packages than between patches or pits on the same waste package and to vary more between pits on different patches of the same waste package than between pits on the same patch.

There is little experimental data currently available as to how the variability within the general or localized CAM or CRM corrosion models should be quantitatively allocated. The experts participating in the WPDEE elicited the fraction of the total variance of the CRM general

corrosion rate distribution to be allocated to the variability and uncertainty of the corrosion rate and the split of the total variability to the variability among waste packages and patches (Pendleton 1998) (see Sections 5.8.2.2 and 5.8.2.3 for the variability and uncertainty allocation). For the CRM general corrosion rate under dripping conditions, the average of the elicited values for the allocation of the total variability to waste package-to-waste package variability is 35 percent, and the average of the elicited values to patch-to-patch variability is 65 percent. When drips are absent, the average of the elicited values for the allocation of the total variability of the (no-drip) CRM general corrosion rate between waste package-to-waste package and patch-to-patch variability is 50 percent. For the localized corrosion model, the average expert-elicited allocation of the total variability is a 50 percent-50 percent split to waste package-to-waste package and patch-to-patch variability. To be consistent with the CRM corrosion models, the same waste package-to-waste package and patch-to-patch variability allocations are used for the CAM.

Uncertainty in Corrosion Model Parameters - Corrosion processes for the CAM are implemented in WAPDEG based on models abstracted from relatively short-term corrosion data and expert assessments. Corrosion processes for the CRM are based largely on expert assessments with some very short term laboratory testing. WAPDEG was developed to evaluate waste package failure while taking all of this variability and uncertainty into account. In addition to the corrosion model parameters discussed earlier that are treated with the patches approach, the various thresholds (temperature, relative humidity, corrosion initiation, etc.) are also variable. As mentioned in the introduction to this subsection, it is likely that most of the parameter distributions input into WAPDEG contain a mixture of variability and uncertainty within them.

The CAM general corrosion models, both humid-air and aqueous, were developed from models and data points appearing in the literature. It was implicitly assumed that the spread in the model parameter distributions was predominately due to the effects of variability among the data sets used to evaluate them. Therefore, the variance-covariance in the model parameters was distributed between waste packages and patches in the manner described earlier in this section.

The CRM general corrosion models, both for dripping and no dripping conditions, were from the WPDEE results. The experts were asked to provide their assessment of the fraction of the total variance in their elicitations of CRM general corrosion rate distributions they would attribute to variability and what fraction they would attribute to uncertainty. The experts' elicitations were averaged and resulted in a 50%/50% uncertainty/variability partition ratio for the case of CRM general corrosion in a dripping environment and a 75%/25% uncertainty/variability partition ratio for the case of CRM general corrosion in the absence of dripping.

Effects of alternative partitioning ratios were investigated with three uncertainty/variability partition ratios (25%/75%, 50%/50%, and 75%/25%) for CRM general corrosion rates in the presence and absence of dripping. Uncertainty/variability partitioning was accomplished through the method of Gaussian Variance Partitioning as discussed in Section 5.7. For the purposes of analysis of this parameter, the variation in the mean value is considered to represent parameter uncertainty, and the variation around the mean parameter variability. The resulting uncertainty distributions were sampled at the 5th, 50th, and 95th percentiles to obtain the median values (not mean values as the distributions are non-normal) to be used for the resulting variability distributions (see Table 5-13). Thus, a total of 54 CRM general corrosion rate CDFs

were generated [(2 drip conditions) × (3 different temperatures) × (3 uncertainty/variability partitioning ratios) × (3 samples of uncertainty percentiles)]. The number of uncertainty/variability partitioning ratios and samples of uncertainty percentiles was limited to three each to allow for preparation and execution of waste package degradation simulations in the time allotted and still reasonably sample the range over which these parameters vary.

The importance of CRM general corrosion rate to the WAPDEG model is illustrated with the "one-off" sensitivity and regression-based sensitivity analyses discussed in Section 5.12. In particular, the regression-based sensitivity analysis results indicate that over 80 percent of the total output variance is explained by the value used for this parameter.

5.10.4 Features and Capabilities of WAPDEG

The WAPDEG stochastic modeling tool was developed to implement and combine the abstracted corrosion models described in the preceding sections. Earlier versions of WAPDEG (CRWMS M&O 1995) modeled general and pitting corrosion of the CAM and pitting corrosion only of the CRM. Several new capabilities have been added to the current version to account for:

- General corrosion of the CRM, including two different models
- Alternate pit growth laws in both the CAM (two models) and CRM (four models)
- Dripping on or pooled water under the waste packages
- Changes in dripping water character (chemistry)
- Differences in corrosion environment depending on waste package location within the repository
- Additional flexibility in distributing variability of model parameters among waste packages, patches that compose waste packages, and pits on the patches
- Additional options such as an modeling of ceramic coatings and variable corrosion rate enhancement factors
- Generally increased input flexibility
- More comprehensive reporting of results and sampled values used during simulations.

The primary objective of WAPDEG is to provide reasonable evaluation of waste package failure time distributions and time-dependent profiles of subsequent degradation processes. Failure could be caused by the penetration of a pit, the complete corrosion of a small area of the waste package called a patch, or by structural failure. The time of failure, the failure mode, and subsequent degradation are important factors that could influence the rate of radionuclide release from the failed waste package to the surrounding environment.

To meet its objectives, WAPDEG must be able to:

- Account for variability of environmental conditions across the lateral extent of the waste package emplacement area

- Account for variability of environmental conditions along the length of a waste package, including the presence or absence of dripping and/or pooled water

- Allow different corrosion mechanisms to occur depending on local environmental conditions

- Allow drips to start, stop, and change chemical character at varying times

- Report waste package failures as a function of time, including the type of failure.

WAPDEG has evolved from the earlier referenced version (CRWMS M&O 1995) while maintaining the capability to recreate earlier results. Also as part of this evolution, several different approaches to modeling corrosion of the CRM were implemented. WAPDEG has been structured to maintain its capability to use all such models. However, only the preferred models were accessed for the TSPA-VA base case runs. The description that follows focuses on the capabilities that are required for the TSPA-VA base case, but the flexibility of WAPDEG is also occasionally evident from some of the text. For a complete discussion of all of the models and capabilities of the WAPDEG code, refer to the *WAPDEG Software Routine Report* (CRWMS M&O 1998c). Most of the modeling parameters discussed below are user-supplied values that are found in the WAPDEG input file (see Section 5.10.7). Parameter values used in the TSPA-VA base case analysis are provided in parentheses.

Number of Waste Packages - WAPDEG can model any number of waste packages in a given run, depending on available computer resources. However. because WAPDEG was written to the FORTRAN 77 standard, arrays whose size depend on the number of waste packages must have a preestablished dimension, currently set at 800. Experience has shown that for typical simulations output variability can be adequately captured through the use of about 400 waste packages per simulation.

Waste Package Groups - The user not only specifies the total number of waste packages, but can also define waste package groups such that each waste package in the group encounters common environmental exposure conditions. Here environmental exposure conditions refer to the time-dependent temperature and relative humidity profiles at the waste package surface. Spatial variability can be accounted for by providing multiple such history groupings within a single simulation and uncertainty in temperature, and relative humidity can be included by randomly perturbing the temperature and relative humidity of a given profile for each waste package within the group. (No temperature or relative humidity perturbations are used in the TSPA-VA base case).

Patches - To facilitate the capability to model variable exposure conditions within a single waste package, the total waste package surface area (~300,000 cm^2) is partitioned into smaller areas called patches (310 cm^2). The user supplies the number of patches per waste package. There is no maximum limit to the number of patches a waste package can have. WAPDEG assumes all patches for a given waste package are the same size. In addition, the user defines the top, sides,

and bottom of the horizontally emplaced package by the angles subtending the top (180 degrees) and bottom (180 degrees). WAPDEG then determines the number of top (482), bottom (482), and side patches (0) for each waste package. Corrosion is modeled at the patch level in WAPDEG.

Surface Area and Pit Density - The user specifies the waste package surface area and the pit densities to be used for the CAM and CRM (10 pits/cm^2 for both) should localized corrosion occur. WAPDEG uses the pit density, the surface area, and the number of patches to calculate the number of pits per patch on a given waste package. The current limit is 32,000 pits per patch. Within WAPDEG, pit sites in the CAM may be regions where roughness factors are applied or where high aspect ratio pitting occurs. Pit sites in the CRM may be regions where localized corrosion, pitting or crevice corrosion occurs. The same surface area is used for both the CAM and the CRM. This introduces little error given the 1.7 m diameter of the typical waste package (Benton 1997).

Number of Patches Contacting Drips - Dripping water can contact patches along the top of a waste package through dripping and along the bottom of the waste package through pooling of dripped water. The user supplies the probability of top patches being dripped on (100 or 0%) and of the bottom patches contacting pooled water (100 or 0%). Side patches are not dripped on based on the WPDEE (CRWMS M&O 1998b, p. 3-9). The probabilities themselves can have a probability distribution. If so, the distribution for top patches is sampled with perfect rank correlation to the distribution for bottom patches. This correlation schema is physically reasonable, as one would expect the frequency of bottom patches contacting pooled water to be highly correlated to the frequency of top patches encountering dripping water.

When Drips Start, Change Character, and Stop - The user provides the time that drips start (0 years), the time that the chemical character of the dripping water changes (never), and the time that drips stop (10^6 years). These three times can be fixed values or can be probability distributions that WAPDEG samples for each waste package. There is an order inherent in these times that can produce up to four different time segments: an initial no-dripping segment, an initial water character segment, a secondary water character segment, and a second no-dripping segment. Any subset of these segments can be modeled as long as the order is maintained. There are corrosion modeling issues that arise at segment time boundaries, which are addressed later in this section. Because the input here can be in the form of probability distributions, there is a possibility of inconsistent sampled times due to overlapping distributions. For example, the sampled value for dripping start time could exceed the sampled value for dripping stop time. In this case, there will be no dripping time segment modeled for the waste package. Similarly, if the sampled time that dripping water changes character is outside the range from the dripping start to dripping end sampled times, then there is only one water type considered for the waste package. If water changes character before dripping starts, all drips are of the second water type and if water changes after dripping stops, all drips are of the initial water type.

Patches Not Dripped On - WAPDEG assumes there is always a need for input describing the corrosion models for patches that see neither drips nor pooled water. In this case, the corrosion model for the CAM is the general corrosion model described in Sections 5.5 (humid-air general corrosion) and 5.6 (aqueous general corrosion). The corrosion model selected for the CRM is the general corrosion model described in Section 5.7, and no localized corrosion is allowed on

the CRM. In addition to corrosion models, the user must supply various thresholds for corrosion initiation on the CAM: (1) the temperature threshold for corrosion initiation, (2) the relative humidity threshold for initiation of humid-air corrosion, and (3) the relative humidity at which the CAM corrosion mode switches from humid-air to aqueous. These thresholds can be fixed values or probability distributions (WPDEE supplied CDFs) that WAPDEG samples for each waste package. The two relative humidity thresholds are sampled with perfect rank correlation, which maintains a constant difference between the two, if both distribution types are uniform, or a relatively constant difference, for other distribution types.

Dripped on Patches - WAPDEG determines if there is a need for input describing the corrosion models for patches that see drips or pooled water based on the dripping start and end times. The corrosion model for the CAM can be either the CAM general corrosion model or CAM pit growth law model discussed in Section 5.6. The corrosion model for the CRM is allowed to be one of the general corrosion models by itself or general corrosion plus one of the pit growth law models. For the base case, the corrosion model for the CRM is the general corrosion model (described in Sections 5.7 and 5.8) plus, if localized corrosion is active, a pit growth law with an Arrhenius temperature-dependence (described in Section 5.9). In addition to corrosion models, the user must supply thresholds for: (1) the temperature threshold for corrosion initiation, (2) the relative humidity threshold for initiation of humid-air CAM corrosion, (3) the relative humidity at which the CAM corrosion mode switches from humid-air to aqueous, and (4) the temperature threshold for the initiation of localized corrosion of the CRM. If the exposure temperature is below this threshold when the CAM is penetrated, localized corrosion will not initiate. These four can be fixed values or probability distributions that WAPDEG samples for each waste package. Under typical circumstances, the dripped-on/pooled patches will be subject to aqueous corrosion, and the user will force this by assigning low values to both relative humidity thresholds for the CAM.

However, to maintain generality, WAPDEG allows for the possibility of humid-air corrosion for water-contacted patches with appropriate relative humidity thresholds for humid-air and aqueous corrosion initiation. This feature is useful for a case with a low dripping rate, for which water on the waste package could evaporate quickly. The two relative humidity thresholds (humid-air and aqueous corrosion initiation) are sampled with perfect rank correlation. If distributions for both thresholds are uniform, a constant difference is maintained between the two thresholds. For other distribution types, a relatively constant difference is maintained. WAPDEG checks the temperature at the beginning of each time segment where the CRM is exposed to water to see if it is sufficiently high for localized corrosion to initiate (Section 5.9.3 and later in this section) by comparing to the threshold for that segment. If so, and if localized corrosion was requested by the user, then localized corrosion initiates and will continue throughout the current and all subsequent segments (as long as the user requested localized corrosion to be modeled in the subsequent segments). If the temperature is too low to initiate localized corrosion and localized corrosion was not initialized in a previous segment, then whether or not the user requested localized corrosion, WAPDEG applies only general corrosion for that time segment.

Transitioning from Segment to Segment (CAM) - Whenever WAPDEG encounters a time boundary between dripping conditions, corrosion processes must be reinitialized for the new time segment. For general corrosion of the CAM, this means applying the previously mentioned thresholds for the new segment and the new corrosion parameter values. Thus, corrosion can

initiate if the new thresholds are more relaxed or cease if they are more stringent. Also, WAPDEG uses the new user-supplied corrosion rate multipliers for the new segment each time it computes a general corrosion rate.

For modeling roughness or high-aspect ratio pitting corrosion of the CAM, some assumptions are made. If WAPDEG is transitioning from one time segment that uses CAM roughness factors or the CAM Pit Growth Law model to a time segment in which CAM roughness factors are used, WAPDEG simply samples a new roughness factor for each pit and the simulation proceeds. For the case of the CAM Pit Growth Law, one could define an "effective" roughness factor at the transition time by the ratio of total pit depth to patch general corrosion depth. If the roughness factor sampled for the new time segment exceeds the old one (or old effective one), this is obviously a conservative approach to modeling the corrosion process as the pit instantaneously deepens. One consequence of this modeling approach is that for some simulations there can be patches that are penetrated precisely on a transition time boundary (the new roughness factor is high enough to cause CAM penetration). If the new roughness factor is smaller than the old (or effective old) one, the pit essentially stops propagation (stifles) until the product of the new roughness factor with the general corrosion depth reaches the total pit depth at transition time. This is consistent with the conceptual model that pitting is stochastic and local corrosion conditions can change at time segment boundaries in such a manner that only shallower pits are able to propagate.

If WAPDEG is transitioning from a time segment which made use of roughness factors to one in which the CAM Pit Growth Law model is used, WAPDEG determines a corrosion time for each pit. That is, it finds the time that would have been required for the pit to reach its incremental depth (its depth beyond general corrosion depth) using the pit growth law parameters sampled for the pit. The time used for simulation of the pit growth law for the pit then becomes the time elapsed since transition plus this corrosion time. The TSPA-VA base case analysis does not use the CAM Pit Growth Law model (see Section 5.12 for a sensitivity study using the CAM Pit Growth Law model).

Transitioning from Segment to Segment (CRM) - During waste package corrosion modeling, whenever WAPDEG encounters a time boundary between dripping conditions, corrosion processes must be reinitialized for the new time segment. For general corrosion of the CRM this means using new sampled values for the corrosion rates in the new time segment, new corrosion rate multipliers, and new corrosion rate maximums.

For localized corrosion of the CRM, some assumptions are made. WAPDEG does not allow different localized corrosion models for the CRM to be used in the same simulation. Thus, for any time segment that includes a localized corrosion model, the model used in that segment is the same for every other time segment. Further, the pit properties are not allowed to change across time segment boundaries. In this way WAPDEG transitions over time segments in a seamless fashion for the CRM and no special treatment is required.

General Corrosion Rate Multipliers - The user can specify multiplication factors that are used to either enhance or lower general corrosion rates. These are used largely for sensitivity analyses, but in combination with other factors available in WAPDEG in the future will likely be used to account for disruptive events such as rock falls. The factors can be constant or can be

assigned probability distributions, one for the CAM and one for the CRM. Also, the fraction of waste package variance in this parameter accorded to waste packages must be specified.

Corrosion Delay (Ceramic Protection) - WAPDEG models the protective effects of an outer layer of ceramic coating around a waste package as a means to delay the onset of corrosion of the CAM. The user specifies a delay time, which can be in the form of a probability distribution. The user also specifies a waste package variance allocation fraction and the remaining variance fraction is assigned to patches. WAPDEG samples a different ceramic protection time for each patch, provided that patches are accorded a nonzero fraction of the variance, and delays onset of corrosion of the CAM for that patch until the sampled time. At that time, corrosion may or may not initiate on the CAM depending on the environment at that time and the temperature and relative humidity thresholds.

Structural Failure of Waste Packages - A waste package can collapse upon itself if it fails to maintain adequate container wall thickness. WAPDEG records average thickness of the CRM at a predetermined set of time points for each waste package. When the average thickness becomes less than the user specified structural integrity thickness, WAPDEG interpolates between the nearest two time steps to estimate the time of structural failure. The value required for input is a percentage. If average thickness becomes less than this percent of the CRM thickness, the waste package can be assumed to have failed structurally although WAPDEG continues to simulate the corrosion process. This information can be used to better represent repository performance. A recent analysis has addressed the issue of what thickness of the inner barrier must remain in order to maintain structural integrity and determined that 9.5 mm or 47.5 percent or the inner barrier is sufficient for this purpose (CRWMS M&O 1996b).

Probability Distributions - WAPDEG input variables may be specified through the use of probability distributions. Some distributions are required to be normal whereas others can be one of several standard types offered by WAPDEG. Table 5-8 shows the theoretical distributions offered and their required parameters.

A fixed distribution indicates to WAPDEG that the variable in question is to be constant at the value provided. In addition to the mean and standard deviation, a bounded normal requires a lower and upper bound that can be used to restrict the range of sampled values. If the bounds are more than 8 standard deviations (often fewer in practice) beyond the mean, they will have no effect on the range for the sampled values. A lognormal distribution is related to the normal distribution through the log transformation. WAPDEG requires the mean and standard deviation of the transformed distribution as input. Uniform distributions are often appropriate for variables whose uncertainty ranges over an order of magnitude or less, whereas loguniform distributions may be called for when the uncertainty ranges over several orders of magnitude. For the latter, there will be about the same number of sampled values in each log decade.

In addition to the theoretical distributions the user can supply an empirically defined distribution. Instead of distribution type, the user specifies a file name for WAPDEG to read. The data in the file must be in the form of a discrete CDF. WAPDEG linearly interpolates the CDF as a lookup table for sampling purposes. Finally, each variable that can be assigned a distribution type has a default distribution and parameters built into WAPDEG. So any such variable can be given the 'Default' distribution type.

Sampling Techniques - WAPDEG uses three sampling techniques. The usual way to sample a distribution for random variable X is to repeatedly obtain numbers p in (0, 1) and find the deviates x such that $p = pr(x < X)$, where pr denotes probability. This can be visualized by drawing the CDF for X, selecting a value for p on the vertical axis, and finding the x value on the horizontal axis that corresponds to p. Sampling techniques differ according to the method used to determine the values for p. In the discussion earlier on how WAPDEG allocates variance, the values for p are selected in a manner to facilitate sharing of the variance between waste packages and patches. WAPDEG also uses random sampling where the values of p are randomly and uniformly selected from the interval (0, 1) using a random number generator (Marsaglia and Zaman 1994). Finally, WAPDEG uses Latin Hypercube Sampling (Iman and Shortencarier 1984) to sample some of the pit properties, where the values of p are found by stratifying the vertical axis into intervals of equal size, and randomly and uniformly selecting a single value for p from each interval.

Waste Package/Patch/Pit Variability Allocation - The variance defined for many of the input variables to WAPDEG is assumed to arise from natural variability. The user has the option for such variables to allocate part of the variance to waste package-to-waste package variability and the rest to patch-to-patch variability (or in some cases both patch-to-patch and pit-to-pit variability). The method used to accomplish variability splitting is identical to Gaussian Variance Partitioning as discussed in Section 5.7.3. The variance share allocated among the waste packages is defined either as a fixed fraction or a probability distribution of fractions that will be sampled for each waste package. Each model parameter that can have its variance allocated is sampled for a waste package using its probability distribution, but with only the waste package's fraction of the distribution's variance. The result is treated as the mean value for the waste package for the sampling of the same property for each of the patches on the waste package, with the latter sampled using the remaining variance. If the model property is a parameter used in a pit growth law model, the variance that remains after the waste package share can be further allocated to both patches and pits. In these cases a second fraction is required, either as a fixed value or a probability distribution. It is used to define the patch share of the variability by multiplying its sampled value by the fraction of variance that remains after the waste package share. Finally, the remaining share is allocated to pit-to-pit variability. The technique used by WAPDEG to implement variance sharing is described under the Variance Allocation Technique below.

The variance allocation feature is available in WAPDEG for

- The parameters that are used to model humid-air and aqueous general corrosion of the CAM. The share of waste package variance can be different for no dripping, and each of the two dripping water conditions.

- The parameters that are used to model general corrosion of the CRM. Again, the share of waste package variance can be different for no dripping, and each of the two dripping water conditions.

- The parameters that are used in the CAM pit growth law model. The fraction of variance that remains after the waste package share can be further allocated to patch-to-patch variability and pit-to-pit variability.

- The parameters that are used to model localized corrosion of the CRM under dripping conditions. The fraction of variance that remains after the waste package share can be further allocated to patch-to-patch variability and pit-to-pit variability. The share of waste package variance can be different for the different dripping water conditions.

- The temperature threshold above which localized corrosion of the CRM will initiate. The share of waste package variance can be different for the different dripping water conditions.

- The rate multiplying factor for general corrosion of the CAM. The share of waste package variance can be different for no dripping and each dripping water condition.

- The rate multiplying factor for general corrosion of the CRM. Again, the share of waste package variance can be different for no dripping and each dripping water condition.

- The ceramic protection time distribution.

Variance Allocation Technique - Given a model parameter that is defined by a probability distribution and whose variance is to be allocated (part for waste package-to-waste package variability and the rest for patch-to-patch variability), the technique used by WAPDEG to implement variance allocation is to:

- Obtain a value for the waste package. WAPDEG randomly samples a value from a normal distribution whose mean is zero and whose variance is the fraction of variance accorded the waste package.

- Obtain a value for a patch on the waste package. WAPDEG randomly samples a value from a normal distribution whose mean is zero and whose variance is the fraction of variance accorded the patch. It then adds the result to the waste package deviate found in step 1 to get the patch value.

- Find the cumulative probability of the patch value. The patch value is normally distributed with mean equal to the package value and variance equal to the fraction of variance accorded the patch.

- Sample the model parameter of interest using the cumulative probability found in the step above.

The last three steps are repeated for each patch on the waste package. If the variance of the model parameter is to be further allocated to pits, steps similar to the last three steps are repeated for each pit on the patch.

The actual distribution for the given model parameter is not used until the last step. Thus, the first three steps represent a systematic approach to finding a probability to be used to sample the actual distribution. The systematic approach is an exact way to allocate variance if the actual distribution for the model parameter is normal and is approximate for other distribution types.

5.10.5 WAPDEG Program Structure

Figure 5-52 shows the main flow chart for WAPDEG. After reading input and initializing, WAPDEG loops over waste packages. It completely simulates each waste package before proceeding to the next. Each waste package is partitioned into small areas called patches, and corrosion is modeled at the patch level.

Input is supplied via a primary input file and history files. History files contain temperature and relative humidity variations with time and are read within the waste package loop. The 'Read input file' box means read the primary input file. The name of the primary input file is prompted by WAPDEG at run time. WAPDEG extracts the root name complete with any path prefix, and uses that root plus various extensions to name the output files associated with the run. In this way, WAPDEG simulations are easily tracked. Output files are discussed in Section 5.10.7.

WAPDEG performs several input data checks. Some errors are fatal, stopping the run, whereas others prompt WAPDEG to issue warning messages. Fatal errors are written to the screen and to the primary (*.out) and auxiliary (*.aux) output files. Warnings are written only to the auxiliary file. Warnings include any changes WAPDEG makes to the user's input, such as normalizing the number of waste packages per group to the total number specified or imposition of any default values.

Provided that there are no errors, WAPDEG next sets the general corrosion parameters for the CAM, denoted by the 'Set CAM parameters' box. These include the mean and standard deviations for each parameter and the covariances amongst parameters for both the humid-air and aqueous general corrosion models. The error variance and the share of variance accorded the waste packages is accounted for when sampling these distributions for each waste package.

In the primary input file, the user provides a seed for the random number generator (Marsaglia and Zaman 1994) used by WAPDEG and the number of waste packages. WAPDEG uses this seed to establish multiple sets of random seeds, one set per waste package, as denoted by the box "Set random seeds." The waste package seeds are based on the total number of waste packages. In a different part of the input file, the user can specify that only a selected subset of waste packages is to be (re)run. If so, the seeds for each of the simulated waste packages can be recovered as long as the same input seed is used. Thus for example, a subset of waste packages rerun will have the same results as they had when they were simulated as part of a larger run. This feature can also be used as a restart capability should the need arise.

As Figure 5-52 shows, the loop over waste packages uses a loop control variable named Pack. The first task for each waste package is to sample all of the waste package level variables. The box "Sample parameters for Pack" refers to a subroutine that will:

- Retrieve the seed for random number generation for the waste package
- Sample the number of patches for the waste package
- Sample parameters for the CAM humid-air and aqueous general corrosion models

- Sample a set of pit multiples to be used for roughness calculations on the CAM for use on patches that do not contact dripping or pooled water

- Sample the general corrosion rates (or general corrosion parameters) for the CRM for use on patches that do not contact dripping or pooled water

- Sample the thresholds for the CAM corrosion initiation temperature and the relative humidities for CAM corrosion initiation and aqueous corrosion transition to be used for patches that do not contact dripping or pooled water

- Sample the multipliers to be applied to the general corrosion rates for both the CAM and CRM for use on patches that do not contact dripping or pooled water.

Note that the sampled values for the general corrosion of the CAM and CRM and for the multipliers of the general corrosion rate are not explicitly used by WAPDEG beyond serving as the mean values for the same properties sampled at the patch level. The sampling of CAM roughness factors at the waste package level is done to speed WAPDEG execution time by re-using the same sample for each patch on the waste package. The drawback to this approach is the potential loss of variability or uncertainty in the WAPDEG results. However, the loss is expected to be minimal especially because WAPDEG resamples the upper tail of the distribution for each patch, and the upper tail drives the first pit penetration times.

If WAPDEG detects that there is to be a time segment (or time segments) during which dripping water will be present, then it will:

- Sample parameters for the CAM humid-air and aqueous general corrosion models for use on patches that contact dripping or pooled water

- Sample a set of pit multiples to be used for roughness calculations on the CAM for use on patches that contact dripping or pooled water

- Sample the general corrosion rates (or general corrosion parameters) for the CRM for use on patches that contact dripping or pooled water

- Obtain a sample for each model parameter, where the sample size is the number of pits per patch, for use on patches that contact dripping or pooled water if localized corrosion is to be simulated on the CRM

- Sample the thresholds for the CAM corrosion initiation temperature and CRM localized corrosion initiation temperature and the relative humidities for CAM corrosion initiation and aqueous corrosion transition to be used for patches that contact dripping or pooled water

- Sample the multipliers to be applied to the general corrosion rates for both the CAM and CRM for use on patches that contact dripping or pooled water.

As with the nondrip case discussed earlier, the sampled values for the general corrosion of the CAM and CRM, the localized corrosion initiation threshold temperature for the CRM, and the multipliers of the general corrosion rate are not explicitly used by WAPDEG beyond serving as the mean values for the same properties sampled at the patch level. The sampling of pit properties at the waste package level for the CRM is done differently depending on how the variance is to be allocated. If the share of the variance of the pit properties accorded to the patches is zero, the complete sample for the pits can be found at the waste package level. Otherwise, it is not found until patches are addressed, as described later in this section.

WAPDEG finishes the waste package setup routine in four more steps.

- If WAPDEG detects that there is to be dripping of any kind, it samples the probability distributions for the probability that top patches and bottom patches contact dripping or pooled water for this waste package. It also samples the dripping start time and stop time, and if water changes character, it samples that transition time. WAPDEG uses the rules of the proceeding section to ensure that the sampled times are ordered properly.

- WAPDEG samples the ceramic protection delay time. This waste package level value is used as the mean for sampling patch level values for patches on this waste package.

- WAPDEG adopts the rule that if there are two different water chemistries encountered during a waste package simulation, the localized corrosion model used for the CRM must be the same for both water chemistries. Further, the values sampled for the parameters used by the selected localized corrosion model are not allowed to change when the water chemistry changes. If the user has supplied distributions for the localized corrosion model parameters as part of the initial dripping time segment properties that are different from those that are part of the final dripping time segment properties, WAPDEG ignores the latter. So in this case, the properties sampled for the initial water chemistry are used for both water chemistries.

- WAPDEG initializes output variables and writes waste package properties to the .aux file.

If the waste package is the first of a new group, shown on Figure 5-52 with the diamond asking "New group?" then the history file for the waste packages of that group is read next. The box that shows "Read history" is for a subroutine that opens and reads the file. A history file contains three columns: time in years, temperature in °C, and relative humidity as a fraction. There can be more columns on the file as long as these are the first three. WAPDEG converts temperatures to Kelvin and relative humidities to percentages for internal use.

The box that says "Refine grid, if requested" is a subroutine that interpolates the history to add time steps so that only small changes in temperature and humidity are allowed from time step to time step. The user defines small in the primary input file as absolute maximums of temperature and relative humidity change allowed. WAPDEG assumes that temperature and humidity vary linearly versus the logarithm of time to do the interpolation (i.e., semi-logarithmic interpolation is used).

Once the temperature and relative humidity history is read and optionally refined, it can be randomly perturbed for the waste package, as indicated by the box "Sample T, RH." The user supplies a standard deviation for temperature and one for relative humidity, and the uncertainty about temperature and humidity at each time step is assumed to follow the form of a normal distribution. There is only one multiple of the standard deviation found for temperature and one for humidity. Thus, even though there is uncertainty in the profile for the waste package, the perturbed history curves are parallel to the mean curve provided by the input.

The box "Set time grids" refers to WAPDEG creating two time grids for the waste package based on the history file for the waste package, possibly refined. It first establishes a time grid to be used for those patches that see neither drips nor pooled water using the no drip thresholds sampled for the waste package. This means that WAPDEG inserts time points to ensure that the crossing of any threshold occurs on a time step boundary. Then if there is a possibility of drips, it also establishes a time grid for patches that are dripped on or are in pools. This could be a different grid because the thresholds sampled for drip conditions are generally different from those sampled for no drip conditions. WAPDEG also inserts time steps into the dripped-on time grid so that the start, stop, and change times for drips occur on time step boundaries.

The patch loop is then initiated for the waste package. The first step is to sample properties for the current patch. The box "Sample parameters for Patch" refers to a subroutine that will:

- Sample a random number and compare to the drip probability for the waste package to determine if the patch sees drips or pooled water.
- Retrieve the appropriate time grid for the waste package depending on whether drips occur.
- Sample the ceramic protection time. If the sampled time is positive, truncate the time grid on the left at the sampled time.
- Create grid-centered temperatures and relative humidities. WAPDEG assumes that the endpoint averaged temperature and relative humidity over a time step applies to the entire time step.
- Sample the CAM general corrosion parameters for the patch based on average values sampled for the waste package and the patch share of the variance for all dripping and no dripping conditions.
- Determine the number of time segments for the patch and number them.
- If there is a no-drip segment (there could be two), resample the largest roughness factor to be used for the CAM, sample the CRM general corrosion rates (or parameters) using the waste package means and the patch share of the variance, and sample the rate multipliers for the CAM and CRM general corrosion rates using the waste package means and the patch share of the variance.

- Determine the type of water involved provided there is an initial drip segment. Then, resample the largest roughness factor for the CAM (if applicable); sample the CRM general corrosion rates (or parameters) using the waste package means and the patch share of the variance; select the appropriate parameters for the CRM pitting model if they have already been sampled at the waste package level or sample them at this time (if localized corrosion applies); sample the localized corrosion initiation temperature threshold for the CRM using the waste package mean and the patch share of the variance; and sample the rate multipliers for the CAM and CRM general corrosion rates using the waste package means and the patch share of the variance.

- Provided there is a second drip segment, determine the type of water involved. Note it must be the alternate to the initial water type. Repeat the steps for the initial drip segment using the properties for the second water type.

In general terms the "Model corrosion" box follows four steps. Each of these steps is expanded in detail in Figures 5-53 through 5-56. To summarize the steps, WAPDEG

- Determines general corrosion depth with time on the CAM using the time grid for the patch and the general corrosion parameters sampled for the patch. Patch general corrosion depth versus time is found from corrosion initiation time until either the patch completely corrodes or the end of simulation time, whichever comes first.

- Determines earliest penetration of the CAM. This can be due to roughness factors or high aspect ratio pitting (CAM Pit Growth Law model).

- Resets the time grid so that time zero is the time when the CAM was first penetrated. Determines general corrosion depth with time on the CRM using the temperatures from the time grid for the patch and the general corrosion rates sampled for the patch. (Two alternative models are available [CRWMS M&O 1998c]). Patch depth versus time is found from corrosion initiation time until either the patch completely corrodes or the end of simulation time, whichever comes first.

- Determines the pit penetration history of the CRM, if applicable. This step is not done if the patch contact neither dripped nor pooled water, the surface temperature was not sufficiently high to initiate localized corrosion, or the user specified use of general corrosion only for the CRM.

Figure 5-53 depicts the procedure for modeling general corrosion of the CAM. The "Initialize" box means set the patch depth arrays to zero and initialize the penetration time variables. Then, the loop over time segments begin. WAPDEG first retrieves the temperature and relative humidity thresholds for the current segment, as denoted by the "Set thresholds" box.

The diamond that asks if the thresholds are met applies to the temperature and relative humidity for the current time step, time step j. If the temperature is too high for corrosion to occur or the relative humidity is too low for humid-air corrosion, WAPDEG sets the patch depth at the end of time step j to that at the end of time step $j - 1$ (i.e., no corrosion occurs during step j). Otherwise, WAPDEG uses either the humid-air general corrosion parameters or the aqueous general

corrosion parameters to find the general corrosion rate for the time step and multiplies the rate by the CAM general multiplying factor for the current segment. Then using the sampled value for the power-of-time exponent in conjunction with the corrosion time concept (discussed in detail in Section 5.10.4), WAPDEG finds the patch depth at the end of the time step.

WAPDEG applies the corrosion time concept by first asking: How much time would be required for general corrosion to reach the depth at the beginning of the time step if the temperature and relative humidity for the current time step would have applied from the beginning of corrosion? This corrosion time, $t_{c(j-1)}$, is found for time step j (t_{j-1}, t_j) by using the terms defined in Equation (5-36):

$$t_{c(j-1)} = (D_{g,j-1} / f_{NFE,j})^{1/d} \tag{5-41}$$

where $D_{g,j-1}$ is the general corrosion depth at the beginning of time step j, $f_{NFE,j}$ is the corrosion rate for time step j, and d is the time exponent. Corrosion time is then augmented by the size of time step j, $(t_j - t_{j-1})$ and is used to find the corrosion depth at the end of time step j by:

$$D_j = f_{NFE,j}(t_{c(j-1)} + t_j - t_{j-1})^d \tag{5-42}$$

The time in parentheses is saved and called the corrosion time for time step j, t_{cj}.

The box "Patch thru?" asks whether the entire patch has failed by general corrosion by the end of time step j. If not, WAPDEG proceeds either to the next time step in the current segment, the next time segment, or exits the segment loop. So, WAPDEG tracks the entire history of the patch general corrosion depth until it fails or the end of simulation is reached. If the patch fails prior to the end of simulation, such as during time step j, WAPDEG again uses the concept of corrosion time to find the exact time the patch failed, as denoted by the box "Find breach time." Corrosion time to reach the CAM thickness, h_{CAM}, is found by:

$$t_c = (h_{CAM} / R_j)^{1/d} \tag{5-43}$$

This corrosion time is subtracted from the corrosion time to reach the depth at the end of time step j and the result is subtracted from the actual time at the end of time step j to obtain patch failure time, t_{PAT}:

$$t_{PAT} = t_j - (t_{cj} - t_c) \tag{5-44}$$

The patch general corrosion depth history for the current patch is added to that for the other patches on the current waste package as noted by the "Accumulate thickness history" box. Later when the waste package is complete, the cumulative depths are divided by the number of patches to find the average waste package depth. The results are reported in the *.cam file (discussed in Section 5.10.7).

Figure 5-54 depicts the procedure for modeling CAM breach with the roughness factor or high-aspect ratio pitting. Because the pitting mechanism and model on the CAM can change when dripping conditions change in WAPDEG, there is a loop over segment. The question in the diamond "Model roughness?" determines which model is to be used for the current segment. An affirmative answer leads down the left side of the flow chart where roughness factors are used to model local variations in the general corrosion depth. There are nested loops over pits, then time in the particular segment. The question "Mp*D(j) > CAM?" is asking whether the product of the roughness factor for the current pit, *Mp*, times the patch general corrosion depth at the end of time step *j*, *D(j)*, exceeds the thickness of the CAM. If so, as indicated by the box stating "Find pit penetration time," WAPDEG computes when the pit broke through the CAM. The procedure is the same as described above for finding the time when an entire patch fails except that the appropriate depth is h_{CAM}/Mp, rather than h_{CAM}. Each time a new pit is to be examined, the time index, j, is reset to the initial time step in the current segment, as denoted by the box "j = SegStart." When all pits are exhausted, WAPDEG checks to see if the CAM has been penetrated. If so, it proceeds to the corrosion of the CRM with the earliest penetration time. If not, it proceeds to the next time segment. If there are no more time segments, then the CAM is not penetrated for the current patch, and WAPDEG proceeds to the next patch. In practice when only roughness is being treated in a WAPDEG simulation, to speed execution time, WAPDEG reduces the number of pits to one and assigns that pit the greatest roughness factor.

If the answer to "Model roughness" is negative, then WAPDEG institutes the CAM Pit Growth Law model for high-aspect ratio pitting. The initial conditions for this model are established for each pit. For the first segment, corrosion time is zero for each pit. For subsequent segments, corrosion time in the current context is the time that would have been required for the pit to reach its incremental depth (the depth beyond the general corrosion depth) using the Pit Growth Law model parameters for the pit. The pit is then allowed to grow using a growth rate appropriate from that time onward. If the incremental pit depth at the beginning of the time segment is I_{pit}, then the corrosion time is:

$$t_c = (I_{pit} / B)^{1/n} \tag{5-45}$$

where B and n are the sampled values for the pit growth law parameters for the current pit (discussed in Section 5.6.4). Incremental pit depth at the end of time step j in the current segment is then

$$P_j = B(t_j - t_c)^n \tag{5-46}$$

The diamond asking "P(j) + D(j) > CAM" becomes: Is the sum of the two depths (the total pit depth) sufficient to penetrate the CAM at the end of time step *j*? If so, WAPDEG linearly interpolates depth versus time over time step *j* to estimate the pit penetration time. The rest of the right hand side of the flow chart functions identically to the left hand side.

Figure 5-55 depicts the procedure for modeling general corrosion of the CRM. The steps are quite similar to those for the simulation of general corrosion of the CAM, Figure 5-53. One

difference is the lack of threshold checking for the CRM. The assumption made for the CRM by WAPDEG is that temperatures decrease with time. So by the time corrosion begins on the CRM, the temperature is sufficiently cooled to allow water to exist on the CRM. A second difference is the time scale. As denoted by the first box "Slide time scale and find LostSeg," WAPDEG adjusts the time grid so that corrosion begins at time zero on the CRM. Because the time of CAM penetration may have occurred after a change in dripping conditions, there may be time segments that the CRM does not experience. So corrosion begins during the first time segment that is not totally lost.

For the TSPA-VA base case model, CRM general corrosion rates are interpolated versus temperature. WAPDEG uses the assumption that the logarithm of the rate varies linearly versus the reciprocal of temperature. If there are temperatures encountered outside the temperature range specified by the user for the corrosion rates, WAPDEG extrapolates using the same relationship. The box "Find corrosion rate & depth for time j" finds the rate, multiplies it by the length of the current time step, and adds the result to the depth at the beginning of the time step.

The box "Patch thru?" asks whether the entire patch has failed by general corrosion by the end of time step *j*. If not, WAPDEG proceeds either to the next time step in the current segment, the next time segment, or exits the segment loop. So, WAPDEG tracks the entire history of a patch until it completely fails or the end of simulation is reached. If the patch fails prior to the end of simulation, WAPDEG linearly interpolates depth versus time to find the time the patch fails, as denoted by the box "Find penetration time."

The patch depth history for the current patch is added to that for the other patches on the current waste package as noted by the "Accumulate thickness history" box. Later when the waste package is complete, the cumulative depths are divided by the number of patches to find average corrosion depth for the waste package. The results are reported on the *.crm file, discussed in Section 5.10.7. WAPDEG also uses this history to report the time of structural failure for the waste package. The time at which the average corroded depth reaches the critical percent of total CRM thickness is interpolated and reported as structural failure time on the *.out file. The user provides the critical percentage in the primary input file.

Figure 5-56 depicts the procedure for modeling localized corrosion (pitting and crevice corrosion) of the CRM. The first question in the segment loop is whether localized corrosion should be treated for the segment, as indicated by the diamond which asks "Pitting?." There are two parts to the question: Was localized corrosion requested by the user for the dripping conditions that apply to this segment, and if so, is the temperature at the beginning of this segment sufficiently high that localized corrosion will initiate? The second part of the question will be overridden if localized corrosion initiated in an earlier segment. That is, once localized corrosion initiates on the CRM, it continues in every subsequent segment in which the user requested it. Also, as part of the decision to initiate localized corrosion, WAPDEG assumes that temperatures are decreasing with time so that only the initial temperature for the segment need be checked.

If localized corrosion is not treated in the segment, WAPDEG checks to see if the patch completely corrodes through during the segment. If so, then the answer to "Patch thru?" is affirmative, and WAPDEG is done modeling the patch because it already knows the failure time.

If not, then WAPDEG either proceeds to the next time segment or finishes with the patch with no breakthrough prior to the end of simulation time.

If the answer to "Pitting?" is affirmative, then WAPDEG institutes the pit growth law model selected by the user. For the base case model, a pit growth law model with the Arrhenius temperature dependence is used. The part of the second box that sets "j = SegStart" is setting the time loop counter to the first time index in the current segment. The incremental pit depth (the pit depth beyond the general corrosion depth) at the end of time step j, P_j, is computed using the temperature for time step j, T_j, and the pit growth law parameters for the pit, A, C, and n, in the equation:

$$P_j = e^{(A-C/T_j)}(t_j^{\,n} - t_{j-1}^{\,n}) + P_{j-1} \tag{5-47}$$

If the total pit depth exceeds the thickness of the CRM, the time of penetration is approximated. Here, WAPDEG uses linear interpolation on total depth versus time if the larger component in the change in total pit depth from the beginning of the time step to the end was because of general corrosion, and logarithmic interpolation otherwise.

When all pits have been exhausted, WAPDEG checks if the general corrosion of the patch was sufficient to penetrate the CRM thickness, as denoted by the lower diamond that asks "Patch thru?" If so, then pits are no longer counted from the time step during which the patch failed onward. This avoids a double counting of the area open for radionuclides to escape. One consequence of this is that the cumulative number of pits penetrating with time need not be monotonically increasing. This can often be seen in the *.bin file (discussed in Section 5.10) and on the columns of the *.out file that report cumulative pits at selected times.

Returning to the main flow chart, Figure 5-52, once all patches have been modeled for a waste package, WAPDEG writes the results for the waste package and proceeds to the next. The results written are described in Section 5.10.7.

5.10.6 Description of WAPDEG Input

Perhaps the most efficient way to describe the inputs for WAPDEG would be by considering its input file. Below is shown an input file (NE1a5set5.inp) for one of the TSPA-VA base case WAPDEG simulations:

```
snf, always drip, 100%, No Backfill, lta nominal i alpha mean, 5/20/98
Uncertainty/Variability=50/50, 50th Quantile

START OF PARAMETERS
3.09                          |Version number of code
12                            |Number of alternate histories
NEsnf00noBFj2204.hst          |History file
15, 0., 0.                    |# packages/group and Temp & RH std deviations
NEsnf01noBFj2204.hst          |History file
59, 0., 0.                    |# packages/group and Temp & RH std deviations
NEsnf10noBFj2204.hst          |History file
6, 0., 0.                     |# packages/group and Temp & RH std deviations
```

```
NEsnf11noBFj2204.hst        |History file
120, 0., 0.                 |# packages/group and Temp & RH std deviations
NEsnf12noBFj2204.hst        |History file
1, 0., 0.                   |# packages/group and Temp & RH std deviations
NEsnf21noBFj2204.hst        |History file
60, 0., 0.                  |# packages/group and Temp & RH std deviations
NEsnf22noBFj2204.hst        |History file
16, 0., 0.                  |# packages/group and Temp & RH std deviations
NEsnf31noBFj2204.hst        |History file
26, 0., 0.                  |# packages/group and Temp & RH std deviations
NEsnf32noBFj2204.hst        |History file
50, 0., 0.                  |# packages/group and Temp & RH std deviations
NEsnf42noBFj2204.hst        |History file
36, 0., 0.                  |# packages/group and Temp & RH std deviations
NEsnf52noBFj2204.hst        |History file
9, 0., 0.                   |# packages/group and Temp & RH std deviations
NEsnf62noBFj2204.hst        |History file
2, 0., 0.                   |# packages/group and Temp & RH std deviations
10.0, 2.0                   |Thickness of outer, inner barriers (cm)
50., 0.35                   |% thick to fail CRM, frac variance to packs
400, 964, 3100, 3100        |Number of packs, patches/pack, pits/patch
1.0, 1.e6, 1200             |Bin start time & end time (y), and # of bins
1.e4, 5.e4, 1.e5, 1.e6      |Output times (y) for cumul. pit penetrations
304058394, F, F             |Random# seed, restart?, ignore CAM variance
0.0, 0.0                    |Max temp, RH change over a time step (C, %RH)
180., 180.                  |Angle defining top/bottom (degrees)
Fixed                       |Distribution for fraction top seeing drips
1.                          |Distribution parameter(s)
Fixed                       |Distribution for fraction bottom seeing drips
1.                          |Distribution parameter(s)
Fixed                       |Distribution for dripping start time
0.                          |Distribution parameter(s)
Fixed                       |Distribution for dripping stop time
1000000.                    |Distribution parameter(s)
T, F                        |Neutral(T/F) water initially, new water (T/F)
Fixed                       |Distr for time range for ceramic protection
0.0                         |Distribution parameter(s)
1.0                         |Package variance share
[No Drip Model, CAM]        |This segment always required
CAMGeneral+PitMultiples     |CAM corrosion model for no drips
B-Normal                    |Distribution for pit multiple
1.5, 0.25, 1.0, 1.0e6       |Mean, StDev, Min, Max
[No Drip Model, CRM]        |This segment always required
CRMGeneralRateOnly          |CRM corrosion model for drips
3, 1.e+6                    |Number of dists (temps), max CRM rate
25.                         |Temp appropriate for dist #1
File                        |Distribution type for #1
gnd17550.cdf                |Distribution parameter (s)
50.                         |Temp appropriate for dist #1
File                        |Distribution type for #1
gnd27550.cdf                |Distribution parameter (s)
100.                        |Temp appropriate for dist #2
File                        |Distribution type for #2
gnd37550.cdf                |Distribution parameter (s)
[No Drip Features]          |This segment always required
File                        |Distr for thermal protection temperature
TThresh.cdf                 |Distribution parameter(s)
```

```
File                                  |Dist type for humid-air initiation
HARH.cdf                              |Distribution parameter(s)
File                                  |Dist type for humid-air/aqueous transition
AQRH.cdf                              |Distribution parameter(s)
1.0                                   |RH correlation factor
0.0, 0.0                              |Galvanic protect depth %, % patches protected
0.0                                   |Spalling depth as a % of thickness
Fixed                                 |Dist for multiple for CAM corrosion rate
1.0                                   |Distribution parameter(s)
Fixed                                 |Dist for multiple for CRM corrosion rate
1.0                                   |Distribution parameter(s)
1.0                                   |Pack variance share for multiples
[Neutral Drip Model, CAM]             |Required if any non-neutral drips can be seen
CAMGeneral+PitMultiples               |CAM corrosion model for no drips
B-Normal                              |Distribution for pit multiple
1.5, 0.25, 1.0, 1.0e6                 |Mean, StDev, Min, Max
[Neutral Drip Model, CRM]             |Required if any non-neutral drips can be seen
CRMGenrate+ArrheniusPit               |CRM corrosion model for drips
3, 1.e+6                              |Number of dists (temps), max CRM rate
25.                                   |Temp appropriate for dist #1
File                                  |Distribution type for #1
g8415050.cdf                          |Distribution parameter (s)
50.                                   |Temp appropriate for dist #1
File                                  |Distribution type for #1
g8425050.cdf                          |Distribution parameter (s)
100.                                  |Temp appropriate for dist #2
File                                  |Distribution type for #2
g8435050.cdf                          |Distribution parameter (s)
Normal                                |Distribution type for A (b0)
11.275, 2.4495                        |Distribution parameter(s)
Fixed                                 |Distribution type for K (b1)
5.5494e+003                           |Distribution parameter(s)
Fixed                                 |Distribution type for n
0.5                                   |Distribution parameter(s)
[Neutral Drip Features]               |Required if any non-neutral drips can be seen
File                                  |Distr for thermal protection temperature
TThresh.cdf                           |Distribution parameter(s)
Uniform                               |Dist type for CRM LC T init
80., 100.                             |Distribution parameter
File                                  |Dist type for humid-air initiation
HARH.cdf                              |Distribution parameter(s)
File                                  |Dist type for humid-air/aqueous transition
AQRH.cdf                              |Distribution parameter(s)
1.0                                   |RH correlation factor
0.0, 0.0                              |Galvanic protect depth %, % patches protected
0.0                                   |Spalling depth as a % of thickness
Fixed                                 |Dist for multiple for CAM corrosion rate
1.0                                   |Distribution parameter(s)
Fixed                                 |Dist for multiple for CRM corrosion rate
1.0                                   |Distribution parameter(s)
1.0                                   |Pack variance share for multiples
```

All of the text that appears above the 'START OF PARAMETERS' statement is copied into the output file (*.out, where the * represents the input file prefix) and can be used for any additional comments the user feels is necessary to distinguish the output. Here we have specified that the waste package size is consistent with that of a spent nuclear fuel waste package, all of the waste

package surface will be dripped on at all times, and we are using temperature and relative humidity histories appropriate to the case of no backfill and long-term average climate with a nominal infiltration and a mean value of alpha (Van Gennchthen parameter, see Chapter 3). Furthermore, the simulation was executed on 5/20/98 and had an uncertainty/variability partition ratio of the CRM dripping general corrosion CDFs of 50%/50% with the uncertainty distribution having been sampled at the 50th percentile.

The version number (3.09) is read and checked against the version of WAPDEG being executed; a mismatch in version numbers will halt program execution. The next line of the input file specifies the number of waste package groups (12, for this particular simulation) that will be used to represent local repository conditions (spatial variability in the drift-scale thermal-hydrology of the repository). The next 24 lines in the input file are composed of 12 pairs of input lines in which the first line specifies the name of the mean history file (*.hst, composed of three columns of data: time, waste package surface temperature, and relative humidity) to be used for each waste package group and is followed by a line composed of three values; the number of waste packages that the history file is to be applied to (the number of waste packages in the group), and the standard deviations for allowed variations in temperature and relative humidity from the waste package group's mean history file. In the TSPA-VA base case, there are no variations allowed from the T and RH data given in the history file. The next input lines:

```
10.0, 2.0                      |Thickness of outer, inner barriers (cm)
50., 0.35                      |% thick to fail CRM, frac variance to packs
400, 964, 3100, 3100           |Number of packs, patches/pack, pits/patch
1.0, 1.e6, 1200                |Bin start time & end time (y), and # of bins
1.e4, 5.e4, 1.e5, 1.e6         |Output times (y) for cumul. pit penetrations
304058394, F, F                |Random# seed, restart flag, ignore CAM variance
0.0, 0.0                       |Max temp, RH change over a time step (C, %RH)
```

allow for input of the outer and inner barrier thicknesses in centimeters. The first value on the next line is related to determination of a structural failure time for the waste package. For each waste package, WAPDEG calculates the average (over all patches) CRM general corrosion depth at each time step. When this average depth exceeds the given percentage (50 percent in this case) of the total CRM thickness, the waste package can be considered to have structurally collapsed (presumably because of static loads from its own weight, the weight of rock, etc.). WAPDEG still continues to model corrosion after this time, and the structural failure time is output (to the .out file) for possible use in other models. The second value on this line (0.35) allows the user to specify the fraction of the total variability in the various model parameters should be assigned to waste package-to-waste package variability and 1 – (this value) is assigned to patch-to-patch variability.

The line following allows the user to specify the number of waste packages (400), patches/waste package (964), and pits/patch (3,100) in both the CAM and CRM to be simulated. The next line contains three values related to the storing of temporal results (number of pit and patch penetrations with time). The start time corresponds to the beginning of the simulation. If the history file does not contain data for this starting time, the simulation is assumed to start with the earliest time step given in the history file. The same is not true for the end time as a time step is added to the end of the history with the same temperature and relative humidity as the last time step in the history file if the history file does not contain data for the simulation end time. The

third value specifies how many (logarithmically distributed) time bins are used to store the cumulative pit penetration profiles. In this way, the resolution of the pit penetration profiles reported by WAPDEG is under user control.

The next line allows the user to specify up to 4 time values that are of particular interest. For each time value, WAPDEG will report (in the *.out file) the cumulative number of pit and patch penetrations in the time bin that contains the specified time value, and not the actual number of pit and patch penetrations at the exact time value specified. The following input line specifies the random number seed used to initialize the random number generator. Also on this line, two boolean flags identify whether the simulation is a "restart" run and whether to ignore the variance in CAM corrosion parameters and use only the mean values, respectively. In a restart run, the first flag discussed above is set to T and the subsequent input line (which must not appear if the flag is set to F) must specify the range of waste package numbers to simulate. The next line allows the user to enter the maximum allowed change in temperature and relative humidity between time steps (0.0, 0.0 causes this option to be ignored). WAPDEG will add time steps to the history file and interpolate T and RH data until these criteria are satisfied. The corrosion models used in WAPDEG require the application of constant environments for the duration of each time step. Through wise application of these values the user may increase the accuracy of the WAPDEG output. The next input lines deal with the application of dripping models.

```
180., 180.                    |Angle defining top/bottom (degrees)
Fixed                         |Distribution for fraction top seeing drips
1.                            |Distribution parameter(s)
Fixed                         |Distribution for fraction bottom seeing drips
1.                            |Distribution parameter(s)
Fixed                         |Distribution for dripping start time
0.                            |Distribution parameter(s)
Fixed                         |Distribution for dripping stop time
1000000.                      |Distribution parameter(s)
```

The user can enter the angle range that defines the top and bottom of the waste package. The remaining angle range (if any) is defined to be the side of the waste package. The side of the waste package differs from the top or bottom in that it can never be dripped on and, thus, never undergoes localized CRM corrosion. WAPDEG allows dripping on a given (top or bottom) patch to start sometime after the beginning of the simulation, to change chemistry sometime after that, and then for dripping to cease. The user must enter the fraction of top and bottom patches that are dripped on, which can be given by one of WAPDEG's built-in distributions that are summarized in Table 5-8. The user may choose "File" in which case the user must supply a the name of a file (look-up table). In the "File" option, the first line of the file used must consist of an integer indicating how many data pairs follow. These data pairs must consist of a value for the property that the file represents and a corresponding CDF value (between 0 and 1). The user may also specify "Default" in which case WAPDEG will use CDF values hardwired in the code.

In addition to dripping start and stop time distributions shown above, the user can cause dripping to change chemistry,(corrosion parameters) at some time during the WAPDEG simulation. The input line:

```
T, F                          |Neutral(T/F) water initially, new water (T/F)
```

allows the user to specify whether the chemistry (corrosion parameters) of the dripping water is initially neutral (T) or chemical (F) in nature and whether the dripping water changes chemistry (T) or not (F). (The words neutral and chemical here have nothing to do with the actual water chemistry, they merely serve to identify groups of user-supplied input parameters that appear later in the input file.). If the dripping water changes chemistry, the user must specify a distribution and parameters for the water chemistry change time on the next input lines. These lines must not be supplied if no change in dripping water chemistry occurs, as in the TSPA-VA base case. In the above example, dripping starts at 0 years, stops at 10^6 years, and never changes chemistry (corrosion parameters). The corrosion parameters from the [Neutral Drip Model, CAM], [Neutral Drip Model, CRM], and [Neutral Drip Features] input segments will be used (see below).

The next input lines:

```
Fixed                          |Distr for time range for ceramic protection
0.0                            |Distribution parameter(s)
1.0                            |Package variance share
```

are concerned with modeling the use of a ceramic coating to offer additional corrosion protection to the waste package. In the current WAPDEG version, the ceramic coating is considered to offer complete corrosion protection to the waste package until it fails. This parameter is not used in the TSPA-VA base case simulations.

The next input segment:

```
[No Drip Model, CAM]           |This segment always required
CAMGeneral+PitMultiples        |CAM corrosion model for no drips
B-Normal                       |Distribution for pit multiple
1.5, 0.25, 1.0, 1.0e6          |Mean, StDev, Min, Max
```

specifies the outer barrier (CAM) and inner barrier (CRM) corrosion models to be used when drips are not present. WAPDEG offers a variety of CAM and CRM models from which to choose (CRWMS M&O 1998h). Here, we discuss only those used in the TSPA-VA analysis (Sections 5.6, 5.7, 5.8, and 5.9).

The CAMGeneral+PitMultiples model for the CAM requires a roughness factor distribution. In the TSPA-VA base case, we make use of a bounded normal distribution with a mean of 1.5, a standard deviation of 0.25, a lower bound of one, and, effectively, no upper bound. The CAMGeneral+PitGrowthLaw for the CAM requires distributions for B and n in the pit growth law equation (Section 5.6.4). Both of these CAM models use the humid-air and aqueous CAM general corrosion models discussed previously (Sections 5.5 and 5.6).

The CRMGeneralRateOnly model, as illustrated in the [No Drip, CRM] general corrosion input segment:

```
[No Drip Model, CRM]           |This segment always required
CRMGeneralRateOnly             |CRM corrosion model for drips
3, 1.e+6                       |Number of dists (temps), max CRM rate
25.                            |Temp appropriate for dist #1
```

```
File                          |Distribution type for #1
gnd15050.cdf                  |Distribution parameter (s)
50.                           |Temp appropriate for dist #1
File                          |Distribution type for #1
gnd25050.cdf                  |Distribution parameter (s)
100.                          |Temp appropriate for dist #2
File                          |Distribution type for #2
gnd35050.cdf                  |Distribution parameter (s)
```

requires specification of up to three temperatures and general corrosion rate distributions. These can be any of the ones built in to WAPDEG. Note that the maximum CRM general corrosion rate is specified just after the number of distributions for the CRMGeneralRateOnly model.

The next set of input lines:

```
[No Drip Features]            |This segment always required
File                          |Distr for thermal protection temperature
TThresh.cdf                   |Distribution parameter(s)
File                          |Dist type for humid-air initiation
HARH.cdf                      |Distribution parameter(s)
File                          |Dist type for humid-air/aqueous transition
AQRH.cdf                      |Distribution parameter(s)
1.0                           |RH correlation factor
0.0, 0.0                      |Galvanic protect depth %, % patches protected
0.0                           |Spalling depth as a % of thickness
Fixed                         |Dist for multiple for CAM corrosion rate
1.0                           |Distribution parameter(s)
Fixed                         |Dist for multiple for CRM corrosion rate
1.0                           |Distribution parameter(s)
1.0                           |Pack variance share for multiples
```

specify the [No Drip Features]. These features include a distribution for the thermal protection temperature, (i.e., the temperature above which no corrosion is allowed to occur). Such a temperature threshold is used primarily because water will not exist in the liquid phase above this temperature, and thus, no corrosion should occur. This threshold could be above the typical boiling point of water due to the presence of impurities in the water film on the waste package and variations in water chemistry. In this example, the temperature threshold is read from a file, TThresh.cdf (CRWMS M&O 1998i), resulting from values elicited from the WPDEE (CRWMS M&O 1997e), and is shown in Figure 5-47. If a negative or zero value is entered, a temperature threshold of 100°C is assumed. Similarly, WAPDEG uses RH thresholds (also from the WPDEE) for the onset of both humid-air and aqueous corrosion modes of the CAM (Figures 5-48 through 5-51).

The next input line allows the user to control the degree to which these RH thresholds are correlated. Entering a value of 1 forces the humid-air and aqueous RH thresholds into perfect correlation, i.e. if the aqueous RH threshold has a Cumulative Probability of 0.56, the humid-air RH threshold with a Cumulative Probability of 0.56 will also be selected. Perfect negative correlation (entering –1) would result in the humid-air RH threshold with the Cumulative Probability of 1 – 0.56 = 0.44 being used.

The "galvanic protection depth %" specifies the percent of the total CAM thickness that must remain in order for the CAM to afford galvanic protection to the "% of patches protected" of the CRM. In this way, the user can control the characteristics of the galvanic protection model used in WAPDEG. The subsequent input line allows specification of how thick a corrosion product film must be before it fails to adhere to the substrate and spalls off the waste package surface. Spalling is not implemented in the current WAPDEG version, but is expected to be in later versions of the code. The "Multiples for the CAM, CRM corrosion rates" are used in sensitivity studies to allow for modeling of corrosive environments that are considered to be more aggressive (multiples > 1) or more benign (multiples < 1) than those typically modeled in WAPDEG simulations. The user is also able to specify what variance share of this parameter is allocated to waste package-to-waste package variability and, thus, the variance share left over for patch-to-patch variability. These multiples are set to one in the TSPA-VA base case analysis.

The next three segments of the input file (and the three succeeding these, if there were a drip change time) are quite similar in form to the preceding three. The user enters [Neutral Drip Model, CAM], [Neutral Drip Model, CRM], and [Neutral Drip Features] in much the same manner as was done for the [No Drip . . .] input segments. If there were a drip change time, the user enters [Chemical Model Drip, CAM], [Chemical Drip Model, CRM], and [Chemical Drip Features], segments. These may differ in salient parameters such as those used to specify the general corrosion rates, RH thresholds, etc., but the form of the input is identical to that described above for the [No Drip . . .] sections with a few exceptions.

Immediately after specification of the three CDFs relevant to CRM general corrosion, the user must specify CRM localized corrosion parameters:

```
Normal                          |Distribution type for A (b0)
11.275, 2.4495                  |Distribution parameter(s)
Fixed                           |Distribution type for K (b1)
5.5494e+003                     |Distribution parameter(s)
Fixed                           |Distribution type for n
0.5                             |Distribution parameter(s)
```

Comparison to Equation (5-35) shows that we have chosen C_{LC} to be *11.275*, ε_{LC} to have a standard deviation of *2.4495*, Q_{LC} equal to *5549.4*, and n to be *0.5*.

The user must also supply two lines of input related to specification of a CRM temperature threshold for initiation of localized corrosion in the [..... Drip Features] section:

```
Uniform                         |Dist type for CRM LC T init
80., 100.                       |Distribution parameter
```

These two lines appear immediately after specification of the temperature threshold for corrosion initiation. The CRM temperature threshold for initiation of localized corrosion is implemented such that if the temperature at the waste package surface is below the CRM temperature threshold for initiation of localized corrosion when the CAM is penetrated, no localized CRM corrosion occurs. However, once localized corrosion (pit or crevice corrosion) initiates, it continues regardless of the temperature, although at a temperature dependent rate.

It is only necessary to enter the input segments that are used by WAPDEG (i.e., if the percent of dripped on patches is zero). It is unnecessary to provide the neutral or chemical drip input segments. Similarly, it is also unnecessary (will result in an error message) to supply input lines related to dripping start/end/chemistry change times if no dripping can occur.

To gain a deeper understanding of the WAPDEG code, the interested reader is directed to the Software Routine Report for WAPDEG (CRWMS M&O 1998h).

5.10.7 Description of WAPDEG Output

WAPDEG creates six output files. All six have the root name of the primary input file, but with a specific extension appended. They are referred to in Table 5-9 by their extension name along with a brief description of their contents. More details about each file are provided below.

The *.out file serves two purposes. It echoes the primary input file data and reports summary failure time results for each package. For the latter there are 24 columns of output. The first six columns include the package number followed by five summary columns, all having units in years:

- *Advection time* as defined by WAPDEG is the earliest time that a *dripped-on, top* patch and any bottom patch have failed, thereby providing a path for advection of seepage water through the waste package. The time does not account for pit penetrations because it is assumed that advective flows are dominant through failed patches, and pit penetrations provide diffusion pathways.

- *Diffusion time* as defined by WAPDEG is the earliest time that any pit or patch on the side or bottom has penetrated, thereby providing a path for diffusion of waste out from the waste package.

- *Structural failure time* is defined as the time when the average thickness of the CRM has thinned to the user specified minimum percentage that can maintain structural integrity of the package.

- *First outer penetration time* is the earliest time the outer barrier (CAM) was penetrated by any mechanism for the package.

- *First inner penetration time* is the earliest time the inner barrier (CRM) was penetrated by any mechanism for the package.

The next 10 columns further break down the first penetration times in years according to barrier, location, and type. The first three are for the outer barrier and represent the earliest penetration for the top, side, and bottom patches. These penetrations are either due to pits (top or bottom patches) or roughness factors.

The next three columns are for the nondripped-on patches for the top, side, and bottom of the inner barrier. If neither dripping nor pooled water is contacting the surface, WAPDEG only allows general corrosion of the CRM. So, these failures are due to general corrosion only and

represent the earliest failure of an entire patch. The last four columns of this group of 10 are for the first penetration times for dripped-on patches of the CRM, for both pits and patches and both top and bottom. Side patches are ignored here because, according to WAPDEG assumption, dripping water runs off the side patches and does not form stable stagnant water film.

The last eight columns provide a summary of overall results with time for the CRM. The user specifies four times in the input file for these columns and WAPDEG reports a cumulative number of penetrated pits (summed over top and bottom) at the four times and the cumulative number of patches completely corroded (summed over top, side, and bottom) at the four times. WAPDEG records pit penetrations of the CRM for a patch up to the point when the entire patch fails. From that point on, all pits have penetrated but to avoid double counting, the pits for the patch are ignored. Thus, WAPDEG reports zero pit penetrations from that time forward for the patch, which can cause the cumulative pit penetration history to be nonmonotonic with time.

The *.aux file is an auxiliary output file. It contains all warning and default messages written while input is being read and checked. This is followed by a summary of sampled values for each package. The number of columns in the summary depends on whether drips occur and the number of water types. One use for the package level sampled values is for sensitivity analyses of package-degradation response variables to package input variables.

The first three columns on the *.aux file are the waste package number, the number of patches for the package, and the ceramic protection time sampled for the package. Then for the most general case there are 3 property sets: one for no drips, one for initial water type drips and one for final water type drips. The property set for the no drip condition consists of

- Sampled values for the temperature threshold for CAM corrosion initiation
- Relative humidity threshold for CAM humid-air corrosion initiation
- Relative humidity threshold for CAM aqueous corrosion initiation, the share of variance accorded the package for the CAM general corrosion parameters
- Share of variance accorded the package for the CAM general corrosion parameters
- Sampled values for all eight CAM general corrosion parameters
- Share of variance accorded the waste packages for the CRM general corrosion parameters
- Either the general corrosion rates sampled for the CRM or the sampled values for the Arrhenius model for the CRM
- Multiplier for the CAM general corrosion rate and the package share of its variance
- Multiplier for the CRM general corrosion rate and the package share of its variance.

Note that the reported thresholds for temperature are in °C and relative humidity is in percent.

If there is dripping, then the next three columns are the probability of a top patch being dripped on, the probability of a bottom patch being in pooled water, and the time of onset of dripping. This is followed by the set of three thresholds mentioned for the no dripping case, the temperature threshold for localized corrosion initiation on the CRM, and the package share of its variance. The share of variance accorded the package for the CAM general corrosion parameters and the sampled values for the CAM general corrosion parameters appear next. If the user has specified that the CAM Pit Growth Law should be used, the next three columns are (1) the variance share accorded the package for this pit growth model, (2) the package mean for the constant term, and (3) the package mean for the time exponent. Next comes the share of variance accorded the waste packages for the CRM general corrosion parameters and either the general corrosion rates sampled for the CRM or the sampled values for the Arrhenius model used for general corrosion of the CRM. If localized corrosion of the CRM is specified for the initial water type, then the next column is the waste package share of the variance of the distributions for the model parameters that describe localized corrosion. Depending on the pit growth model specified, there are two or three parameters required. The waste package level values of those parameters appear next. The initial water property set is finished off with the multiplier for the CAM general corrosion rate and the waste package share of its variance and the multiplier for the CRM general corrosion rate and the waste package share of its variance.

If there is a second dripping water segment, the next property is the time that the dripping water changed chemical character. The same properties are reported for the second segment as were reported for the initial water segment just described. The final column of the *.aux file for the most general case is the time that dripping stops.

If dripping water does not change chemical character, then properties for the initial water are used throughout time, and there are no columns for the final water property set nor for the time when water character changes. Similarly if there are no drips possible, then neither property set for dripping water appears and none of the dripping start, change, and stop times appear.

The *.cam file contains the average corrosion depth into the CAM versus time for each package. Here time is in years, and depth (lost thickness) is expressed in millimeters. There is a header line for each package containing the waste package number and the number of records to follow for the package. This is followed by that number of records where each record consists of two columns. The first column is time, and the second is the average corrosion depth at that time. The first time in the list is the last time step before corrosion began for any patch on the CAM. The last time in the list is either the simulation time (the CAM did not completely corrode) or the time that the CAM completely corroded. The time steps used to report the depths here are those of the history file for the waste package. The user has the option to refine the time grid, which can be useful when the results of this file are of interest.

The *.crm file contains the average corrosion depth into the CRM versus time for each waste package. Here time is in years, and depth (lost thickness) is expressed in millimeters. There is a header line for each waste package containing the waste package number and the number of records to follow for the waste package. This is followed by that number of records where each record consists of two columns. The first column is time, and the second is the average corrosion depth at that time. The first time in the list is the last time step before corrosion began for any patch on the CRM. The last time in the list is either the simulation time (the CRM did

not completely corrode) or the time that the CRM completely corroded. The time steps used to report the depths here are those of the history file for the waste package. The user has the option to refine the time grid, which can be useful when the results of this file are of interest.

The *.pat file contains the failure history for the patches of each waste package. Each waste package has a header record containing four values: the waste package number, first bin number (b_1), the total number of bins ($N_B + 1$), and the earliest failure time for any patch for the waste package in years. Note that N_B is specified by the user in the primary input file and is the same for each waste package. WAPDEG uses a logarithmic binning scheme to record these results. The time interval that encompasses the results for record j, (t_j^L, t_j^R) can be found by first finding the logarithms

$$\ln(t_j^{\ L}) = \ln(u_0) + \ln(u_f / u_0)(j + b_1 - 2) / N_B \tag{5-48}$$

and

$$\ln(t_j^{\ R}) = \ln(u_0) + \ln(u_f / u_0)(j + b_1 - 1) / N_B \tag{5-49}$$

and then taking the antilogs. Times u_0 and u_f are the user specified start and end times for the binning. The final time, u_f, is the problem simulation time in years, and the initial time, u_0, is usually one year.

Each record has five entries corresponding to (1) top patches that see drips, (2) bottom patches in pooled water, (3) top patches that do not see drips, (4) side patches, and (5) bottom patches that are not in pooled water. In each case the number reported is the cumulative number of completely corroded patches in the appropriate time bin for the waste package.

The *.bin file contains the failure history for the pits of each waste package. It is structured like the *.pat file. Each waste package has a header record containing four values: the waste package number, first bin number (b_1), the total number of bins ($N_B + 1$), and the earliest time of any pit penetration for the waste package in years. WAPDEG uses the same logarithmic binning scheme to record these results as described for the patches in the *.pat file. Each record here has two entries corresponding to top pits and bottom pits. In both cases the number reported is the cumulative number of penetrated pits in the appropriate time bin for the waste package. However, recall that WAPDEG subtracts the number of pits per patch from the cumulative sum whenever a patch completely fails. So, the cumulative sum may not be monotonically increasing.

5.10.8 Post Processing of WAPDEG Output for Result Abstraction

The output files discussed above provide an adequate description through time of the location (top, bottom, side) and type (patch or pit) of penetrations experienced by each waste package. It is necessary to sort and abstract this large body of information for use by the TSPA model, Repository Integration Program (RIP) (Golder 1998), as well as to produce data files suitable for

graphing. Post308 is a postprocessor for WAPDEG output files that accomplishes these tasks. Post308 is discussed in detail within the WAPDEG Software Routine Report (CRWMS M&O 1998h). It reads the *.out, *.bin, and *.pat files produced by WAPDEG and produces columnar output that can be used to plot:

- The fraction of waste package failures (penetration either by a pit or patch) versus simulation time
- The fraction of waste package failures by pit penetration versus simulation time
- The fraction of waste package failures by patch penetration versus simulation time
- The fraction of waste packages versus number of pit penetrations at four given (in the input file) simulation times
- The fraction of waste packages versus number of patch penetrations at four given (in the input file) simulation times
- The average number of pits per failed waste package versus time
- The average number of patches per failed waste package versus tie.

The first plot and the last two plots are also abstracted (the data is time averaged to decrease the number of data points) and reformatted to RIP input table specifications (Golder Associates 1998). The post processor writes a header on each RIP input table it produces containing:

- The WAPDEG input file prefix
- The version of WAPDEG the input file was designed for
- The post processor version used
- Copies of the WAPDEG input file header lines.

In this manner, the WAPDEG postprocessor adds to the traceability of the WAPDEG simulations.

5.11 BASE CASE ANALYSIS

The base case analysis for waste package degradation constitutes a WAPDEG simulation that uses the base case values of the individual corrosion model parameters and the simulation parameters. The base case values are listed in Tables 5-10 and 5-11. The base case analysis was conducted with WAPDEG Version 3.07 (CRWMS M&O 1998c). Because of the time constraints imposed on the TSPA-VA analysis, interim expert assessment results were provided for the TSPA-VA base case analysis (Pendleton 1998). Therefore, the experts' assessments used in the base case analysis are not identical to those in the final WPDEE report (CRWMS M&O 1998b). However, the differences are small, and the analysis results are should not affected. Information on the WAPDEG version used and the status of input and output data for the base case analysis is given in Table A-2 in Appendix A.

Among the potential modes for waste package degradation discussed in Section 5.2, general and localized corrosion of the barriers are considered in the base case analysis. As additional information becomes available for other degradation modes, they may need to be included in the future analysis.

WAPDEG 3.07 is a FORTRAN program 9470 lines in extent. It conforms to the FORTRAN 77 standard. Computer Software Configuration Item (CSCI) Identifier of the software is 30048 v 3.07. WAPDEG 3.07 was installed on a Dell PowerEdge 2200 (CRWMS-M&O tag 112371) computer which operates at 266 MHz, and a variety of Hewlett-Packard HP-UX 20 workstations (CRWMS-M&O tags 102877, 112515, 108319, 107436, 107437, 108335, 111031). The software was appropriate for the base case analysis discussed in this section, used only within the range of validation, and obtained from Software Configuration Management in accordance with appropriate procedures. Details of the software are documented in CRWMS M&O (1998c).

5.11.1 Base Case Description

The conceptual model (Section 5.4) and individual corrosion models and their parameters (Sections 5.5 to 5.9) for the base case waste package degradation analysis were described in the preceding sections. This section provides additional descriptions of the base case waste package degradation analysis and summarizes major assumptions employed in the analysis.

A. The drift-scale thermal-hydrologic modeling divides the repository area into six different regions, and the division is based mainly on infiltration rate in the repository. The total number of waste packages were grouped into the six regions proportional to the areas of each region. The varying thermal-hydraulic properties in the repository would create different thermal-hydraulic environments in the emplacement drifts of the six regions. The base case analysis uses the waste package surface temperature and relative humidity histories of the waste package groups from only one of the six regions of the repository, the northeast (NE) region simplification was invoked because sensitivity of waste package degradation to different thermal-hydrologic environments (in terms of temperature and relative humidity profiles at the waste package surface) in the other regions is not insignificant (see Section 5.12).

B. All the WAPDEG simulations for the base case analysis are for the commercial spent nuclear fuel waste packages only, i.e., defense high-level waste and DOE-owned spent nuclear fuel waste packages are not included. Our analyses have shown that there are little differences in the degradation behavior of the different-waste-type waste packages in the same location of the potential repository. Differing thermal outputs from different waste-type waste packages would result in differing thermal conditions around the waste packages, especially during the initial periods after waste emplacement. In the current thermal-hydrologic model, these effects are expressed by differing temperatures and relative humidities at the waste package surface. As demonstrated in Section 5.12.2.1, such differing temperatures and relative humidities at the waste package surface have insignificant effects on the waste package degradation. In addition, the base case analysis ignores small variations of the dimensions of the waste packages for different types of spent nuclear fuels. The dimensions of those waste packages are found in Benton (1997). The temperature and relative humidity at the

surface of the waste package groups in the NE region are shown in Figures 5-57 and 5-58 respectively. After passing through the peak temperature, the waste package surface temperatures decrease to 100°C at time periods ranging from 100 to 1,200 years. As the waste package surface temperature decreases, the relative humidity at the surface increases. At 1,000 years when most of the waste packages in the region have cooled to or below 100°C, the relative humidity at the surface of the waste packages has reached about 90 percent. About 3 percent of the waste packages experience drier conditions with about 80 percent relative humidity at the surface at 1,000 years. However, the near-field conditions for the waste packages become much wetter (about 90 percent relative humidity) within a few hundred years.

C. In the WAPDEG simulations, the waste package surface is divided into two parts: top and bottom. The top and bottom corresponds to the arc subtended by an angle of 180 degrees at the top and bottom of the waste package, respectively. However, for the analysis results presented in this chapter and the abstraction of the results for the TSPA model, no distinction was given to the failure sites on the top and bottom of the waste package.

D. In the base case analysis, two water contact modes for the waste package are simulated: no dripping and always dripping. The waste packages that do not see drips are assumed never dripped on and to be in humid-air conditions for the entire simulation period. The waste packages that are dripped on are assumed to be under dripping conditions for the entire simulation period, and the entire surface of the waste package is assumed wetted by the drips. This assumption is based on the conceptual model that seepage could move along the waste package length with time, potentially wetting the entire waste package surface. This assumption is very conservative considering the current conceptual model assumes that localized corrosion of the CRM initiates only under dripping conditions, and the CRM general corrosion rates for the dripping conditions—especially the right-hand tails of the distributions—are much higher than for the no-dripping condition. The total system performance assessment model determines the number of waste packages that are under dripping conditions or that are under no-drip conditions. This parameter is determined mainly by the climate changes, which is represented as a function of time (see Chapter 2 for details of the number of waste packages with drips).

E. In the base case analysis, the same corrosive conditions, once assumed under dripping conditions, are applied to the entire simulation period. That is, the effect of potential run-off of salt solutions from the waste package surface under sustained dripping is not considered. Sustained drips could leave accumulated salt deposits initially on the waste package surface, providing aggressive conditions to waste package corrosion. However, when the waste package temperature cools well below boiling temperature, the sustained drips would wash off the salt solutions from the waste package surface and lead to potentially less corrosive conditions.

F. Temperature threshold for the CAM corrosion initiation used in the base case analysis is for the case without salt present from the WPDEE (Figure 5-47).

G. Relative humidity thresholds for humid-air and aqueous corrosion initiation of the CAM are taken from the WPDEE results for the case without salts present (Figures 5-49 and 5-51 respectively).

H. The CAM humid-air general corrosion is modeled with Equation (5-8) and the CAM aqueous general corrosion with Equation (5-13).

I. Local variations of the CAM general corrosion in humid-air and aqueous conditions are modeled with the roughness factor (or localization factor) approach and use the distribution from the WPDEE, i.e., the roughness factor is normally distributed with a mean of 1.50 and a standard deviation of 0.25.

J. The CRM general corrosion rate with no drips is modeled with the rate distributions for three temperatures presented in Section 5.7.

K. The CRM general corrosion rate under dripping conditions is modeled with the composite rate distributions for three temperatures discussed in Section 5.8. The composite distributions include the effect of the three local corrosion environment scenarios provided from the WPDEE.

L. The CRM localized corrosion is modeled with the pit growth law model presented in Section 5.9. The critical temperature threshold discussed in Section 5.9 is used for the initiation of CRM localized corrosion.

M. Variability in the degradation of the waste packages to be modeled is represented by allocating the total variances of the individual corrosion models and their parameters to waste package-to-waste package variability and to patch-to-patch variability within a single waste package. Details of the methodology for the variance allocation are discussed in Section 5.7.

N. Each simulation uses 400 waste packages. Each waste package has a total of 964 patches with a uniform area of 310 cm^2 for each patch. A pit density of 10 pits/cm^2 is used.

A summary of the corrosion models and parameters, and their values, which were employed in the base case analysis are given in Table 5-10. The input parameters and their values used for the base case analysis are summarized in Table 5-11.

5.11.2 Results

The base case results are analyzed in terms of the following waste package degradation profiles:

- The first breach (either by a pit or patch perforation) profile of waste packages with time
- The first pit-breach profile of waste packages with time
- The first patch-breach profile of waste packages with time
- The number of pit perforations in waste packages at 10^4, 5×10^4, 10^5, and 10^6 years
- The number of patch perforations in waste packages at 10^4, 5×10^4, 10^5, and 10^6 years.

The results for the base case waste package degradation analysis are shown in Figures 5-59 through 5-61. Figure 5-59 shows the first breach profiles of waste packages with time for the drip and no-drip cases. The first pit-breach and first patch-breach profiles and the CAM first breach profiles are for the drip case. For the no-drip case, there is no waste package failure until about 700,000 years, and only about 5 percent of the waste packages fail by 1,000,000 years. Because the number of waste packages that fail under no drip conditions are negligibly small, the no-drip case will not be discussed any further.

Under dripping conditions, the CAM failure initiates at about 980 years, and all the waste packages have the CAM failure by about 7,000 years. The first waste package breach initiates at about 2,700 years, with about 1 percent of the waste packages failing by 10,000 years, and about 23 percent of the waste packages failing by 100,000 years. Comparison of the first breach profiles with the first pit-breach and first patch-breach profiles show that the early breaches are due to pit penetrations from the CRM localized corrosion, and the later breaches are due to patch penetration from the CRM general corrosion. The first patch-breach initiates at about 12,500 years.

The number of pit perforations in the waste packages at the different times are shown in Figure 5-60. Those waste packages that are breached by a pit penetration have only a small number of pit penetrations over 100,000 years. As mentioned above for the base case analysis, only 1 percent of waste packages have at least one pit perforation at 10,000 years. At 50,000 years, about 2 percent of waste packages have at least one pit perforation. The most pitted waste package has about 10 pit perforations at 50,000 years, and about 20 pit perforations at 100,000 years. The number of pit perforations on the breached waste packages is used to calculate the radionuclide release rate from the breached waste packages. Although a small number of waste packages fail early by a pit penetration, the radionuclide release rate from the breached waste packages should be insignificant because of a small number of pit perforations.

The number of patch perforations in the waste packages at different times are shown in Figure 5-61. As mentioned earlier, no waste packages have a patch perforation until 12,500 years. At 50,000 years, about 8 percent of the waste packages have at least one patch perforation, and the most degraded waste package has 10 patch perforations. At 100,000 years, about 22 percent of waste packages have at least one patch perforation, and 33 patch perforations were predicted for the most degraded waste package.

The base case results showed that only a small fraction of waste packages fail by pit penetrations, and the dominant degradation mode is general corrosion (or passive dissolution) of the CRM under dripping conditions. The general corrosion rates with drips that were used in the base case analysis were provided by the experts and have a range over three to five orders of magnitude. This is due mainly to a lack of information on local chemical and electrochemical conditions on the CRM and limited experience with the relatively new alloy. As discussed in the following section, sensitivity analyses evaluated potential impacts of alternative uses of the expert-elicited CRM general corrosion rate parameters for dripping conditions.

5.11.3 Guidance for Sensitivity Studies

The base case analysis employs assumptions on some waste package corrosion processes and parameters that are not readily definable. The base case also uses the expected values (or best estimates) of the corrosion parameters and input variables. Thus, sensitivity analysis needs to be done to evaluate potential effects of the simplifications made for the corrosion processes and assumed values for the corrosion parameters and input variables. The sensitivity analysis will be done by using a reasonable range of the values for the processes and parameter and input values. As will be discussed further in Section 5.12, two types of sensitivity analysis techniques will be employed to evaluate the sensitivity of waste package degradation to the package corrosion parameters. One technique is termed "one-off" sensitivity analysis, in which only one parameter is varied while other parameters are kept as in the base case model. The other technique is termed "regression-based" sensitivity analysis, in which a number of candidate parameters are varied over certain ranges. Their impacts on waste package degradation are ranked against waste package performance measures using a regression technique.

As discussed earlier, the CRM general corrosion rate under dripping conditions has significant impacts on the waste package performance. Sensitivity analysis was conducted to evaluate potential impacts of alternative uses of the expert-elicited CRM general corrosion rate parameters for dripping conditions. The sensitivity cases that will be studied are (1) alternative allocations of variability and uncertainty of the CRM general corrosion rate variance for dripping conditions, and (2) two end-members of the elicited CRM general corrosion rates for dripping conditions.

As discussed in Section 5.11.1, assumptions and simplifications were made in the base case analysis for the waste-package property parameters and repository condition parameters. This was to simplify the waste package degradation analysis and the total system performance analysis. Those assumptions and simplifications are

- Inclusion of the waste packages only in the northeast region
- Inclusion of the waste packages only for the commercial spent nuclear fuel (CSNF)
- Assumption that the entire surface of the waste package experiences dripping conditions if the waste package is dripped on
- Use of a uniform area of 310-cm^2 for each patch.

Thus, sensitivity analysis was conducted for the following cases: (1) sensitivity to six repository region conditions in terms of temperature and relative humidity at the waste package surface, (2) sensitivity to the fraction of the waste package surface wetted by drips, and (3) sensitivity to the patch size in the waste package degradation modeling.

Although the base case analysis indicated that the CAM degradation may not be very significant to the overall waste package degradation, there are processes that could potentially enhance the CAM corrosion and thus, potentially shorten the waste package lifetime. Among the processes that were discussed in Section 5.2, potentially important processes that may enhance the CAM

degradation significantly include (1) pitting corrosion in the presence of high pH drips, (2) MIC, (3) galvanic corrosion in contact with the CRM, and (4) SCC in the closure welds. The cases to be studied are (1) sensitivity to alkaline (pH≥10) dripping on the waste package, which could result from dripping water interacting with the degrading concrete liners in the emplacement drift; and (2) sensitivity to potentially enhanced corrosion of the CAM under an assumed sustained microbial activity in the near-field. Other cases are not analyzed because of a lack of information on the effect of the processes.

Sensitivity analysis will be conducted for waste package degradation to key waste package and engineered-barrier-system design options. The design options are to improve long-term performance of waste package and the engineered-barrier-system, and ultimately overall repository performance. The design options to be analyzed include (1) backfill, (2) Alloy 22 drip shield with different thicknesses and with backfill, (3) ceramic coating on the waste package (CAM) surface with backfill, (4) alternative thicknesses of the CAM barrier, and (5) alternative thicknesses of the CRM barrier.

5.12 SENSITIVITY STUDIES

Sensitivity analyses were conducted as part of the TSPA-VA analysis on a number of waste package corrosion parameters and alternative waste package and engineered barrier system design options to evaluate their importance to waste package performance. In particular, some of the abstractions developed from the WPDEE results were evaluated in a sensitivity framework. This section discusses the development of the sensitivity cases and scenarios and their results.

A list of sensitivity study cases that were analyzed in this report is discussed in Section 5.12.1. Section 5.12.2 discusses the results for the sensitivity of waste package degradation to the parameters that are related to the waste package level properties and the repository conditions. Sensitivity of the waste package degradation to CAM corrosion-related parameters are presented in Section 5.12.3, and those to CRM corrosion-related parameters are in Section 5.12.4. The waste package degradation results for alternative waste package and engineered barrier system design options are discussed in Section 5.12.5. Regression analysis was used to quantify the significance of various waste package degradation parameters, and the results are presented in Section 5.12.6. Information on the WAPDEG version used and the input and output files for all the sensitivity cases discussed in this section is given in Table A-2 in Appendix A.

5.12.1 Overview of Sensitivity Studies

For the current analysis, two types of sensitivity analysis techniques were employed to evaluate the sensitivity of waste package degradation to the package corrosion parameters. One technique is termed "one-off" sensitivity analysis, in which only one parameter is varied while other parameters are kept as in the base case model. The other technique is termed "regression-based" sensitivity analysis, in which a number of candidate parameters are varied over certain ranges. Their impacts on waste package degradation are ranked against waste package performance measures using a regression technique. For the one-off sensitivity analysis, the results are analyzed in terms of the following waste package degradation profiles:

- The first breach (either by a pit or patch perforation) profile of waste packages with time

- The first pit-breach profile of waste packages with time
- The first patch-breach profile of waste packages with time
- The number of pit perforations in waste packages at 10^4, 5×10^4, 10^5, and 10^6 years
- The number of patch perforations in waste packages at 10^4, 5×10^4, 10^5, and 10^6 years.

Where applicable, the results of the five degradation profiles are compared with those of the base case results. However, only those that show significant sensitivity are presented and discussed. The one-off sensitivity cases analyzed in this report and a brief description for the cases are listed in Table 5-12.

The same waste package degradation profiles to the one-off sensitivity analysis are used in the regression-based sensitivity analysis with the exception that the second and fourth performance measures (first pit breach time, and number of pit perforations) were not used in the analysis because of the small number of waste packages breached by pit penetrations and also the small number of pit perforations for those waste packages that were breached by localized corrosion (see Section 5.12.6).

WAPDEG Version 3.09 was used for the one-off sensitivity analysis, and Version 3.11 for the regression-based sensitivity analysis. Those codes were documented in the Software Routine Reports of the respective version (CRWMS M&O 1998h; CRWMS M&O 1998k). These updates to WAPDEG were needed for additional features to allow the sensitivity analysis. WAPDEG 3.09 is a FORTRAN program 9607 lines in extent. It conforms to the FORTRAN 77 standard. Computer Software Configuration Item (CSCI) Identifier of the software is 30048 v 3.09. WAPDEG 3.09 was installed on a Dell PowerEdge 2200 (CRWMS-M&O tag 112371) computer which operates at 266 MHz, and a variety of Hewlett-Packard HP-UX 20 workstations (CRWMS-M&O tags 102877, 112515, 108319, 107436, 107437, 108335, 111031, 700805, 700889). The software was appropriate for the sensitivity analysis discussed in this section, used only within the range of validation, and obtained from Software Configuration Management in accordance with appropriate procedures. Details of the software are documented in CRWMS M&O (1998h). WAPDEG 3.11 (CRWMS M&O 1998k) and SATOOL Version 1.3 (Iman et al 1980), which were used for the regression-based sensitivity analysis discussed in Section 5.12.6 were not baselined at the time of the analysis.

5.12.2 Waste-Package Property and Repository Condition Parameters

This section discusses the sensitivity analysis results for the waste package property parameters and repository condition parameters. The cases presented are (1) sensitivity to six repository region conditions in terms of temperature and relative humidity at the waste package surface, (2) sensitivity to the fraction of the waste package surface wetted by drips, and (3) sensitivity to the patch size in the waste package degradation modeling.

5.12.2.1 Sensitivity to Six Repository Region Conditions

The drift-scale thermal-hydrologic modeling divides the repository area into six different regions, and the division is based mainly on infiltration rate in the repository. Then the total number of waste packages was grouped into the six regions proportional to the areas of each region. The varying thermal-hydraulic properties in the repository would create different

thermal-hydraulic environments in the emplacement drifts of the six regions. In addition, in conjunction with the varying thermal-hydraulic properties, different types of waste packages with different heat-output characteristics in each region would cause further variations of the temperature and relative humidity profiles at the waste package surface, which could affect waste package degradation processes. Detailed discussions of the above modeling approach and assumptions and the temperature and relative humidity profiles at the waste package surface in the six repository regions are given in Chapter 3.

As was discussed in Section 5.11, the base case model uses the waste package surface temperature and relative humidity histories of the waste package groups in the NE region, one of the six regions of the repository. Sensitivity of waste package degradation to different thermal-hydrologic environments (in terms of temperature and relative humidity profiles at the waste package surface) in the other regions were analyzed using the temperature and relative humidity histories from the other regions. In this analysis, other parameters were kept the same as the base case model. The results are shown in Figures 5-62 through 5-64. All the runs used the base case parameter values for the dripping case: that is, spent nuclear fuel waste packages, no-backfill, always dripping, and 100 percent of the waste package surface wetted by drips.

Sensitivity of the first breach profiles of waste packages with time in six different regions is shown in Figure 5-62, along with the CAM breach profiles. As was discussed for the base case results in Section 5.11, the early breaches are due to pit penetrations, and the later breaches are due to patch penetration from general corrosion. The results show that the temperature and relative humidity variations among the different histories representing the six repository regions do not significantly affect the waste package first breach profiles, although there is some impact on the CAM breach profiles. When the CAM is breached, some 1,000 or more years after emplacement, there is less exposure temperature variation among the different histories than at earlier times in the simulation. Therefore, there are no significant variations in the CRM degradation rates, which in the current model are a function of exposure temperature only. The results indicate that the impact from the variations in the CAM failure time (CRM corrosion initiation time) are not significant to the waste package breach profiles an additional conclusion from this analysis is that the CRM degradation rate is a more important factor than CAM degradation rate to waste package degradation as a whole.

Results for the first pit-breach profiles with time are shown in Figure 5-63. There is not much difference in the initiation time for the first pit-breach failure of waste packages among the six regions, with failure initiation times only ranging from 1,700 to 2,500 years. The central-central region shows the most waste packages breached by pitting corrosion, having about 2 percent of waste packages breached by a pit penetration at 10,000 years and about 10 percent at 100,000 years. Those waste packages that are breached by a pit penetration have only a small number of pit penetrations (less than 10 pit penetrations) over 100,000 years. Results for the first patch-breach profiles with time are shown in Figure 5-64. Again, the difference in the initiation time of the waste package breach by a patch-perforation from general corrosion among the six regions is relatively small ranging from 7,000 to 10,000 years. The first patch-breach profiles for the waste packages in the six regions are almost identical to each other. By 100,000 years, all six regions have about 20 percent of the waste packages breached by a patch perforation.

The analysis results presented here demonstrate that the variable temperature and relative humidity at the waste package surface in the six different repository regions does not significantly affect long-term waste package performance. The differing temperatures and relative humidities in different repository regions have some impacts on the CAM degradation, but there is insignificant effect on the CRM degradation rate by both the localized and general corrosion. This is because when the CAM breach is initiated, the waste package temperature is low and only a small number of waste packages are subject to localized corrosion of the CRM. Therefore, no significant differences are observed for the number of waste packages breached by a pit penetration (Figure 5-63). For waste packages that are breached by general corrosion of the CRM, because the CRM general corrosion rate is very low, two to three thousand-year differences in the CAM breach time have little impact on the CRM first-patch breach time (Figure 5-64). In addition, the temperature dependence of the CRM general and localized corrosion rate is relatively small (see Figure 5-37 for the general corrosion rate, and Equation (5-29) for localized corrosion rate).

5.12.2.2 Sensitivity to Waste Package Surface Fraction Wetted by Drips

The base case conservatively assumes that if the waste package experiences dripping, the entire surface of the waste package is wetted by the drips. As was discussed for the base case model description in Section 5.11, the 100 percent wetting is based on the assumption that drips may move along the waste package length over time. Sensitivity analyses were conducted to evaluate the effect of this parameter on the waste package degradation by reducing the surface area fraction wetted by drips to 1 and 10 percent. The results are shown in Figures 5-65 through 5-69. All the runs were made with the base case parameter values, except for the fraction of the waste package surface area wetted by drips.

The first breach profiles of waste packages with time are shown in Figure 5-65. The CAM breach profiles are almost identical, with CAM breach times ranging from about 800 years to 7,000 years. Although there are no significant differences in the first breach initiation time of the waste packages, which spans from 2,100 to 3,300 years, there are considerable differences in the fraction of waste packages breached after 10,000 years for the different surface fractions wetted. At 100,000 years, about 25 percent of waste packages are breached for the base case with the 100 percent surface wetted, but only 2 percent of waste packages are breached for the case with the 1 percent surface wetted. For all the cases studied, the early breaches are by pitting corrosion as shown in Figure 5-66, and the later breaches by a patch penetration from general corrosion (Figure 5-67).

The first pit-breach profiles with time (Figure 5-66) show insignificant sensitivity to the different surface fractions wetted by drips. However, considerable sensitivity is seen for the first patch-breach profiles with time shown in Figure 5-67. The initiation time for the first patch-breach of waste packages for the 100 percent wetted surface is about 9,500 years. However, it comes much later for smaller surface area wetted, that is, it is about 16,000 years for the 10 percent wetted surface case and 53,000 years for the 1 percent wetted surface case. In terms of the number of waste packages breached by a patch perforation, about 25 percent of waste packages are breached at 100,000 years for the 100 percent wetted surface, about 6 percent for the 10 percent wetted surface, and less than 1 percent for 1 percent wetted surface. Figures 5-68 and 5-69 show the number of patch perforations for the different surface fractions wetted at 50,000

and 100,000 years, respectively. For 100,000 years most waste packages that have been breached by patch failure have less than 10 patch perforations.

5.12.2.3 Sensitivity to Patch Size

The base case uses a patch size of 310 cm^2, which is based on the ASTM standard test coupon size (ASTM 1992). In the TSPA-VA analysis, a patch size is defined as the maximum area in which relatively uniform local conditions exist, and thus, a uniform general corrosion rate is applied. Because the WAPDEG is based on a stochastic approach, different patch sizes (i.e., different patch numbers per waste package) could have an impact on the model results. The effect of patch size on the waste package degradation modeling results was analyzed by increasing or decreasing the patch size by a factor of 10 from the base case patch size (i.e., 31 and 3,100 cm^2). The results are shown in Figures 5-70 to 5-74. All the runs were made with the base case parameter values, except for the patch size which was varied. A pit density of 10 pits/cm^2 was used for all the runs; thus the smaller patch has 3,100 pits and the larger one has 31,000 pits.

The results for the first breach profiles with time are shown in Figure 5-70. While there is little difference for the CAM breach profiles, considerable sensitivity is shown for the waste package first breach profile. With increasing patch size, the waste package breach initiates earlier; that is, 5,000 years for 31-cm^2 patch size, 2,500 years for 310-cm^2 patch size, and 1,700 years for 3,100-cm^2 patch size. A comparison of Figures 5-71 and 5-72 indicates that early waste package breaches for 310-cm^2 and 3,100-cm^2 patch sizes are by pit penetrations, and those for 31-cm^2 patch size are by patch penetrations. As was discussed in the base case model description in Section 5.11, initiation of localized corrosion of a given CRM patch requires the exposure temperature at the time of CAM penetration to be greater than the threshold temperature sampled for each patch. For the larger patch size, the total number of pits in a patch is 10 times higher than the base case. Thus, there is a greater probability for pits in the larger patch to sample higher pitting rates than the base case if localized corrosion initiates on the patch. This resulted in earlier pit penetrations for the waste packages with the larger patches than the base case. For the smaller patch size case in which there are 10 times more patches per waste package but 10 times less pits per patch than the base case, more CRM patches would be subject to localized corrosion, but the pits in the patches that are subject to localized corrosion are likely to have lower pitting rates sampled than the base case because of a smaller number of pits in each patch. This is seen in Figure 5-71, which shows the first pit-breach profiles with time. As shown in the figure, although waste packages with the larger patches have an earlier pit penetration, the number of waste packages with the first pit-breach for the different patch sizes are not much different.

For the first patch-breach profiles of waste packages, the initiation time of waste package breach initiation time is earlier with a smaller patch size as shown in Figure 5-72. The first patch-breach initiation times are significantly different for the different patch sizes: about 5,000 years with 31-cm^2 patch size; about 9,500 years with 310-cm^2 patch size (base case patch size); and about 29,000 years with 3,100-cm^2. The number of waste packages with at least a patch-breach are also sensitive to the patch size. At 100,000 years, about 55 percent of waste packages have a patch-breach for 31-cm^2 patch size, about 25 percent of waste packages for 310-cm^2 patch size, and it is only about 8 percent for 3,100-cm^2 patch size.

Figures 5-73 and 5-74 show the results for the number of patch perforations at 50,000 and 100,000 years respectively. At 50,000 years (Figure 5-73), for waste packages with 31-cm^2 patch size, 5 percent of them have at least 10 patch perforations, and 0.5 percent have more than 100 patch perforations. For waste packages with 310-cm^2 patch size, only 0.3 percent have more than 10 patch perforations. At 100,000 years, as shown in Figure 5-74, for waste packages with 31-cm^2 patch size, about 18 percent have at least 10 patch perforations, and about 2 percent have more than 100 patch perforations. A small fraction of waste packages (0.5 percent) have more than 400 patch perforations. With 310-cm^2 patch size, about 2 percent of waste packages have at least 10 patch perforations, and about 0.2 percent have more than 40 patch perforations.

The patch size used in the waste package degradation analysis is an uncertain parameter. As discussed earlier, a patch size is defined as the maximum area in which relatively uniform local conditions exist, and a uniform general corrosion rate is applied. The base case patch size (310 cm^2) was used to represent the CAM corrosion data in the waste package degradation analysis because most of the corrosion data used to develop the CAM corrosion models were developed according to the ASTM standard procedures. The uncertainty associated with the patch size may be better represented by randomly sampling the patch size within a reasonable range.

5.12.3 CAM Corrosion Parameters

This section discusses the sensitivity analysis results for two CAM corrosion parameters: (1) sensitivity to alkaline (pH≥10) dripping on the waste package, which could result from dripping water interacting with the degrading concrete liners in the emplacement drift, and (2) sensitivity to potentially enhanced corrosion of the CAM under an assumed sustained microbial activity in the near-field. Other CAM corrosion parameters that are potentially important to waste package degradation but not analyzed in this report are summarized in Section 5.12.7.

5.12.3.1 Sensitivity to Alkaline Dripping with pH≥10

The near-field geochemical environment abstraction analysis has shown that interaction of seepage water with the degrading concrete liners could result in elevation of the dripping water pH above 10 for the first 10,000 years (see Chapter 4 for details). As was discussed in Sections 5.4 and 5.6, the current conceptual model dictates that carbon steel undergoes high-aspect ratio pitting corrosion when in contact with alkaline solutions with pH≥10. This conceptual model is supported by the recently conducted WPDEE (CRWMS M&O 1998b). Sensitivity analysis was conducted to evaluate the effect of alkaline dripping on the CAM and waste package degradation. The CAM pitting corrosion was modeled using a pit growth law that was developed using input from the expert elicitation. Details of the model abstraction are discussed in Section 5.6. All the runs were made with the base case parameter values, except for the first 10,000-year period with alkaline drips with pH≥10.

The analysis results are shown in Figures 5-75 and 5-76. As shown in Figure 5-75, the CAM breach starts at 30 years, 50 percent of the waste packages have their CAM breached by about 300 years. All the waste packages have their CAM breached by 2,000 years. This rapid failure

of the CAM is due to very high pitting rates of carbon steel under alkaline conditions (pH≥10) as dictated by the pit growth law that was developed from the expert elicitation results. The six-month and one-year carbon-steel corrosion data from the concentrated J-13 water tank, in which the solution pH is maintained between 9.8 and 9.9, do not show such high-aspect ratio pitting (CRWMS M&O 1998d). These data do not support the pit growth law provided by the experts. Some experts on the panel suggested that mixed anions presented in the concentrated J-13 water may inhibit such high-aspect ratio pitting corrosion of carbon steel in alkaline conditions (CRWMS M&O 1998b). Because early breaches of the CAM patches expose the CRM patches to the exposure environment when the temperature is still high, localized corrosion would initiate for most of the CRM patches, and this would result in substantial localized corrosion attack on most of the waste packages. These are shown in the figure with the waste package first breach starting as early as 250 years. The first pit-breach profile with time overlaps exactly with the first breach profile, indicating the first breaches of the waste packages are all by localized corrosion processes. The first patch-breach also initiates very early, starting at about 2,000 years, compared to about 9,500 years for the base case. Comparison of the current results for the first breach profiles with the base case results is shown in Figure 5-76. It shows that the waste package failure rate is significantly higher in the alkaline dripping case than the base case. While, for the alkaline dripping case, about 25 percent of waste packages have breached at 10,000 years, only 2 percent of waste package have failed for the base case. At 100,000 years, the alkaline dripping case predicts about 75 percent waste packages fail, whereas only 25 percent fail in the base case.

As mentioned earlier, the current high-aspect ratio pit growth law model for carbon steel in contact with alkaline water, which was suggested by the expert panel, does not represent the corrosion behavior of the carbon steel samples under testing at Lawrence Livermore National Laboratory. The current model appears unrealistically conservative, and it needs to be re-evaluated for its applicability to the long-term waste package degradation prediction in the potential repository environments.

5.12.3.2 Sensitivity to Microbiologically Influenced Corrosion of CAM

The WPDEE suggested a mass balance inventory analysis for potential microbial activity in the post-closure repository be undertaken before considering the MIC effects on waste package degradation. This is to determine whether there is a limiting factor (or factors) to continued microbe growth in the potential repository to the extent that it could affect waste package corrosion (CRWMS M&O 1998b). Because such analysis is not yet available, it was assumed in this sensitivity analysis that sustained and sufficient microbe activities exist all the time in the post-closure repository at a level high enough to affect waste package corrosion. As discussed in Section 5.2.9, no cases were documented for the susceptibility of Alloy 22 to the MIC. The expert panel agreed that Alloy 22 would not be affected by the MIC, thus, it was assumed only corrosion of the CAM is affected by the MIC. In addition, because drips are required for microbe growth, as indicated by the expert panel, MIC is assumed to be operative only for the dripping case.

This sensitivity analysis was conducted using a simple MIC-enhancement factor (or multiplication factor) to the CAM general corrosion rate. A recent study by Horn et al (1998) reported that the corrosion current of the inoculated carbon steel samples was increased by five

to six folds over the sterile samples at ambient room temperature. Because the corrosion current is proportional to the corrosion rate, the test results for the corrosion current differences were used for an enhancement factor to the CAM corrosion rate. For this analysis, the enhancement factor to the CAM general corrosion rate was assumed to have a uniform distribution between 1 and 5. In the simulation, the factor was sampled randomly from the distribution and applied as a multiplier to the aqueous general corrosion rate. The results are shown in Figures 5-77 through 5-79. All the simulations were made with the base case parameter values, except for the increased CAM general corrosion rate.

The first breach profile for the CAM and waste packages with time are shown in Figure 5-77. The first CAM breach starts at about 350 years, and all the waste packages have CAM failure by about 3,400 years. For the base case, the CAM breach initiation time is about 1,000 years and by about 7,000 years all the waste packages had at least one CAM patch breached (see Figure 5-59). The effect of early exposure of the CRM from the early CAM breaches is shown by an earlier waste package breach initiation and a substantially greater number of breached waste packages, compared to the base case results. With the MIC-enhanced corrosion of the CAM, the first waste package breach initiates at about 900 years. About 10 percent of waste packages fail by 10,000 years, and about 45 percent by 100,000 years. For the base case, the first breach initiation time is about 2,500 years, and only about 1 percent of waste packages fail by 10,000 years and about 23 percent fail by 100,000 years. Also, compared to the base case results (Figure 5-60), much more extensive pit perforation is predicted for the MIC case, as shown in Figure 5-78. For patch perforations by general corrosion, there is not much difference between the base case and the MIC case (see Figure 5-61 for the base case and Figure 5-79 for the MIC case).

Although the WPDEE results indicated that there is no documented cases for the MIC susceptibility of Alloy 22 and the CRM is immune to the MIC (CRWMS M&O 1998b), the alloy has a relatively short history of field applications (about 15 years). As discussed in Section 5.2.9, the formation of MIC colonies could potentially create locally acidic and oxidizing environments, which could increase the susceptibility of the CRM to localized corrosion. Data are needed to demonstrate with confidence that the CRM is not subject to MIC.

5.12.4 CRM Corrosion Parameters

The candidate CRM, Alloy 22, is highly resistant to corrosion. The base case results showed that only a small fraction of waste packages fail by pit penetrations, and the dominant degradation mode is general corrosion (or passive dissolution) of the CRM under dripping conditions. However, the general corrosion rates with drips that were provided by the experts and used in the base case model have a range over three to five orders of magnitude. This is due mainly to a lack of information on local chemical and electrochemical conditions on the CRM and limited experience with the relatively new alloy. This section discusses the sensitivity analysis results conducted for the CRM general corrosion rate parameters under dripping conditions. The cases studied in this section are (1) for alternative allocations of variability and uncertainty of the general corrosion rate variance, and (2) for two end-members of the elicited general corrosion rates.

5.12.4.1 Sensitivity to Alternative Allocation of the Variability and Uncertainty of General Corrosion Rate with Drips

The experts of the WPDEE provided their representation of the Alloy 22 general-corrosion rate distribution for dripping conditions and the allocation of the total variance to variability and uncertainty. For the base case analysis, 50 percent of the total variance was allocated to the variability of the corrosion rate. The remaining 50 percent was allocated to the uncertainty variance. Then the 50th percentile value of the uncertainty variance was used as the median corrosion rate for the variability distribution. The above allocation was based on the average of the individual expert's assessment. However, as indicated above, the general corrosion rates provided by the experts have a wide range of values, and there are high degrees of uncertainty associated with the assessment. This is mainly due to a limited understanding of the local exposure conditions on the CRM after CAM breach and a limited experience with the relatively new material. Thus, the effect of the general corrosion rate on the waste package degradation was evaluated with three alternative variability and uncertainty allocations and three alternative median rates from the uncertainty variance. Details of the approach used for the variance split are discussed in Section 5.8.

As mentioned above, the base case model for the general corrosion rate under dripping conditions is with the 50 percent variability and 50 percent uncertainty split of the total variance and with the median general corrosion rate sampled at the 50th percentile of the uncertainty variance. Two additional variability and uncertainty splits of the total variance were considered: 25 percent variability and 75 percent uncertainty, and 75 percent variability and 25 percent uncertainty. For each of the variance splits including the base case split, the median corrosion rate was sampled from the 5th, 50th,and 95th percentile of the uncertainty variance. Thus, for this sensitivity analysis, a total of nine cases including the base case were analyzed. The summary of these variance splits and the median corrosion rate sampling are given in Table 5-13, along with the designation of each of the nine cases (Sets 1 to 9). The results are shown in Figures 5-80 through 5-83. All the simulations were made with the base case parameter values for the drip case, except for the CRM general corrosion rates from the alternative allocations of the variability and uncertainty.

The results for the first breach profiles of waste packages with time, shown in Figure 5-80, show that the median general corrosion rates of the CRM sampled from the uncertainty variance (i.e., 5th, 50th, and 95th percentile values) have the most dominant effect on the waste package failure profile. That is, Sets 7, 8, and 9, which have the median corrosion rate sampled at the 95th percentile value of the corresponding uncertainty variance show the most rapid waste package failures. All the cases use the same localized corrosion model, and the waste package failure initiation time is the same for all the cases, starting at about 2,500 years. For a given sampled median corrosion rate, the waste package failure rate is higher with a greater allocation to the variability from the total variance. For example, for Sets 4, 5, and 6, which have the median corrosion rate sampled from the 50th percentile of the corresponding uncertainty variance

- Set 4 (25 percent uncertainty and 75 percent variability) has the highest waste-package failure rate

- Set 5 (50 percent uncertainty and 50 percent variability) shows the medium failure rate

- Set 6 (75 percent uncertainty and 25 percent variability) shows the lowest failure rate.

In particular, only few waste packages fail for Set 3 (75 percent uncertainty and 25 percent variability, and the median rate at the 5th percentile of the uncertainty variance): less than 2 percent of waste packages fail by 100,000 years, and about 3 percent fail at 1,000,000 years.

Similar observations are shown for the first patch-breach profiles with time for the nine cases, which are shown in Figure 5-81. The first patch-breach initiation time ranges from 4,600 to 7,200 years for Sets 7, 8, and 9; 6,800 to 9,700 years for Sets 4, 5, and 6; and 9,500 to 13,700 years for Sets 1, 2, and 3. For the number of patch perforations at 10,000 years shown in Figure 5-82, Sets 7 and 8 show that 10 to 20 percent of waste packages have at least one patch perforation, and a small fraction of waste packages have more than 10 patch perforations. For Set 9 a small fraction of waste packages have one or two patch perforations. As shown in Figure 5-83, at 100,000 years for Sets 7, 8, and 9, almost all the waste packages have at least one patch perforation; about 75 percent of them have at least 10 patch perforations; and about 25 percent have at least 100 patch perforations. A small fraction of waste packages have about 600 (out of total 964 patches) patch perforations.

The sensitivity analysis results demonstrate that different uncertainty and variability allocations of the CRM general corrosion rate for the dripping condition and different median corrosion rates sampled from the uncertainty variance have a significant impact on the long-term waste package degradation results. As will be discussed in Section 5.12.6 for the regression-based sensitivity analysis results, the median rate of the CRM general corrosion rate under dripping conditions and the allocation of the total variance of the rate to the uncertainty and variability are the two most important parameters for long-term waste package degradation. Additional information on the following may reduce the uncertainty of the waste package degradation model: (1) data for the repository-relevant conditions to characterize the local exposure conditions on the CRM with confidence will assist development of a predictive model for the evolution of the local exposure conditions with time and different near-field conditions and (2) data for the CRM general corrosion (or passive dissolution) rate for the conditions that bound reasonably the local exposure conditions expected on the CRM.

5.12.4.2 Sensitivity to End-Member Assessments of General Corrosion Rate with Drips

As mentioned in the above section, the CRM general corrosion rates under drips from the WPDEE span a wide range of values (over three to five orders of magnitudes). This wide range of the distribution has resulted from combining each expert's assessment with an equal weight, so the resulting aggregate distribution covers the entire range of the individual expert's assessment (See Section 5.8 for details for the development of the aggregate distributions). The sensitivity analysis discussed in this subsection is intended to evaluate the effects of two end-members of the experts' assessments for the CRM general corrosion rate under drips on the long-term waste package degradation. The end-member assessments were selected based on the elicited rates, especially, the right-hand tails of the distributions (see Figures 5-30 through 5-32) and the elicited probabilities for the local corrosion exposure conditions, particularly the most corrosive condition, i.e. pH 2.5 and 640 mV SHE (see Table 5-6). Based on these two criteria, the assessments given by Dr. Peter Andresen were chosen as the most optimistic and those by Dr. Joseph Farmer as the most conservative among the five experts' assessments.

The composite distributions at three temperatures for each end-member were developed using the probabilities for the three local exposure conditions given by the expert. That is, for Andresen, the probabilities for the most benign (pH=3–10), 340 mV SHE), intermediate (pH=2.5, 340 mV SHE), and most corrosive (pH=2.5, 640 mV SHE), conditions are 0.99, 0.01, and 10^{-5},respectively. For Farmer, those are 0.45, 0.45, and 0.1, respectively. The resulting composite CDFs for the general corrosion rate at the three temperatures (25, 50, and 100°C) are shown in Figure 5-84 for Andresen and 5-85 for Farmer. The analysis results are shown in Figure 5-86 for the first breach profiles of waste package with time, Figure 5-87 for the first patch-breach profile with time, and Figure 5-88 for the number of patch perforations at different times. All the simulations were made with the base case parameter values for the drip case, except for the differing CRM general corrosion rates from the end-member assessments.

As shown in Figure 5-86, there is a very significant difference in the waste package failure profile with time between the two experts. Compared to the base case results, it shows that the results with the Farmer assessment are comparable to the base case results. There is no difference in the early breach profile including the first breach initiation time, because the same localized corrosion model was used and the early breaches are by pit penetrations. The analysis with the Andresen assessments predicts insignificant failure of waste packages, less than 2 percent of waste packages failed by about 150,000 years, and considerable increases in failure at about 700,000 years. The first patch-breach profiles with time shown in Figure 5-87 show similar results. The results with the Farmer assessments are comparable to the base case results, indicating the base case results were driven by the assessments provided by Farmer. The number of patch perforations predicted for the two cases also show similar trends (Figure 5-88). With the Farmer assessment, a large fraction of waste packages have patch perforations.

The results demonstrate again that the wide range of the distribution of the elicited CRM general corrosion rates in presence of drips causes a wide spread in the waste package degradation prediction. Reduction of the uncertainty in the general corrosion rate model would reduce the uncertainty in the waste package performance model. Additional characterization of the local exposure conditions on the CRM and development of corrosion data in the established exposure conditions would assist in reducing this uncertainty.

5.12.5 Design Option Parameters

This section discusses the results of the sensitivity analysis of waste package degradation to key waste package and engineered-barrier-system design options. The design options to be discussed here are intended to improve long-term performance of the waste package and the engineered-barrier-system, and ultimately overall repository performance. The cases studied include (1) backfill, (2) Alloy 22 drip shield with different thicknesses and with backfill, (3) ceramic coating on the waste package (CAM) surface with backfill, (4) alternative thicknesses of the CAM barrier, and (5) alternative thicknesses of the CRM barrier.

5.12.5.1 Sensitivity to Backfill

One design option is to have backfill in the emplacement drifts over the waste packages. The backfill design option would potentially reduce the amount of liquid water in contact with the waste package, leading to longer waste package lifetimes. Backfill also may result in a reduction

in relative humidity for a longer period of time after waste emplacement leading to slower degradation of waste package. Alternatively, backfill could provide a focusing pathway for dripping water to the waste package, which could enhance the waste package corrosion.

This design option was incorporated in a limited manner into the drift-scale thermal-hydrologic model. The backfill was assumed to have the properties of crushed tuff and to be emplaced 100 years after the waste package was emplaced. The results for the temperature and relative humidity profiles at the waste package surface for the NE region are shown in Figures 5-89 and 5-90, respectively. Compared to the base case temperature and relative humidity profiles without backfill (Figures 5-57 and 5-58), the primary effect on the waste package exposure environment is the increase in temperature following the time of backfill emplacement and corresponding delay in the relative humidity increase as the repository cools. The large temperature increase at 100 years corresponds to the time of emplacement of the backfill. For the empty emplacement drift, the dominant mode of heat transfer is radiation, which is an efficient mode of heat transfer between the waste package surface and the drift wall. For a backfilled drift, heat transfer rate in the porous backfill material by primarily conduction and convection is greatly reduced, and this results in the increase of the waste package temperature. Accompanying the increase in surface temperature is a corresponding decrease in the relative humidity around the waste package. Note that potential changes in the seepage contacting the waste package as a result of backfill were not included in the modeling.

Waste package degradation simulations were conducted for six repository regions, and the results are shown in Figures 5-91 through 5-93. The simulations were made with the base case parameter values for the drip case, except for the temperature and relative humidity histories with the backfill. Figure 5-91 shows the results for the CAM breach and waste package breach profiles with time for the six repository regions. For all the repository regions the CAM breach initiation time is delayed by more than 1,000 years compared to the results for no-backfill case (Figure 5-62). The bend in the CAM breach curves after about 80 percent of the waste packages have a CAM breach is because a few of the waste packages have very low relative humidity compared to the rest of the waste packages, leading to longer CAM lifetime. The waste package breach initiation time for the backfill case ranges from about 5,000 years to about 12,000 years. This represents a delay from 3,000 to 10,000 years, depending on the repository regions considered and compared to the no-backfill cases presented earlier in Figure 5-62. However, there are no significant differences in the overall waste package failure profiles between the no-backfill and backfill cases, both cases having about 20 to 23 percent of the waste packages breached by 100,000 years. The early breaches are by pit perforations as indicated by Figure 5-92, which shows the results for the first pit-breach profiles with time. The first pit-breach profiles are similar to those for the no-backfill case except for the later breach initiation time. In both cases, the central-central region shows the most pit perforations, and this is due to higher waste package temperatures in the region, which would in turn have a higher probability for the pit initiation. The first patch-breach profiles with time shown in Figure 5-93 show that the patch-breach initiation time ranges from 9,000 to 15,000 years, depending on the regions. This is comparable to the no-backfill case that has the initiation time ranging from 7,000 to 10,000 years.

As discussed earlier, there are no significant differences in the overall waste package failure profiles between the no-backfill and backfill cases. However, for the backfill case, potential

effects of backfill on the water seepage into the emplacement drifts and its contacts with the waste packages were not included. Backfill could cause diversion of the seepage, reducing the contact of the seepage with the waste packages. Or, it could provide preferential passages to the waste packages, which could increase focused flow of the seepage to the waste packages. Some of other potential effects of backfill on the seepage include (1) concentration of salts in the backfill from evaporation of the seepage water percolating through the backfill; and (2) enhanced water condensation by capillary condensation at the dust particles that have settled on the waste package surface during the backfill emplacement, and at the contacts between the backfill gravel and the CAM surface.

5.12.5.2 Sensitivity to Dripshield

Numerous configurations for the dripshield on waste package have been proposed. However, only a single representative dripshield was evaluated. The design for the dripshield evaluated was a 2-cm thick "inverted U-shaped" plate made of Alloy 22 emplaced over the waste package (the so-called waste package dripshield). The dripshield was assumed to have half of the surface area of the waste package. The simulation assumed backfill emplacement at 100 years.

For this analysis, two simulations were performed: (1) for the degradation of dripshield only and (2) for the waste package degradation. In the second simulation, waste packages that were subject to dripping were assumed to undergo CRM corrosion in humid-air conditions until the dripshields failed. Once the dripshield was modeled to fail, the waste package was subject to dripping, switching from a humid-air CRM corrosion condition to an aqueous CRM corrosion condition under dripping.

In the first simulation, dripshields were assumed to have the same temperature as the respective waste packages underneath the dripshields. The temperature and relative humidity profiles for the waste packages and dripshields were for the backfill case discussed in the previous section; that is, the effect of the dripshield was not included in the thermal-hydrologic simulation. If drips occurred, the dripshields were assumed to have 100 percent of the upper surface wetted by drips This is based on the base case assumption that drips may move along the waste package length. Because no substantial amounts of oxidants other than oxygen will be available to the wetted surface and because there is no potential to form tight crevices on the wetted surface, the dripshields were assumed to degrade by general corrosion only and—not be subject to localized (pitting and crevice) corrosion. It was also assumed that the drip shield general corrosion rate under dripping corresponds to that of the Alloy 22 inner barrier for the least corrosive condition (moderately acidic and moderately oxidizing—see Section 5.8). Although there is a potential for the formation of crevices between the inner surface of the dripshield and the CAM of the waste package, it was assumed crevice corrosion does not initiate because of the lack of aggressive species such as chloride ions. Potential galvanic coupling between the dripshield and the CAM barrier would reduce the general corrosion rate of the dripshield and increase the corrosion rate of the CAM, but it was not considered.

In the second simulation, as mentioned earlier, the waste package was assumed to undergo degradation under humid-air conditions while the dripshield was functioning. After failure of the dripshield, the waste package was assumed to be subject to dripping, and 10 percent of its surface area wetted by the drips. The area of the waste package surface wetted is dependent on

the opening size and number on the dripshield. Because the dripshield degrades by general corrosion only (i.e., patch failure), there will be one patch opening, transmitting some of the dripping water to the waste package underneath the dripshield at the time of dripshield failure. Thus, only a fraction of the waste package surface directly underneath the patch opening in the dripshield will get wetted by drips. As additional patches fail in the dripshield, more water could potentially contact the waste package. Ten percent of the waste package surface area wetted were chosen as a conservative assumption and used for the simplicity in the simulations. For this sensitivity analysis, the effect of dripshields with different thicknesses (other than 2-cm) was analyzed. The simulations were performed with the base case parameter values for the drip case, except for those indicated otherwise: NE region, spent nuclear fuel waste packages, backfill, always dripping, and 100 percent of the surface wetted by drips.

The first breach profiles of waste packages with time for the 2-cm thick dripshield are shown in Figure 5-94, along with the results for the 1-cm thick and 4-cm thick dripshield cases. Also shown in the figure are the CAM first breach profiles and dripshield first breach (patch-breach) profiles for the different thicknesses. The CAM breach profile even in the presence of the dripshields is very close to that of the backfill-only case (Figure 5-91). This is because the CAM corrosion rate and modes are dependent on temperature and relative humidity, which quickly rises above the relative humidity threshold for transition from CAM humid-air to aqueous corrosion, and thus, the elimination of the dripping onto the waste package has a negligible impact on CAM degradation. The results show significant performance gains of waste packages with the dripshield. Waste packages with a thicker dripshield perform better given the modeling assumptions. With the 2-cm thick dripshield for which the initial breach starts at about 19,000 years, waste package failure is not predicted for over 100,000 years. With the dripshields considered in this analysis, no waste packages are breached by localized corrosion. This is due to the exposure temperature at the time of drip shield failure (drip initiation time for the underlying waste package) being lower than the localized-corrosion-initiation threshold temperature. Initial breach of the 1-cm thick dripshields starts at about 7,800 years, and that of the waste packages is about 59,000 years. For the 4-cm thick dripshield case, initial dripshield failure begins at 48,000 years, and no waste packages fail before 134,000 years.

The sensitivity analysis results indicated that significant waste package performance gains are achieved through the use of a dripshield. The most important benefit offered by the dripshields is to eliminate the contacts of the seepage water to the waste package during the early period of the repository lifetime, when waste packages are still at elevated temperatures and the water contacting waste packages could be concentrated carrying aggressive species to the waste packages. By eliminating these conditions with dripshields, waste packages are not subject to localized corrosion and degrade dominantly by general corrosion in much less corrosive conditions. As shown in the analysis, relatively benign exposure conditions in the vicinity of the waste package provided by the dripshield has extended the waste package lifetime significantly. One major uncertainty associated with the current analysis is that potential effects of the alteration of the thermal-hydrologic (and possibly chemical) processes in the near-field due to the presence of dripshield was not included.

5.12.5.3 Sensitivity to Ceramic Coating on Waste Package

One of the design options to enhance the waste package performance is to coat the CAM (i.e., waste package) surface with a thin layer of an impermeable material to delay the contact of seepage water with the waste package as long as the coating is intact. One candidate material to be considered for the coating is ceramic material. The current assessment indicates that the sprayed ceramic coating would have about 2 percent interconnected porosity. A preliminary model for the ceramic coating degradation was developed based on the assumption that fracture of the coating because of the stresses that are developed by the volume expansion from the corrosion products of the CAM substrate is the only mechanism leading to the coating failure.

The ceramic coating degradation model is based on the process that the CAM substrate corrosion rate (i.e., the rate of stress generation from the substrate corrosion) is directly proportional to the oxygen transport rate to the corroding substrate, and the water-filled interconnected pores in the ceramic coating retards the oxygen transport rate. Thus, the degradation of the ceramic coating as an oxygen transport barrier is expressed with the reduction factor for the CAM substrate corrosion rate and a threshold general corrosion depth in the CAM substrate in which the volume expansion by the corrosion products generate stresses sufficient enough to fail the coating. The reduction factor for the CAM general corrosion rate is expressed with a distribution to represent the uncertainty. The reduction factor and the threshold general corrosion depth for the CAM used in the simulation are given in Table 5-14. More details of the preliminary ceramic-coating degradation model are discussed in Pasupathi (1998).

The ceramic coating design option requires backfill over the waste packages to prevent damage to the coating by rockfall, so the waste package surface temperature and relative humidity profiles for the backfill case were used in these analyses. For these analyses, two WAPDEG simulations were conducted: the first one for the ceramic coating failure only, and the second one for the waste package degradation. The simulations were performed with the base case parameter values for the drip case. As mentioned above, in the first simulation, the ceramic coating failure time was calculated applying the CAM general corrosion rate reduction factor and the threshold CAM general corrosion depth. It was assumed that the pores in the coating are all filled with water under the dripping condition, and thus, the CAM general-corrosion rate reduction factor for aqueous condition was used. It was also assumed that failure of one coating-patch for a given waste package constitutes the failure of the entire coating of that waste package. This is based on the assumption that at the time of the first coating-patch failure, there would be multiple sites on the waste package undergoing similar coating-patch failure stages, and the spread of the degradation to the neighboring patches from the multiple failure sites progresses in a relatively short period of time. In the second simulation, the ceramic coating time from the first simulation was distributed among the waste packages, and corrosion of each waste package was delayed until the ceramic coating for that waste package fails.

The results for the ceramic coating failure profiles and the first breach profiles of waste packages with time are shown in Figure 5-95 and are compared with the base case results. The failure of the ceramic coating does not begin until after 300,000 years and results in less than 6 percent of waste packages with the coating failure over 1,000,000 years. There are no waste package breaches until about 500,000 years, and less then 4 percent of waste packages fail by 1,000,000 years.

The preliminary coating degradation model considers that stresses developed by the volume expansion of the corrosion products of the CAM substrate is the only mechanism leading to the coating failure. However, there are other potential mechanisms to damage the currently proposed thin ceramic coating on the waste package. These could include damages and cracks caused by handling, transportation, local stress concentration at the contacts, especially over the bottom of the waste package, impact by a large rockfall, ground motion by earthquakes. The presence of fabrication defects would accelerate the ceramic coating degradation. Analyses for the effects of the processes have not been completed.

5.12.5.4 Sensitivity to CAM Thickness

Sensitivity analysis was conducted to evaluate the effect of alternative thicknesses of the CAM barrier. The reference design for the CAM barrier is 10-cm thick. Two other thicknesses (15 and 30 cm) for the CAM barrier were considered in this analysis. The simulations were performed with the base case parameter values for the drip case, except for the differing CAM thicknesses.

The results for the first breach profiles are shown in Figure 5-96. The CAM breach is delayed with a thicker CAM barrier: the 15-cm thick CAM barrier delays the first CAM breach by about 700 years, and the 30-cm thick CAM barrier delays CAM breach by about 1,600 years. For the waste package breach profiles, there is no significant difference between the waste packages with the 10-cm CAM and 15-cm CAM barriers. The first breach initiates at about 2,500 and 3,000 years with the 10-cm and 30-cm thick CAM barriers, respectively. Similar fractions for breached waste packages are predicted at 100,000 years, i.e., 27 and 23 percent for the 10-cm and 15-cm thick CAM barriers, respectively.

However, with the 30-cm thick CAM barrier, significant improvements of the waste package performance are predicted. The CRM is not breached by pit penetrations, and all the failures are by general corrosion. This is demonstrated in Figure 5-97 showing the first pit-breach profiles and Figure 5-98 showing the first-patch profiles. With the 30-cm thick CAM barrier, the first waste package breach initiates at about 41,000 years by a patch perforation by CRM general corrosion. This delay in the first breach is accounted for by the fact that the exposure temperature is lower than the localized corrosion initiation threshold when the 30-cm thick CAM has failed, eliminating the potential for the localized corrosion initiation on the CRM.

5.12.5.5 Sensitivity to CRM Thickness

Additional sensitivity analyses were conducted to evaluate the effect of alternative CRM thicknesses on long-term waste package performance. In addition to the base case CRM thickness (2 cm), three different CRM thicknesses (1, 4, and 6 cm) were considered. The simulations were performed with the base case parameter values for the drip case, except for differing CRM thicknesses.

The results for the first waste package breach are shown in Figure 5-99. In terms of the first breach initiation time, which is by a pit penetration, waste packages with a 6-cm thick CRM have a delay over 5,000 years compared to the 1-cm thick CRM case. It is over 4,000 years compared to the base case results. This may not be a substantial performance benefit in light of the costs

for the increase CRM thickness. However, significant performance improvements are predicted for the number of waste packages that are breached at 100,000 years. For the base case, about 27 percent of the waste packages are breached. With the 4-cm thick CRM barrier, about 10 percent of the waste packages fail, and it is only 4 percent with the 6-cm thick CRM barrier. For the first pit-breach profiles with time shown in Figure 5-100, little performance improvement is predicted with an increase in the CRM thickness as was discussed for the first breach profiles. The first patch-breach profiles shown in Figure 5-101 indicate the long-term waste package failures are dominated by the patch perforations from the general corrosion of the CRM. An increase of the CRM thickness from 2-cm to 6-cm delays the first patch-breach initiation time over 5,000 years. The number of waste packages with first patch-breach over time are about the same as the first breach profile as shown in Figure 5-99.

5.12.6 Quantification of Parameter Uncertainty and Sensitivity

The one-off sensitivity analyses discussed in the earlier sections address the effects of a single parameter on waste package degradation by varying the parameter value over a prescribed range but allowing the values of other parameters to vary as in the base case. This approach has limitations on analyzing the relative importance of each parameter on the model results. In Monte Carlo simulations as applied in WAPDEG, the variability of the input parameters or variables are propagated through the computational model to evaluate the variability of the output. Sensitivity analysis was conducted to identify the dominant input variables responsible for variability in the model results. It is important to identify the relationship between input variability supplied to a model and the variability in its predictions. Knowledge of which inputs have a significant effect on model output and their relative importance can aid in model validation and improvement.

5.12.6.1 Model Inputs and Outputs

The primary objective of the WAPDEG code is to provide an evaluation of waste package performance because of corrosion over the life span of the repository. WAPDEG was created as a general purpose code to model waste package performance dependent on a large number of inputs including corrosion parameters and environmental exposure conditions. The WAPDEG user is also able to specify how much of the total variability is allocated among the waste packages and how much among patches within individual waste packages, i.e., aspects of sample design are under user control. Full details of the WAPDEG implementation can be found in Section 5.10. For the purposes of this study, two different WAPDEG simulations were analyzed. The first studied only those parameters that were varied in the base case analysis (labeled as WPSA1; see Table 5-15). The second allowed a somewhat larger number of input parameters to vary, including the total variability allocations discussed above (labeled as WPSA2; see Table 5-16). The input parameters studied include the temperature and relative humidity thresholds for corrosion initiation, both in the presence and absence of dripping, various CAM humid-air and aqueous corrosion model parameters, and various CRM general and localized corrosion model parameters.

In WAPDEG a certain number of input variables are correlated by design. Because these variables are statistically redundant in terms of the sensitivity analysis and may cause singularities in the correlation matrix calculations, only one variable out of a set of correlated

variables was retained. For example, the CRM general corrosion rates for different temperatures are perfectly rank-correlated so only the rate at 50°C is used in the list of input variables. The humid-air and the aqueous relative humidity thresholds are perfectly rank-correlated so only the former is retained. Percentages of the top and bottom surface of the waste package that see dripping condition are perfectly correlated if they are sampled from the same distribution and rank-correlated if sampled from different distributions. Again only the former variable is retained. The CAM general corrosion model coefficients for the dripped-on and not-dripped-on patches differ only if different variance partitions are used in the respective cases. In this study, the CAM humid-air general corrosion coefficients for the not-dripped-on patches and CAM aqueous general corrosion coefficients for the dripped-on patches were retained. In addition, as the CAM coefficients are from a correlated multivariate normal distribution, certain coefficients were judged to have high enough correlation to merit their removal.

The WAPDEG model outputs considered are listed in Table 5-17. They include the first breach time of waste packages by either a pit or patch penetration, the first pit-breach time, and the first patch-breach time as well as the fraction of failed patches at 10,000, 50,000, 100,000, 500,000, and 1,000,000 years.

5.12.6.2 Sensitivity Analysis Procedures

The approach to sensitivity analysis used in this section is based on a regression analysis method for ordering the importance of the input variables. This approach involves fitting a response surface using a stepwise regression technique to the output and input variables and performing sensitivity analysis on the fitted linear model. Helton (1993) has documented this methodology based on linear multiple regression models, as adopted here.

Two important indicators used are the coefficient of multiple determination (R^2) and the partial correlation coefficients (PCC). R^2 is the ratio of the measures of variation explained by the regression model to the total variation present in the output variable under consideration. Values of R^2 will vary between 0 (no variation explained and a very poor regression model) to 1 (perfect explanation of the model variation by the regression model). The PCC for a particular input variable measures the correlation between the output and the selected input variable, after both have been adjusted to account for the other variables in the fit, so that any correlation measured is due only to that variable. PCC are also useful because their sign (±) indicates whether the selected input variable has a positive or negative effect on the performance measure. To make the PCC more meaningful in the context of sensitivity analysis, RamaRao et al. (1998) showed that the square of a PCC is proportional to the gain in R^2 (expressed as a fraction of the currently unexplained variation) as the selected variable is brought into the regression model.

The technique of stepwise regression, more specifically a forward selection approach, is used to build a multiple regression model. The single input variable, which best explains variability in the response, will be chosen as the first variable to enter the model. Then, among the remaining input variables, the next input variable that best explains the remaining (or residual) variability enters. This process continues, building the multiple regression models, until none of the remaining input variables contribute substantially to reducing residual variability in the predicted response. At each step, the set of variables in the current regression model is ranked using the PCC and the changes in R^2, the coefficient of determination. Tests of significance, based on

whether the current coefficients provide a statistically significant regression, are applied to determine if variables enter or leave the regression model. Details of this technique are discussed by Iman et al. (1980). In this study the significance levels (α-values) have been prescribed as 0.10 for entering variables and 0.20 for departing variables. The stepwise procedure terminates when no additional variables qualify to enter the model.

This Monte Carlo-based method allows self-verification because the effectiveness of the PCC as a measure of sensitivity is conditional upon the model coefficient of determination, R^2. R^2 can be computed together with the PCC and gives the fraction of the model output variance accounted for by the linear regression model. If R^2 is close to one (the regression model explains the output well), the absolute value of the PCC can be used to rank the relative influence of the input variable on the output measures. When the raw data does not provide a good linear regression model, the rank transformed data (i.e., regression models built between the ranks of input and output variables) usually provide a better linear relationship. If the original data is nonlinear, but monotonic, then a linear relationship will exist between their ranks. However the rank transformation approach is completely inappropriate and will fail for nonmonotonic relationships. In this study, rank transformations have been adopted to achieve a higher R^2 value for all the regression fits. If the R^2 still shows a poor fit, the analyst must use techniques that work for nonlinear (or nonmonotonic, if ranks transformations are used) models. Such analysis is beyond the scope of this study.

5.12.6.3 Sampling Input Variables

The code SATOOL (Sensitivity Analysis TOOL) has been developed by enhancing an existing step-wise regression code (Iman et al. 1980) with the capability to compute PCCs at every step and provide importance ranking of the input variables at each step. The code SATOOL has been used for the importance ranking of the input variables in this study. The same code and approach were used for the uncertainty and sensitivity analysis of the total system performance assessment results (see Section 11.3 of Chapter 11-Summary and Conclusions).

For this analysis, each waste package is treated as a sample or data point. Thus, the input variables are those used to define waste package properties for the computer model, and potential output variables are those computer outputs defined for each waste package. Eleven output variables were selected:

- The time of the first breach by either a pit or patch penetration (waste package failure time)
- The time of the first patch failure on the waste package
- The time of the first pit failure on the waste package
- The number of patch failures at five simulation times (Table 5-17).

As mentioned earlier, there were two WAPDEG runs made for the purpose of stepwise regression sensitivity analysis. The first case evaluated the dripping scenario of the base case and was labeled as WPSA1. In the second case, labeled as WPSA2, additional variables, mainly

those dealing with sampling design (i.e., the number of patches, and variance partitioning for waste-package to waste-package variability and patch to patch variability) were allowed to vary. SATOOL was initially run for the entire suite of input values. SATOOL reported those input variables that were fixed and those that were highly correlated (on their ranks) to other input variables. Input variables that met either criterion were then eliminated from the SATOOL input for a final run of SATOOL.

5.12.6.4 Analysis of Results

For the first sensitivity run, referred to as Case WPSA1, thirteen input variables were used (Table 5-15). Results of the stepwise analysis, using SATOOL, where the output variable chosen was the first patch time, show that the input variable explaining the most variability is the CRM general corrosion rate under dripping conditions. This variable has a R^2 of 0.8098 for the rank transform fit. While approximately 20 percent of the remaining variation is left unaccounted for, the strong influence of this single variable on the WAPDEG model can be seen in a scatter plot of the first patch-breach times versus the CRM general corrosion rate under dripping condition (Figure 5-102). The regression model obtained using the first breach time as the output variable also shows a strong dependence on the CRM general corrosion rate with a R^2 of 0.7459 for the rank transform fit. The magnitude of R^2 is not as large because of a small number of waste package failures caused by localized corrosion (pit penetration). The sensitivity analysis of the pitting degradation output variables, both first pit-penetration time and the number of pit penetrations at differing times, was not successful. For the first pit-penetration time, this is because the small number of actual pitting failures in this model. For the number of pits at differing times, the relationship is essentially nonmonotonic due to the way pit-penetration numbers are defined in WAPDEG. This is because the number of pit penetrations on a given patch are removed from the cumulative count when the patch fails.

For the second sensitivity run (Case WPSA2), a total of 21 input variables were included in the study (Table 5-16). The first breach times and the first patch-breach times were nearly the same in Case WPSA2. This is because no waste package first breaches are caused by pitting failure until after 500,000 years. This delay in pitting failure is probably due to values of the localized corrosion time exponent being allowed to vary down to low values, coupled with the fact that the number of failures caused by pit perforation were low, as in Case WPSA1. The six most important variables, using waste package first breach time as our output variable, are shown in Table 5-18. The values of Standardized Rank Regression Coefficients (SRRC) and Partial Rank Correlation Coefficients (PRCC) and the R^2-loss are shown in this table. The ranking is the same based on PRCC or SRRC, indicating little impact of input variable correlation on the results. The regression model from which these results are drawn has six input variables, with a R^2 of nearly 0.85. While a higher R^2 would be desirable, it is considered adequate for the purpose of inferring the importance of the variables. The top four important variables are:

- Variance partition for the CRM general corrosion model
- Dripping CRM general corrosion rate
- Percent of waste package surface dripped on
- Number of patches simulated on the waste package.

The R^2-loss for these variables ranges from 0.49 to 0.02. The R^2-loss for other variables is insignificant being much smaller than those for the top four variables. Intuitively, from the physics of the model, one would expect those variables to be important, and the results of analysis thus appear very plausible. The R^2-loss indicates that redefining the top two important variables with a very small variance would reduce the variability in first breach times.

The analysis of the fraction of failed patch area on a waste package with time shows the time dependence of R^2-loss (Figure 5-103) and PRCC (Figure 5-104) on the top three inputs above, along with a forth variable, the no-dripping-CRM-general-corrosion rate. This time dependence illustrates how the regression model fit improves and stabilizes after 500,000 years, once the number of patch failures became statistically significant enough for a good regression fit. At very late times the no-dripping-CRM rate ranking (based on PRCC) increases, presumably because of an increase in the number of failures under no drip conditions.

5.12.6.5 Summary from Regression-Based Sensitivity Analysis

The primary results from this regression-based sensitivity analysis are:

A. For the response variables listed in the table, there were two input variables that consistently appeared as the two most important: the general corrosion rate of the CRM under dripping condition, and the waste package share of the variance of the distributions that define this corrosion rate. These two traded positions as the first and second most important variables, but in most cases they were both significantly more important than the third most important variable.

B. The most frequent variable to appear as the third most important variable, at a significant level of importance was the fraction of the top (or bottom) patches contacting dripping water.

These results indicate the importance of refined estimates of the general corrosion rate of the CRM under dripping condition to reduce the overall uncertainty in the waste package degradation prediction. Also, the allocation of variability to waste packages and patches should be further examined to see if there is any justification for narrowing its possible values. Finally, a better estimate for the fraction of patches that contact drips would also help reduce the variance of the output. These conclusions are based on the analysis of waste package failure time and the results for the number of patch failures.

The WAPDEG outputs that report the pit penetrations (in terms of first pit-penetration and number of pit penetrations) are poor choices of response variables for the sensitivity analysis. One reason for this is the preponderance of zeroes in the output. A second reason is the absence of monotonicity in the relationship of the number of pits to the input variables. Both of these reasons arise at least partially from the WAPDEG treatment of pit penetrations. That is, the number of pit penetrations are accumulated up to the point that the entire patch that they are on fails, then they are zeroed out to avoid double counting. Thus, reporting the number of pit penetrations at any given time will not necessarily show any consistent behavior from waste package to waste package.

5.13 SUMMARY AND RECOMMENDATION

5.13.1 Introduction

As part of the characterization efforts for the potential repository at Yucca Mountain, Nevada, which is being studied for the disposal of the nation's high-level radioactive waste including commercial spent nuclear fuels and vitrified high-level waste, the Viability Assessment (VA) of the potential repository is being conducted (CRWMS M&O 1997b). The current design concept for a multibarrier waste container provides the primary component of the engineered barrier system of the potential repository. Fulfillment of the requirements for substantially complete containment of the waste and subsequent controlled/gradual release of radionuclides from breached waste package into the geosphere will rely upon a robust waste container design, among other engineered barrier system components.

The current reference design specifies a two-layer barrier system, with a 100-mm thick CAM as the outer barrier and a 20-mm thick CRM as the inner barrier. The candidate materials are carbon steel (or ASTM A516) for CAM, and Alloy 22 (or UNS N06022) for the CRM (CRWMS M&O 1998a). Although failure of the waste container will most likely occur in the form of perforations created by localized corrosion of the corrosion-resistant inner barrier, high-performance corrosion-resistant alloys such as the candidate inner-barrier material could undergo corrosion degradation dominantly by general corrosion (CRWMS M&O 1998b). An additional small fraction of waste containers may fail prematurely because of material and manufacturing defects, damage during handling and/or by rockfall during emplacement, and other processes such as ground motions from earthquake and fault displacement. *Waste package failure is defined as having an opening through the wall of the waste package through which advective or diffusive transport of gas or radionuclide can occur.* Even if perforated with holes and cracks, the waste container should still be able to provide a substantial barrier to radionuclide release (Lee 1997; Lee, Chambré, and Andrews 1996; Lee, Atkins, McNeish, and Vallikat 1996; Pigford 1993).

The primary role of the waste package degradation modeling and abstraction, which is the subject of this chapter, is to provide information on the lifetime and overall degradation of the waste package. The key outputs from the waste package degradation modeling and abstraction are a quantitative assessment of the waste package degradation. The output from the waste package degradation model (WAPDEG) is presented as a time to initial penetration of the waste packages—in the form of either small holes (pits) resulting from localized corrosion or large openings ("patch" perforations) resulting from general corrosion—and subsequent perforations (or openings) of the waste packages as a function of time. The time of the initial perforation is assumed to lead to the initiation of the waste form degradation inside the breached waste package. The perforated or opened area on the waste package provides the area through which radionuclides are released. The uncertainty and spatial variability of the degradation information also are provided as an output from the waste package degradation model (WAPDEG).

5.13.2 Waste Package Degradation Expert Elicitation

Data for corrosion and other degradation processes of the candidate materials and their process models are being developed under the comprehensive corrosion testing and modeling programs

at Lawrence Livermore National Laboratory (McCright 1997). However, long-term testing data are not yet available under prototypic conditions, and, as a result, the models for waste package performance have large uncertainties. Consequently, an expert elicitation was conducted with the objective of developing additional information and models that are needed for waste package degradation modeling for TSPA-VA (CRWMS M&O 1998b).

Another major objective of the expert elicitation was to capture the uncertainties involved in assessing waste package degradation processes, including uncertainty both in the models used to represent corrosion processes and the parameter values used in those models. To ensure that the analysis included a range of perspectives, multiple individual judgements were elicited from members of an expert panel. The resulting assessments and probability distributions, therefore, provide a reasonable aggregate representation of the knowledge and uncertainties about key issues regarding waste package degradation.

In the elicitation, the experts provided an overview of the processes for waste package degradation in the potential repository, taking into consideration potential evolutions of the exposure conditions in the emplacement drifts. Then, the experts developed assessments for the models of various key corrosion processes and the parameters of the corrosion models for the CAM (carbon steel) and CRM (Alloy 22) barriers. The assessments for the above models and parameters also expressed uncertainties in the respective model and parameter values.

5.13.3 Waste Package Degradation Model

The current subsystem model for evaluating degradation of the waste package is WAste Package DEGradation (WAPDEG) model. Three different versions of WAPDEG were used for the analyses presented in this chapter. The base case analysis (Section 5.11) was conducted with Version 3.07 (CRWMS M&O 1998c), and the sensitivity analysis (Section 5.12) was with Versions 3.09 and 3.11 (CRWMS M&O 1998h, 1998k). This was due to the continued development of the code to meet the needs for various sensitivity analyses. The WAPDEG model is based on a stochastic simulation approach and provides a description of waste package degradation, which occurs as a function of time and repository location for specific design and thermal-hydrologic modeling assumptions.

A substantial amount of information for the individual corrosion model parameters and waste package degradation parameters, which are employed in the current waste package degradation model were derived from the recently conducted WPDEE. Because of the time constraints imposed on the completion of the TSPA-VA analysis and extended elicitation processes, the interim elicitation results were provided to facilitate the analysis (Pendleton 1998), and those interim results were used in the base case analysis (Section 5.11) and subsequent sensitivity analysis (Section 5.12). Consequently, the elicitation results for some parameters that were used in the analyses reported in this chapter are not exactly same as those in the final WPDEE report (CRWMS M&O 1998b). However, the differences in the parameter values between those two versions are insignificant to the extent that they should not affect the analysis results.

The stochastic waste package degradation model incorporates the following individual corrosion models:

- Humid-air general corrosion model for the CAM outer barrier
- Humid-air "roughness" factor (or localization factor) model for the outer barrier
- Aqueous general corrosion model for the outer barrier
- Aqueous roughness factor (or localization factor) model for the outer barrier
- Aqueous pitting corrosion model for the outer barrier when contacted with an alkaline solution (pH≥10)
- General corrosion model for the CRM inner barrier without drips
- General corrosion model for the CRM inner barrier in the presence of drips
- Localized corrosion (pitting and crevice corrosion) model for the CRM inner barrier.

In addition, the following corrosion parameters were abstracted and implemented in the waste package degradation model:

- Temperature threshold for the initiation of corrosion of the CAM outer barrier
- Relative humidity threshold for the initiation of humid-air corrosion of the CAM outer barrier
- Relative humidity threshold for the initiation of aqueous corrosion of the CAM outer barrier
- Local exposure conditions on the CRM inner barrier (after breach of the outer barrier) and their probability to attain
- Critical temperature threshold for the initiation of localized corrosion of the CRM inner barrier.

In TSPA-VA, the waste package degradation is modeled by dividing the waste package surface into patches and populating the corrosion rates stochastically over the patches, depending on the local corrosion conditions. The patches approach is an attempt to explicitly represent the variability in corrosion rates within a single waste package and to address multiple corrosion modes underway within a single waste package at a given time.

Variability in waste package degradation across the repository because of varying exposure conditions is modeled by incorporating explicitly the spatial distribution of the exposure conditions. These exposure condition parameters to be included in the waste package degradation modeling are temperature, relative humidity, in-drift water dripping, and pH of the contacting water. In addition, variability in waste package degradation due to *uncertain variations* of corrosion processes and local exposure conditions are not readily quantifiable.

These may include local (or micro-scale) electrochemical conditions of solution contacting waste package, uncertain long-term post-closure exposure conditions (such as water dripping and rockfalls), manufacturing of waste package, variation of the materials properties (especially microstructure-scale) etc. Where quantitative information for those uncertain parameters is available, the information was implemented explicitly in the waste package degradation modeling. For example, the WPDEE provided allocation of the elicited parameter values to its variability and uncertainty (see Sections 5.3 and 5.7 to 5.9). Otherwise, effects of those parameters for which quantifiable information is not available were represented by stochastically varying the corrosion rate parameters over the waste packages to be simulated and the patches in each waste package.

5.13.4 Summary of Waste Package Degradation Modeling Results

The base case results for the no-drip case show that there is no waste package failure until about 700,000 years, and only about 5 percent of the waste packages fail by 1,000,000 years. This is due to the excellent resistance of Alloy 22 to humid-air corrosion. Under dripping conditions, the first waste package breach occurs earlier, starting at about 2,700 years with only about 1 percent of the waste packages failing by 10,000 years, and about 23 percent of the waste packages failing by 100,000 years. The early breaches are caused by pit penetrations from the CRM localized corrosion, and the later breaches by patch penetration from the CRM general corrosion. The first patch-breach occurs at about 12,500 years.

The base case results showed that only a small fraction of waste packages fail by pit penetrations, and the dominant degradation mode is general corrosion (or passive dissolution) of the CRM under dripping conditions. The general corrosion rates with drips that were used in the base case analysis were provided by the experts and have a range over three to five orders of magnitude. This is due mainly to a lack of information on local chemical and electrochemical conditions on the CRM and limited experience with the relatively new alloy. As discussed in the following section, sensitivity analyses evaluated potential impacts of alternative uses of the expert-elicited CRM general corrosion rate parameters for dripping conditions.

A suite of sensitivity analyses was conducted to evaluate potential effects of alternative assumptions and values for the corrosion processes and parameters that were used in the base case analysis. In these analyses, two types of sensitivity analysis techniques were employed to evaluate the sensitivity of waste package degradation to the various waste package corrosion parameters. One technique is termed "one-off" sensitivity analysis, in which only one parameter is varied while other parameters are kept as in the base case model. The other technique is termed "regression-based" sensitivity analysis, in which a number of candidate parameters are varied over certain ranges and their impacts on waste package degradation are ranked against waste package performance measures using a regression technique. The major findings from the sensitivity analyses are summarized below.

The most important parameters to the long-term waste package degradation are (1) the CRM general corrosion rate under dripping conditions and (2) the allocation of the corrosion rate variance to waste package-to-waste package variability variance. For the base case analysis, 50 percent of the total variance was allocated to the variability of the corrosion rate, and the remaining 50 percent to the uncertainty variance, then the 50th percentile value of the uncertainty

variance was used as the median corrosion rate for the variability distribution. The above allocation was based on the average of the individual expert's assessment (Pendleton 1988). However, the general corrosion rates provided by the experts have a wide range of values, and there are high degrees of uncertainty associated with the assessment. This is mainly due to a limited understanding of the local exposure conditions on the CRM after CAM breach, and a limited experience with the relatively new material. To evaluate the effect of the general corrosion rate on waste package degradation, three alternative variability and uncertainty allocations and three alternative median rates from the uncertainty variance were defined. Two additional variability and uncertainty splits of the total variance were considered: 25 percent variability and 75 percent uncertainty, and 75 percent variability and 25 percent uncertainty. For each of the variance splits including the base case split, the median corrosion rate was sampled from the 5th, 50th, and 95th percentile of the uncertainty variance. Thus, for this sensitivity analysis, nine cases including the base case were analyzed (see Table 5-13 for a summary of the variance splits and median corrosion rates sampled).

The sensitivity analysis results demonstrate that different uncertainty and variability allocations of the CRM general corrosion rate for the dripping condition and different median corrosion rates sampled from the uncertainty variance have a significant impact on the long-term waste package degradation results. The regression-based sensitivity analysis results also show that the median rate of the CRM general corrosion rate under dripping conditions and the allocation of the total variance of the rate to the uncertainty and variability are the two most important parameters for long-term waste package degradation.

The sensitivity analysis results for the dripshield design option indicated that significant waste package performance gains are achieved through the use of a dripshield. The most important benefit offered by the dripshields, based on the modeling assumption is to eliminate seepage water from contacting the waste package during the early period of the repository lifetime. During these periods, waste packages are still at elevated temperatures, and the water contacting waste packages could be concentrated carrying aggressive chemical species to the waste packages. By eliminating these conditions with dripshields, waste packages are not subject to localized corrosion and degrade dominantly by general corrosion in much less corrosive conditions. As shown in the analysis, the reduction of water contacting the waste package because the dripshield extends the waste package lifetime significantly. One major uncertainty associated with the current analysis is that potential effects of the alteration of the thermal-hydrologic (and possibly chemical) processes in the near-field due to the presence of dripshield were not included.

A preliminary ceramic coating degradation model was developed to evaluate the ceramic coating design option. The preliminary model assumes that stresses developed by the volume expansion of the corrosion products of the CAM substrate is the only mechanism leading to the coating failure. The sensitivity analysis results based on the preliminary model showed that the ceramic coating itself could last more than 300,000 years if the pores in the ceramic coating are filled with water, providing a barrier to the oxygen transport to the corroding carbon steel substrate. However, the effect of other potential mechanisms on damaging the proposed thin ceramic coating on the waste package has not been analyzed. Other potential failure mechanisms include damages and cracks caused by handling, transport, local stress concentration at the contacts (especially at the bottom of the waste package), impact by a large rockfall and ground motion by

earthquakes. A complete analysis of the effects of these processes should be conducted before potential benefits of the ceramic coating can be substantiated.

The base case model uses the waste package surface temperature and relative humidity histories of the waste package groups in the NE region only, one of the six regions of the repository. Sensitivity of waste package degradation to the different thermal-hydrologic environments (in terms of temperature and relative humidity profiles at the waste package surface) in the other regions were analyzed using the temperature and relative humidity histories from the other regions. The analysis showed that the variable temperature and relative humidity at the waste package surface, from the six different repository regions, did not significantly affect long-term waste package performance.

The sensitivity analysis for a case with backfill showed that there are no significant differences in the overall waste package failure profiles between the no-backfill and backfill cases. However, for the backfill case, potential effects of backfill on the water seepage into the emplacement drifts and its contacts with the waste packages were not included in the analysis. Backfill could cause diversion of the seepage, reducing the contact of the seepage with the waste packages, or it could provide preferential passages to the waste packages, which could increase focused flow of the seepage to the waste packages and enhance waste package corrosion. Some other potential effects of backfill on the waste package degradation include (1) concentration of salts in the backfill from evaporation of the seepage water percolating through the backfill; and (2) enhanced water condensation by capillary condensation at the dust particles that have settled on the waste package surface during the backfill emplacement, and at the contacts between the backfill and the CAM surface.

5.13.5 Recommendation for Future Work

This section discusses key areas of uncertainty in the waste package degradation modeling for future analysis.

CRM Local Exposure Condition and General Corrosion Rate under Dripping Condition - The current analysis indicates that the CRM general corrosion rate for dripping condition is the most important parameter to long-term degradation of waste package in the potential repository. However, the general corrosion rates for dripping conditions that were provided by the experts have a range of three to five orders of magnitude. This uncertainty is due mainly to a lack of characterization of the local chemical and electrochemical conditions on the CRM and limited experience with the relatively new alloy. Additional data for the repository-relevant conditions could reduce uncertainty in characterizing the local exposure conditions on the CRM and thus the CRM general corrosion rate. Those data are also needed to develop a predictive model for the evolution of the local exposure conditions with time and varying near-field bulk conditions. Also, additional data for the CRM general corrosion (or passive dissolution) rate for the conditions that reasonably bound the local exposure conditions expected on the CRM would reduce the uncertainty in the waste package degradation prediction.

Evolution of Salt Concentrations on Waste Package with Drips - In the current waste package degradation model, for dripping conditions, the same corrosive conditions and the same corrosion rates for the CRM are applied to the entire simulation period. That is, effect of

potential run-off of salt solutions from the waste package surface under sustained dripping is not considered. Sustained drips could leave accumulated salt deposits on the waste package surface while the waste package is at elevated temperatures and potentially provide aggressive conditions for waste package corrosion. However, when the waste package temperature cools below boiling temperature, the sustained drips could wash off the salt solutions from the waste package surface, leading to potentially less corrosive conditions. Additional data and a predictive tool to characterize evolution of the local exposure conditions on the CRM as a function of the bulk exposure condition and time could reduce the uncertainty in the waste package degradation model prediction.

Characterization of Seepage Behavior – For dripping conditions in the current model the entire surface of the waste package is assumed to be wetted. This is based on the assumption that seepage could move along the waste package length with time and potentially wet the entire waste package surface. This assumption is very conservative considering the current conceptual model assumes that localized corrosion of the CRM initiates only under dripping conditions and the CRM general corrosion rates for the dripping conditions—especially the right-hand tails of the distributions—are much higher than those for the no-dripping condition. Such a conservative assumption is employed because of a lack of information on the process, but has an important effect on waste package degradation. The seepage conditions that are important to waste package performance and, thus, repository performance include the repository area that is subjected to dripping (i.e., the number of waste packages that experience dripping), the dripping rate and frequency, and the fraction of the waste package surface that is wetted by drips. Improved understanding of the seepage behavior could reduce the uncertainty in the waste package degradation model.

Galvanic Coupling Effects - Galvanic coupling of the CAM and CRM barriers may have an impact on the waste package degradation. One example of such interactions is galvanic protection of the CRM, which may contribute to enhanced waste package performance. Potential adverse effects to long-term waste package performance, which could result from the galvanic coupling, are enhanced corrosion of the CAM and hydrogen embrittlement of Alloy 22.

CRM Localized Corrosion Initiation Threshold - Localized corrosion (pitting and crevice corrosion) of high performance alloys such as Alloy 22 does not initiate if the local exposure conditions are below certain threshold values. As discussed in Section 5.9.2.6, in the waste package degradation model, the critical temperature threshold for the initiation of localized corrosion in the CRM is taken as an absolute. That is, localized corrosion initiates in the CRM if the waste package temperature is above the sampled critical threshold temperature, but never initiates if the waste package temperature is below the critical threshold temperature. The initiation threshold should include also other important exposure condition parameters. Those exposure parameters considered important are temperature, pH, chloride concentration, and concentration of oxidants such as Fe^{3+}. In addition, potential effect of prolonged exposure should be also considered in the future analysis. Additional testing and analysis for the initiation threshold in the repository-relevant conditions could help reduce uncertainty in the waste package degradation model.

CRM Localized Corrosion Stifling Criteria - Potential exists that localized (pitting and crevice) corrosion in the CRM may stifle before it penetrates through the 2-cm thick CRM.

Testing and detailed analysis to establish the localized corrosion stifling criteria in the repository-relevant conditions could help reduce uncertainty in the waste package degradation model.

Stress Corrosion Cracking - In many alloy systems, localized corrosion and stress corrosion cracking are interrelated because the sites of localized corrosion attack become the sources of initiation of stress corrosion (Farmer and McCright 1989; Farmer et al. 1988). In particular, because of potential technical difficulties associated with the relieving of stresses in the closure welds of the double-walled waste container, SCC of the closure welds may occur. Additional data and analysis could help reduce uncertainty in the waste package degradation model.

Enhanced Corrosion of CAM under Dripping - Preliminary testing results of carbon steel samples covered with salts indicate that the corrosion rate is higher than those without salt deposits. Additional data and analysis for the implication of the salt-deposit-enhanced corrosion could help reduce uncertainty in the waste package degradation model.

MIC Effect - The sensitivity analysis discussed in Section 5.12.3.2 showed that the early exposure of the CRM from the early CAM breaches by the MIC caused an earlier waste package breach initiation and a substantially greater number of waste packages with breached, compared to the base case results. The analysis was conducted under the assumption that sustained and sufficient microbe activities exist all the time in the post-closure repository at a level high enough to affect the CAM corrosion. It was also assumed in the analysis that the CAM general corrosion rate is increased by the MIC and the enhancement factor is represented by a multiplication factor to the CAM general corrosion rate, which was based on the recent preliminary test results (Horn et al. 1998). In addition, although the WPDEE results indicated that there are no documented cases for the MIC susceptibility of Alloy 22 and the CRM is immune to the MIC (CRWMS M&O 1998b), the alloy has a relatively short history of field applications. MIC colonies could potentially create locally acidic and oxidizing environments, which could increase the susceptibility of the CRM to localized corrosion.

Detailed mass balance inventory analyses, along with the data for site-relevant conditions, could help to reduce the uncertainty in the long-term microbial activity in the post-closure conditions of the potential repository. The uncertainty in the effect of microbial activity on the CAM and CRM corrosion could be reduced with additional data from the site relevant conditions.

Dripshield Design Option - The analysis results indicate that long-term waste package performance could be enhanced with the use of dripshield. Additional analyses could reduce the uncertainties associated with potential effects from the alteration of the thermal-hydrologic (and possibly chemical) processes in the near-field because of the presence of dripshield.

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