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# **Total System Performance Assessment (TSPA) Data Input Package for General Corrosion and Localized Corrosion of Waste Package Outer Barrier**

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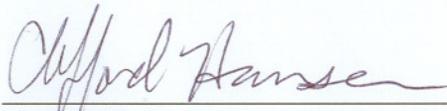
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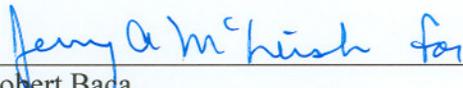
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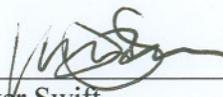
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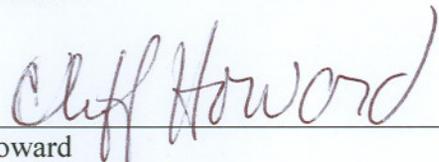
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## CHANGE HISTORY

<u>Revision Number</u>	<u>Interim Change No.</u>	<u>Date</u>	<u>Description of Change</u>
00	00	02/28/07	Initial issue
01	00	05/09/07	Crevice corrosion initiation model revised

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## ACRONYMS

ASW	as-welded
BSW	basic saturated water
CPP	cyclic potentiodynamic polarization
DIRS	Document Input Reference System
DTN	data tracking number
LTCTF	Long-Term Corrosion Testing Facility
MA	mill-annealed
MCA	multiple crevice assembly
MIC	microbially influenced corrosion
PCA	prism crevice assembly
QA	quality assurance
QARD	Quality Assurance Requirements and Description
SAW	simulated acidified water
SCW	simulated concentrated water
SDW	simulated dilute water
SSC	saturated silver chloride electrode
TDIP	TSPA data input package
THE	Tsujikawa-Hisamatsu electrochemical
TSPA	total system performance assessment
TWP	technical work plan
WPOB	waste package outer barrier
YMP	Yucca Mountain Project

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## 1. TSPA PARAMETER IDENTIFICATION AND DESCRIPTION

The purpose of this technical report is to document and transmit parameter names, values, uncertainties, and other relevant information from *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (WPOB) (SNL 2007 [DIRS 178519]), as planned in *Technical Work Plan for Postclosure Engineered Barrier Degradation Modeling* (SNL 2007 [DIRS 178849]) to total system performance assessment (TSPA). This report, a TSPA data input package (TDIP), is required to provide a documented data trail and usage description that is pertinent to the qualification of parameters and their associated values for use in the TSPA model. This TDIP is prepared in accordance with LS-PRO-001, *Technical Reports and Technical Work Plan for: Total System Performance Assessment (TSPA) Parameter Selection and Documentation with TSPA Data Input Package (TDIP)* (SNL 2007 [DIRS 179320]).

As mentioned in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (WPOB) (SNL 2007 [DIRS 178519], Section 1), the WPOB will be constructed of Alloy 22 (UNS N06022), a highly corrosion-resistant nickel-based alloy. The corrosion behavior of Alloy 22 has been evaluated in terms of two main corrosion processes—general corrosion and localized corrosion (SNL 2007 [DIRS 178519], Section 6). The general corrosion model will be used by TSPA to evaluate the extent of WPOB degradation by general corrosion under repository relevant environmental conditions over the regulatory performance period. The WPOB general corrosion model considers several submodels, which account for dry oxidation, aqueous general corrosion, the effects of aging and phase instability, and microbially influenced corrosion (MIC). However, dry oxidation and aging and phase instability have been determined to have insignificant effect on the general corrosion rate of the WPOB under repository exposure conditions (SNL 2007 [DIRS 178519], Sections 6.4.2 and 6.4.6). Consequently, they will not be considered in the TSPA. The waste package outer barrier localized corrosion model will be used by TSPA to evaluate the extent of WPOB degradation by localized corrosion under the expected repository relevant environmental conditions over the regulatory performance period. The submodels included in the waste package outer barrier localized corrosion model are the crevice repassivation potential, long-term corrosion potential, and crevice corrosion propagation models. These models are limited in their application to repository relevant exposure conditions. Additional limitations on the evaluation of the crevice repassivation and long-term corrosion potential models are expressed as implementation rules in Section 2.2.1.

Model development in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* was accomplished following an approved technical work plan (TWP) and other applicable quality assurance (QA) procedures and qualified software (SNL 2007 [DIRS 178519], Sections 2 and 3). Direct inputs to the models included Yucca Mountain Project (YMP) data and outside data along with a few properly justified assumptions (SNL 2007 [DIRS 178519], Sections 4 and 5). Lists of direct and indirect inputs to each submodel are presented in the Document Input Reference System (DIRS) database report. Data tracking numbers (DTNs) of the YMP data and their Q-status are documented in the DIRS database report.

### 1.1 TSPA PARAMETER NAME

A complete list of parameter inputs from *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]) to TSPA is provided in Table 1-1. As seen

in Table 1-1, these parameters include: the natural logarithm of the general corrosion rate for Alloy 22 at 60°C (i.e.,  $\ln R_o$ ), the shape and scale parameters for Weibull distribution of  $R_o$ , relative humidity threshold for MIC, MIC general corrosion enhancement factor,  $C_1$  parameter giving the temperature dependence of general corrosion rate, crevice repassivation potential model coefficients/parameters, long-term corrosion potential model coefficients/parameters, and percentage of surface area affected by crevice corrosion and crevice corrosion propagation rate.

## 1.2 TSPA PARAMETER DEFINITION/DESCRIPTION

All TSPA input parameters from *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]) are defined and briefly described in Table 1-1 as well as in Section 2. The sources of these parameters are also documented in Table 1-1.

## 1.3 PARAMETER TYPE

As mentioned in column 4 of Table 1-1, all input parameters into TSPA from *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]) are of a statistical nature. The name of the statistics for each parameter distribution is mentioned in Table 1-1.

## 1.4 PARAMETER VALUE(S)

The value(s) of the TSPA parameters provided in column 5 of Table 1-1 are contained in DTN: MO0703PAGENCOR.001 [DIRS 180663]. Uncertainty in the parameter values and their distribution characteristics are also presented in Table 1-1.

## 1.5 DTN/NAME OR OTHER REFERENCE

The source for all TSPA input parameters listed in Table 1-1 is DTN: MO0703PAGENCOR.001 [DIRS 180663], which, in turn, is prepared on the basis of outputs from *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 8).

Table 1-1. TSPA Parameter Information/Specification

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Model Name	Parameter Name	Parameter Definition/ Description	Parameter Type	Parameter Value and Uncertainty/Variability	Parameter Source DTN
General corrosion	lnR <sub>o</sub> TSPA Model file names are WDlnR_ESC_L_cdf WDlnR_ESC_M_cdf WDlnR_ESC_H_cdf	Cumulative distribution function for the natural logarithm of the general corrosion rate for Alloy 22 (R <sub>o</sub> ) R <sub>o</sub> is the general corrosion rate of Alloy 22 at 60°C. Variance in R <sub>o</sub> represents spatial variability in the general corrosion process.	Stochastic	Three sets of values corresponding to low, medium, and high levels of uncertainties in GC_shape and GC_scale parameters (see second and third rows of this table and also see Table 2-1)	Source: Developed by TSPA from GC_Scale and GC_Shape parameters.
General corrosion	GC_scale	Scale parameter for Weibull distribution (b)	Stochastic	6.628 (low): 5% of realizations 8.134 (medium): 90% of realizations 9.774 (high): 5% of realizations Different values are uncertainty. Overall distribution is spatial variability	DTN: MO0703PAGENCOR.001 [DIRS 180663]. Filename: <i>BaseCase GC CDFs.xls</i> .
General corrosion	GC_shape	Shape parameter for Weibull distribution (c)	Stochastic	1.380 (low): 5% of realizations 1.476 (medium): 90% of realizations 1.578 (high): 5% of realizations Different values are uncertainty. Overall distribution is spatial variability	DTN: MO0703PAGENCOR.001 [DIRS 180663]. Filename: <i>BaseCase GC CDFs.xls</i> .
General corrosion	C1_GenCorr_A22_a	Parameter for the temperature dependence of general corrosion rate (C1)	Stochastic	Truncated (at ±2 standard deviations) normal distribution. Mean: 4,905 K, standard deviation: 1,413 K. Uncertainty	DTN: MO0703PAGENCOR.001 [DIRS 180663]. Filename: <i>BaseCase GC CDFs.xls</i> .
General corrosion	MIC_A22_a	MIC general corrosion enhancement factor	Stochastic	Uniform distribution between 1 and 2 Spatial variability	DTN: MO0703PAGENCOR.001 [DIRS 180663]. Filename: <i>MIC Summary.pdf</i> .
General corrosion	MIC_RHThresh_a	Relative humidity threshold for MIC	Stochastic	Uniform distribution between 75% to 90% Uncertainty	DTN: MO0703PAGENCOR.001 [DIRS 180663]. Filename: <i>MIC Summary.pdf</i> .
Localized corrosion	LC_a0 LC_a1 LC_a2 LC_a3 LC_a4	Coefficients of crevice repassivation potential model Equation 2-3 (SNL 2007 [DIRS 178519], Section 8). (a <sub>0</sub> , a <sub>1</sub> , a <sub>2</sub> , a <sub>3</sub> , a <sub>4</sub> )	Stochastic	Mean LC_a0 = 190.242 Mean LC_a1 = -3.008 Mean LC_a2 = -46.800 Mean LC_a3 = 535.625 Mean LC_a4 = 0.061 Covariance matrix given in Equation 2-4 (SNL 2007 [DIRS 178519], Section 8) Uncertainty	DTN: MO0703PAGENCOR.001 [DIRS 180663]. Filename: <i>LC_Initiation.pdf</i> .

Table 1-1. TSPA Parameter Information/Specification (Continued)

Model Name	Parameter Name	Parameter Definition/ Description	Parameter Type	Parameter Value and Uncertainty/Variability	Parameter Source DTN
Localized corrosion	LC_eps_rcrev_a	Error term of crevice repassivation potential model Equation 2-3 ( $\epsilon_{rcrev}$ )	Stochastic	Normal distribution with a mean of zero mV versus SSC and a standard deviation of 45.055 mV versus SSC Uncertainty	DTN: MO0703PAGENCOR.001 [DIRS 180663]. Filename: <i>LC_Initiation.pdf</i> .
Localized corrosion	LC_c0 LC_c1 LC_c2 LC_c3 LC_c4 LC_c5 LC_c6	Coefficients of long-term corrosion potential model, Equation 2-5 (SNL 2007 [DIRS 178519], Section 8) ( $C_0, C_1, C_2, C_3, C_4, C_5, C_6$ )	Stochastic	Mean LC_c0 = 1051.219 Mean LC_c1 = -3.024 Mean LC_c2 = -155.976 Mean LC_c3 = -1352.040 Mean LC_c4 = 10.875 Mean LC_c5 = 137.856 Mean LC_c6 = -8.498 Covariance matrix given in Equation 2-6 (SNL 2007 [DIRS 178519], Section 8). Uncertainty	DTN: MO0703PAGENCOR.001 [DIRS 180663]. Filename: <i>LC_Initiation.pdf</i> .
Localized corrosion	LC_eps_corr_a	Error term of long-term corrosion potential model Equation 2-5 ( $\epsilon_{corr}$ )	Stochastic	Normal distribution with a mean of zero mV versus SSC and a standard deviation of 85.265 mV versus SSC Uncertainty	DTN: MO0703PAGENCOR.001 [DIRS 180663]. Filename: <i>LC_Initiation.pdf</i> .
Localized corrosion	LC_WP_Frac_Area_a	Percentage of surface area affected by crevice corrosion	Stochastic	Minimum: 0.05% of waste package area Maximum: percentage of waste package area wetted by seepage. Uniform distribution: if both minimum and maximum values are of the same order of magnitude. Log-uniform distribution: if maximum value is greater than minimum value by one order of magnitude (or larger) Uncertainty	DTN: MO0703PAGENCOR.001 [DIRS 180663]. Filename: <i>LC_Initiation.pdf</i> .
Crevice corrosion propagation rate	LC_Rate_a	Crevice corrosion propagation rate	Stochastic	0 percentile = 12.7 $\mu\text{m}/\text{yr}$ 50th percentile = 127 $\mu\text{m}/\text{yr}$ 100th percentile = 1,270 $\mu\text{m}/\text{yr}$ Log-uniform distribution Uncertainty	DTN: MO0703PAGENCOR.001 [DIRS 180663]. Filename: <i>LC_Propagation.pdf</i> .

NOTE: SSC = saturated silver chloride electrode.

## 2. TSPA IMPLEMENTATION

The waste package outer barrier (WPOB) can be subject to a variety of corrosion processes depending on exposure conditions during its expected unusually long service life in the repository. For example, general corrosion of the waste package outer barrier is possible under conditions in which a stable aqueous water film can exist on the waste package surface. The WPOB general corrosion model was developed using data obtained from experiments conducted in mixed ionic environments as well as simple salt solutions including highly concentrated chloride brines and chloride brines containing nitrate ions. The general corrosion model has been validated against data obtained at temperatures as high as 180°C. Therefore, the general corrosion model should be applicable over all repository exposure environments.

Microbially influenced corrosion (MIC) effects are applied when the relative humidity at the waste package surface is greater than a threshold relative humidity sampled from a uniform distribution between 75% and 90%. The effect of MIC on general corrosion of the WPOB is represented by an enhancement factor applied to the general corrosion rate determined from Equation 2-1. The MIC general corrosion enhancement factor is uniformly distributed between 1 and 2 (see Section 2.1). The effect of MIC on localized corrosion is considered to be inconsequential.

Localized corrosion can be either pitting corrosion on boldly exposed surfaces or crevice corrosion, which takes place in occluded regions. In the WPOB degradation model report (SNL 2007 [DIRS 178519]), the only form of localized corrosion is assumed to be crevice corrosion as opposed to pitting corrosion. This assumption conservatively includes all other forms of localized corrosion including pitting. This is a conservative and bounding assumption because initiation thresholds for crevice corrosion, in terms of exposure parameters such as chemistry and temperature, are lower than those required for pitting corrosion (SNL 2007 [DIRS 178519], Section 5.3). Crevices may be formed on the waste package surface at occluded regions such as in between the waste package and its supports and potentially beneath mineral scales, corrosion products, dust, rocks, etc. The chemical environment in a creviced region may be more severe than the near-field environment due to hydrolysis of dissolved metals in the creviced region. Metal ion hydrolysis can lead to the accumulation of hydrogen ions and a corresponding decrease in pH. Electromigration of chloride ions (and other anions) into the crevice must occur to balance the charge within the creviced region. Chloride ions can cause initiation of crevice corrosion on Alloy 22 WPOB surface.

### 2.1 WPOB GENERAL CORROSION MODEL IMPLEMENTATION

The general corrosion model is applied to all environmental conditions in the repository and is based on corrosion measurements in the presence of an aqueous electrolyte. The base-case general corrosion model for the WPOB (SNL 2007 [DIRS 178519], Section 6.4.3.4) is based on a temperature dependence of the general corrosion process, represented by an apparent activation energy using a modified Arrhenius relation. The model is expressed as follows:

$$\ln(R_T) = \ln(R_o) + C_1 \left( \frac{1}{T_0} - \frac{1}{T} \right) \quad (\text{Eq. 2-1})$$

where  $R_T$  is the temperature-dependent general corrosion rate in nm/yr,  $T$  is absolute temperature in Kelvin,  $T_0 = 333.15$  K ( $60^\circ\text{C}$ ), and  $R_o$  and  $C_1$  are uncertain constants.

The temperature dependence term ( $C_1$ ) was obtained from short-term polarization resistance data for Alloy 22 specimens tested for a range of sample configurations, metallurgical conditions, and exposure conditions. The temperature dependence term,  $C_1$ , is represented as a truncated (at  $\pm 2$  standard deviations) normal distribution with a mean of 4,905 K and a standard deviation of 1,413 K. These values correspond to an apparent activation energy of 40.78 kJ/mol with a standard deviation of 11.75 kJ/mol. As mentioned in Section 6.4.3.4 of the WPOB model report (SNL 2007 [DIRS 178519]), the selection of a normal distribution for this parameter is based on the observation of a linear quantile-normal plot. In addition, a Shapiro-Wilk goodness-of-fit test calculated a p-value, which is consistent with normal distribution. Truncation of the  $C_1$  distribution at  $\pm 2$  standard deviations is appropriate given that the resulting range in apparent activation energies spans a large range of values from extremely low temperature dependence (e.g., 17.3 kJ/mol) to a high temperature dependence (e.g., 64.3 kJ/mol).

The parameter  $R_o$  follows a Weibull distribution (with parameters given in Table 2-1) that was fit to general corrosion rates derived from weight-loss data of five-year exposed crevice specimens. The five-year data were considered to represent the distribution of long-term general corrosion rates of the WPOB at  $T_0 = 333.15$  K ( $60^\circ\text{C}$ ).

As will be discussed in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 6.4.3), weight loss specimens with two different geometries (uncreviced weight loss and creviced) were analyzed after five years of exposure either immersed in solution or exposed to the vapor phase above the solution (a limited number of specimens were exposed at the water line). The weight-loss values of the creviced specimens were observed to be higher than those of the uncreviced weight-loss specimens. This may have been caused by different surface polishing treatments between the two specimen groups (Wong et al. 2004 [DIRS 174800]). The weight-loss specimens were polished on both sides, and the crevice specimens were only polished on one side. It is possible that the mill-annealed oxide left on the unpolished side of the crevice specimen resulted in a greater measured weight-loss when the specimen cleaning was undertaken (i.e., the mill-annealed oxide was removed resulting in a greater measured weight-loss). Furthermore, creviced specimens exposed to the vapor phase and immersed creviced specimens exhibited comparable weight losses while, for uncreviced specimens, the weight loss for specimens in the vapor phase was lower than that for immersed specimens. It is possible that the differences in immersed versus vapor exposed weight loss behavior between the different specimen geometries was a result of the different surface polishing treatments. The primary source of uncertainty in the weight loss measurements is the measurement of the weight loss itself (SNL 2007 [DIRS 178519], Section 6.4.3). Because the measured weight losses of the creviced specimens were higher than those of the uncreviced weight-loss specimens, the measurement uncertainty (relative to the measured weight loss) for the creviced specimens is less than that of the uncreviced weight-loss specimens. Due to their higher weight losses, it is conservative to use the general corrosion rates derived from the weight loss of the creviced specimens in evaluating waste package performance in the repository.

Table 2-1. Results of Uncertainty Analysis of Weibull Fitting of 60°C General Corrosion Rate Distribution

Uncertainty Level	Scale Parameter, b (nm/yr)	Shape Parameter, c (no units)
Low	6.628	1.380
Medium	8.134	1.476
High	9.774	1.578

Source: As listed in Table 1-1.

In TSPA, the low, medium, and high general corrosion rate distribution parameters should be randomly selected in such a way that the low and high general corrosion rate distributions are each used for 5% of realizations and the medium general corrosion rate distribution is used for the remaining 90% of realizations. These parameters are discussed further in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 6.4.3.3).

Comparing the above specification with the parameters listed in Table 1-1 indicates that  $R_o$  is given by a Weibull distribution with a shape parameter given by GC\_shape ( $c$  in Table 2-1) and a scale parameter given by GC\_scale ( $b$  in Table 2-1).

The variance in  $R_o$  is very likely the result of the uncontrolled surface treatment for the creviced specimens. However, this variance is being used to represent the spatial variability in the general corrosion process for the purposes of modeling the general corrosion behavior. The general corrosion rate variability is applied among local areas on the surfaces of the waste packages. The entire variance in the temperature dependence term ( $C_1$ ) (i.e., C1\_GenCorr\_A22\_a in Table 1-1) is due to uncertainty, and the uncertainty is limited to  $\pm 2$  standard deviations. This treatment of temperature dependence accounts for over 95% of the variance in this term (i.e.,  $C_1$ ).

The general corrosion model (SNL 2007 [DIRS 178519], Section 6.4.3.4) was developed using data in both mixed ionic environments and data from simple salt solutions including highly concentrated chloride brines and chloride brines containing nitrate ions. *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 7.2) validates the general corrosion model against data obtained at temperatures as high as 180°C. The general corrosion model extrapolates corrosion rates below 60°C. This approach is justified because the anodic dissolution of the passive film on Alloy 22 is expected to decrease with a decrease in the temperature. This view is supported by the results published by Dunn et al. (2005 [DIRS 178104], Sections 3.1 and 3.2; 2004 [DIRS 171452]) and Lloyd et al. (2003 [DIRS 167921]). Dunn et al. (2005 [DIRS 178104], Sections 3.1 and 3.2; 2004 [DIRS 171452]) studied the effect of temperature on the general corrosion rate of Alloy 22 in 0.028 M NaCl at a pH of 5.5 over a temperature range of 25°C to 95°C. They reported an apparent activation energy of 46.3 kJ/mol. This apparent activation energy is consistent with that documented in this TDIP (i.e., 40.78 kJ/mol obtained by polarization resistance method). Also, a temperature dependence of 46 kJ/mol was observed by Lloyd et al. (2003 [DIRS 167921]) in acidic chloride- and sulfate-containing solutions (pH about 1) over a temperature range of 25°C to 85°C using a potentiostatic method. This value also corroborates well with that reported in this report and provides further confidence in the apparent activation value documented in this report.

*General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 7.2) validates the general corrosion model against data obtained at temperatures as high as 180°C. Repository maximum temperatures are on the order of 200°C (BSC 2005 [DIRS 173944], Figure 6.3-53). Based on the discussion provided above and the small region of extrapolation (approximately 20°C), the general corrosion model should be valid for modeling of general corrosion at repository maximum temperatures. Therefore, the general corrosion model should be applicable over all repository exposure environments.

The WPOB is considered subject to MIC when the relative humidity at the WPOB surface is equal to or greater than a relative humidity threshold. The effect of MIC on general corrosion of the WPOB is represented by an enhancement factor applied to the general corrosion rate determined from Equation 2-1 (SNL 2007 [DIRS 178519], Section 6.4.5). The current waste package modeling TWP (SNL 2007 [DIRS 178849], Section 2.1.1), requires reevaluation of the relative humidity threshold for MIC and the MIC enhancement factor. The reevaluation led to the conclusions that the relative humidity threshold for MIC should be uniformly distributed between 75% and 90%, and the MIC enhancement factor should be uniformly distributed between 1 and 2. In addition, the reevaluation attributed the entire variance of the distributions to 100% uncertainty and 100% spatial variability, respectively (Table 1-1). Justifications for the selection of upper and lower bound values for the relative humidity threshold for MIC and the MIC enhancement factor, as well as the selection of statistical distributions to represent the variance of these parameters are documented in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 6.4.5).

The technical product outputs of the WPOB general corrosion model are documented in DTN: MO0703PAGENCOR.001 [DIRS 180663] and summarized in Table 2-2. More detailed information is available in *General and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 8).

It should be noted that the crevice geometry specimens used to determine the  $R_o$  distribution had dimensions of 2 in × 2 in × 1/8 in with a 0.312-in. (7.9-mm)-diameter hole in the center for sample mounting. Using Equation 2-2:

$$A = 2ab + 2bc + 2ac - \left( \frac{\pi d^2}{2} \right) + \pi dc \quad (\text{Eq. 2-2})$$

where  $a$  is the length of the specimen,  $b$  is the width of the specimen,  $c$  is the thickness of the specimen, and  $d$  is diameter of the hole, the exposed surface area for a crevice sample (converted to mm<sup>2</sup>) is 5,787 mm<sup>2</sup>. If a patch area that is greater than this is used to analyze general corrosion of waste packages, the general corrosion rates used should be adjusted to account for the effects of this change of scale. A methodology to accomplish this change of scale has been supplied to TSPA in the past (BSC 2004 [DIRS 169996], Section 6.3.4).

Table 2-2. Summary of General Corrosion Model Output for Waste Package Outer Barrier

Name	Output Description	Output Uncertainty		
		Source of Uncertainty	Uncertainty Distribution	Characteristic Values
Parameter $R_0$ of temperature-dependent general corrosion model, Equation 2-1	Weibull distribution	Fitting to distribution	Three sets of values for low, medium, and high levels of uncertainty Table 2-1	Table 2-1
Parameter $C_1$ of temperature-dependent general corrosion model, Equation 2-1	Truncated normal distribution	Measurement	Entire distribution	Mean 4,905 K, standard deviation 1,413 K. Limited to $\pm 2$ standard deviations.
MIC enhancement factor	Uniform distribution	N/A	All spatial variability	Minimum = 1 Maximum = 2
MIC initiation threshold	Uniform between 75% and 90% relative humidity	Microbial identity/environment	Entire distribution	Minimum = 75% Maximum = 90%

Source: As listed in Table 1-1.

## 2.2 WPOB LOCALIZED CORROSION MODEL IMPLEMENTATION

Localized corrosion of the WPOB is modeled with two model components: an initiation model and a propagation model (SNL 2007 [DIRS 178519], Section 6.4.4).

### 2.2.1 Waste Package Outer Barrier Localized Corrosion Initiation Model Implementation

Crevice corrosion of the WPOB initiates when the long-term corrosion potential ( $E_{corr}$ ) is equal to or greater than a critical potential ( $E_{critical}$ ), that is,  $\Delta E (= E_{critical} - E_{corr}) \leq 0$ . The crevice corrosion initiation model uses the crevice repassivation potential ( $E_{rcrev}$ ) as the critical potential. The **crevice repassivation potential model** ( $E_{rcrev}$ ) is expressed as follows:

$$E_{rcrev} = a_0 + a_1 T + a_2 \ln[Cl^-] + a_3 \frac{[NO_3^-]}{[Cl^-]} + a_4 T \cdot [Cl^-] + \varepsilon_{rcrev} \quad (\text{Eq. 2-3})$$

where  $a_0$ ,  $a_1$ ,  $a_2$ ,  $a_3$ , and  $a_4$  are coefficients of the model parameters,  $T$  is the temperature ( $^{\circ}\text{C}$ ),  $[Cl^-]$  is the molal ( $m$ , moles/kg water) chloride ion concentration,  $[NO_3^-]$  is the molal nitrate ion concentration, and  $\varepsilon_{rcrev}$  is the error term. The mean values of the coefficients of the model parameters from the fitting were determined to be:  $a_0 = 190.242 \pm 18.373$ ,  $a_1 = -3.008 \pm 0.225$ ,  $a_2 = -46.800 \pm 3.126$ ,  $a_3 = 535.625 \pm 26.140$ , and  $a_4 = 0.061 \pm 0.010$ . The variance of the model coefficients is calculated via a covariance matrix (Equation 2-4), and the entire variance is due to uncertainty. Equation 2-4 is the covariance matrix mentioned in Table 1-1. The model

coefficients are sampled from a multivariate normal distribution with the above-mentioned mean values consistent with the covariance matrix given in Equation 2-4.

$$r\Sigma = \begin{pmatrix} 3.376E+002 & -3.909E+000 & -9.310E+000 & 8.236E+001 & 3.559E-002 \\ -3.909E+000 & 5.077E-002 & 9.271E-002 & -1.202E+000 & -8.308E-004 \\ -9.310E+000 & 9.271E-002 & 9.770E+000 & 1.930E+000 & -2.048E-002 \\ 8.236E+001 & -1.202E+000 & 1.930E+000 & 6.833E+002 & -2.790E-002 \\ 3.559E-002 & -8.308E-004 & -2.048E-002 & -2.790E-002 & 1.011E-004 \end{pmatrix} \quad (\text{Eq. 2-4})$$

The error term,  $\varepsilon_{rcrev}$ , is a term representing data variance not explained by the fitting procedure and has a normal distribution with a mean of zero mV versus the saturated silver chloride electrode (SSC) and a standard deviation,  $s_{rcrev}$ , of 45.055 mV versus SSC. Variance in the error term,  $\varepsilon_{rcrev}$ , is attributed to uncertainty (DTN: MO0703PAGENCOR.001 [DIRS 180663], filename: *LC\_Initiation.pdf*).

The prediction intervals for the *unconstrained* crevice repassivation potential model are calculated by adding to the median estimate (i.e., the expected value of  $E_{rcrev}$  obtained by using the mean values of the model coefficients from Equation 2-3) an adjustment based on the standard deviation of the error term ( $s_{rcrev}$ ), the covariance matrix of the model coefficients (Equation 2-4), and the values of the exposure parameters for the data point being evaluated. The adjustment factor is written in matrix form as,

$$\pm 2 \sqrt{\left[ 1 \quad T \quad \ln[Cl^-] \quad \frac{[NO_3^-]}{[Cl^-]} \quad T \cdot \ln[Cl^-] \right] r\Sigma \left[ 1 \quad T \quad \ln[Cl^-] \quad \frac{[NO_3^-]}{[Cl^-]} \quad T \cdot \ln[Cl^-] \right]^T + s_{rcrev}^2} \quad (\text{Eq. 2-5})$$

The values of the crevice repassivation potential are *constrained* to be within the range defined by the  $\pm 2$  standard deviation prediction interval of the *unconstrained* crevice repassivation potential model. That is, the  $\pm 2$  standard deviation prediction intervals of the *unconstrained* crevice repassivation potential relationship (Equation 2-3 adjusted by Equation 2-5) are used as bounds on the value that the crevice repassivation potential may have. Thus, if the calculated *unconstrained* crevice repassivation potential exceeds the +2 standard deviation prediction bound of the *unconstrained* crevice repassivation potential model, the crevice repassivation potential value of the +2 standard deviation prediction bound of the *unconstrained* crevice repassivation potential model should be used as the value of the crevice repassivation potential for the given exposure conditions. Similarly, if the calculated *unconstrained* crevice repassivation potential does not exceed the -2 standard deviation prediction bound of the *unconstrained* crevice repassivation potential model, the crevice repassivation potential value of the -2 standard deviation prediction bound of the *unconstrained* crevice repassivation potential model should be used as the value of the crevice repassivation potential for the given exposure conditions.

The **long-term corrosion potential model** ( $E_{corr}$ ) for the WPOB is expressed as follows (SNL 2007 [DIRS 178519], Section 6.4.4):

$$E_{corr} = c_o + c_1 T + c_2 pH + c_3 \frac{[NO_3^-]}{[Cl^-]} + c_4 T \frac{[NO_3^-]}{[Cl^-]} + c_5 pH \frac{[NO_3^-]}{[Cl^-]} + c_6 pH \ln[Cl^-] + \varepsilon_{corr} \quad (\text{Eq. 2-6})$$

where  $c_0, c_1, c_2, c_3, c_4, c_5,$  and  $c_6$  are coefficients of the model parameters,  $T$  is the temperature ( $^{\circ}\text{C}$ ),  $[\text{Cl}^-]$  is the molal chloride ion concentration,  $[\text{NO}_3^-]$  is the molal nitrate ion concentration, and  $\varepsilon_{corr}$  is the error term. The estimated regression coefficients and their uncertainty ( $\pm 1$  standard deviation) are:  $c_0 = 1,051.219 \pm 119.774$ ,  $c_1 = -3.024 \pm 0.977$ ,  $c_2 = -155.976 \pm 11.495$ ,  $c_3 = -1,352.040 \pm 252.224$ ,  $c_4 = 10.875 \pm 1.890$ ,  $c_5 = 137.856 \pm 23.158$ , and  $c_6 = -8.498 \pm 0.801$ . The variance of the model coefficients is calculated via a covariance matrix (Equation 2-6), and the entire variance is due to uncertainty. Equation 2-6 is the covariance matrix mentioned in Table 1-1. The model coefficients are sampled from a multivariate normal distribution with the above-mentioned mean values consistent with the covariance matrix given in Equation 2-6.

$$r\Sigma^2 = \begin{pmatrix} 1.435\text{E}+004 & -1.031\text{E}+002 & -9.152\text{E}+002 & -2.762\text{E}+004 & 1.802\text{E}+002 & 1.884\text{E}+003 & -1.660\text{E}+001 \\ -1.031\text{E}+002 & 9.539\text{E}-001 & 2.770\text{E}+000 & 1.846\text{E}+002 & -1.519\text{E}+000 & -6.817\text{E}+000 & -7.543\text{E}-002 \\ -9.152\text{E}+002 & 2.770\text{E}+000 & 1.321\text{E}+002 & 1.971\text{E}+003 & -6.909\text{E}+000 & -2.515\text{E}+002 & 4.409\text{E}+000 \\ -2.762\text{E}+004 & 1.846\text{E}+002 & 1.971\text{E}+003 & 6.362\text{E}+004 & -4.223\text{E}+002 & -4.107\text{E}+003 & 5.959\text{E}+001 \\ 1.802\text{E}+002 & -1.519\text{E}+000 & -6.909\text{E}+000 & -4.223\text{E}+002 & 3.573\text{E}+000 & 1.337\text{E}+001 & -2.622\text{E}-001 \\ 1.884\text{E}+003 & -6.817\text{E}+000 & -2.515\text{E}+002 & -4.107\text{E}+003 & 1.337\text{E}+001 & 5.363\text{E}+002 & -6.697\text{E}+000 \\ -1.660\text{E}+001 & -7.543\text{E}-002 & 4.409\text{E}+000 & 5.959\text{E}+001 & -2.622\text{E}-001 & -6.697\text{E}+000 & 6.418\text{E}-001 \end{pmatrix} \quad (\text{Eq. 2-7})$$

The error term,  $\varepsilon_{corr}$ , is a term representing data variance not explained by the fitting procedure and has a normal distribution with a mean of zero mV versus SSC and a standard deviation,  $s_{corr}$ , of 85.265 mV versus SSC. Variance in the error term,  $\varepsilon_{corr}$ , is attributed to uncertainty (DTN: MO0703PAGENCOR.001 [DIRS 180663], filename: *LC\_Initiation.pdf*).

The prediction intervals for the *unconstrained* long-term corrosion potential model are calculated by adding to the median estimate (i.e., the expected value of  $E_{corr}$  obtained by using the mean values of the model coefficients from Equation 2-6) an adjustment based on the standard deviation of the error term ( $s_{corr}$ ), the covariance matrix of the model coefficients (Equation 2-7), and the values of the exposure parameters for the data point being evaluated. The adjustment factor is written in matrix form as:

$$\pm 2 \sqrt{\left[ 1 \quad T \quad pH \quad \frac{[\text{NO}_3^-]}{[\text{Cl}^-]} \quad T \cdot \frac{[\text{NO}_3^-]}{[\text{Cl}^-]} \quad pH \frac{[\text{NO}_3^-]}{[\text{Cl}^-]} \quad pH \ln[\text{Cl}^-] \right] r\Sigma^2 \left[ 1 \quad T \quad pH \quad \frac{[\text{NO}_3^-]}{[\text{Cl}^-]} \quad T \cdot \frac{[\text{NO}_3^-]}{[\text{Cl}^-]} \quad pH \frac{[\text{NO}_3^-]}{[\text{Cl}^-]} \quad pH \ln[\text{Cl}^-] \right]^T + s_{corr}^2} \quad (\text{Eq. 2-8})$$

The values of the long term corrosion potential are *constrained* to be within the range defined by the  $\pm 2$  standard deviation prediction interval of the *unconstrained* long-term corrosion potential model. That is, the  $\pm 2$  standard deviation prediction interval of the *unconstrained* long-term corrosion potential relationship (Equation 2-6 adjusted by Equation 2-8) are used as bounds on the value that the long-term corrosion potential may have. Thus, if the calculated *unconstrained* long-term corrosion potential exceeds the +2 standard deviation prediction bound of the *unconstrained* long-term corrosion potential model, the long-term corrosion potential value of the +2 standard deviation prediction bound of the *unconstrained* long-term corrosion potential model should be used as the value of the long-term corrosion potential for the given exposure conditions. Similarly, if the calculated *unconstrained* long-term corrosion potential does not exceed the -2 standard deviation prediction bound of the *unconstrained* long-term corrosion

potential model, the long-term corrosion potential value of the -2 standard deviation prediction bound of the *unconstrained* long-term corrosion potential should be used as the value of the long-term corrosion potential for the given exposure conditions.

The empirical correlations used in the WPOB crevice corrosion initiation model for the long-term corrosion potential ( $E_{corr}$ ) and crevice repassivation potential ( $E_{rcrev}$ ) are expressed as functions of temperature,  $pH$  (for  $E_{corr}$  only), chloride ion concentration, and nitrate ion concentration. Based on the range of environmental conditions in which the input data were obtained and on the model validation activities, the application of the WPOB crevice corrosion initiation model can be summarized as follows.

To implement the WPOB crevice corrosion initiation model, the following criteria are applied:

Initiation of crevice corrosion may be possible when seepage water contacts the waste package outer barrier surface. If the exposure temperature is greater than or equal to 20°C, and less than or equal to 120°C, then the empirical correlations for the long-term corrosion potential ( $E_{corr}$ ) and crevice repassivation potential ( $E_{rcrev}$ ) are evaluated in accordance with the following implementation rules. If crevice corrosion is determined to initiate, then crevice corrosion continues to occur regardless of changes in the bulk chemical exposure environment. This is a conservative modeling assumption and is used because the model does not account for the possibility of crevice corrosion repassivation or stifling.

- a) If the nitrate-to-chloride ion ratio in the environment exceeds 1, then evaluate  $E_{rcrev}$  and  $E_{corr}$  at a nitrate-to-chloride ion ratio of 1. If the molality of chloride ion is less than 0.0005 molal, the nitrate-to-chloride ion ratio should be evaluated with a chloride ion concentration of 0.0005 molal.
- b) If the molality of chloride ion in the environment exceeds 20 molal, then evaluate  $E_{rcrev}$  and  $E_{corr}$  at a molality of chloride ion of 20 molal. If the molality of chloride ion is less than 0.0005 molal, then evaluate  $E_{rcrev}$  and  $E_{corr}$  at a molality of chloride ion of 0.0005 molal.
- c) If the  $pH$  in the environment exceeds 10, then evaluate  $E_{corr}$  at a  $pH$  of 10. If the  $pH$  in the environment is less than 1.9, then initiate crevice corrosion.

The origin of these bounds and the rationale for them are discussed further in *General and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 6.4.4.6). Plots showing comparisons between  $E_{rcrev}$  and  $E_{corr}$  versus  $pH$ , temperature, and chloride and nitrate concentrations are provided in DTN: MO0703PAGENCOR.001 [DIRS 180663].

Nitrate ions inhibit crevice corrosion initiation. In addition, carbonate and sulfate ions may have an inhibitive effect on crevice corrosion. Therefore, because only nitrate ions are accounted for in the model, the results for solutions with significant amounts of other potentially inhibitive ions in addition to nitrate ions are conservative. The model results for the beneficial effects of the inhibitive ions combined with alkaline  $pH$  conditions of the typical carbonate-containing waters

in the repository are consistent with the experimental observations on the immunity of Alloy 22 to crevice corrosion in those waters.

The entire variance of the crevice corrosion initiation model (i.e., crevice repassivation potential model and long-term corrosion potential model) is due to uncertainty. Variability in the crevice repassivation potential and long-term corrosion potential among the waste packages to be modeled is represented with the temporally and spatially varying waste package temperature and water chemistry contacting the waste packages. In the absence of specific information regarding local environments on the waste package, the area affected by crevice corrosion due to seepage water can be, as a maximum, the percentage of the waste package surface that is exposed to seepage. The minimum fraction of the waste package surface area affected by crevice corrosion was estimated in SNL 2007 [DIRS 178519], Section 6.4.4.9, to be 0.05%. This value (i.e., 0.05%) represents a conservative estimate of the waste package-pallet contact area. The variation in distribution of the maximum and minimum waste package area affected by crevice corrosion due to seepage water is attributed to uncertainty. These results are summarized in Table 2-3.

Table 2-3. Summary of Localized Corrosion Model Output for WPOB

Output Name	Output Description	Output Uncertainty		
		Source of Uncertainty	Uncertainty Distribution	Characteristic Values
Coefficients of crevice repassivation potential model, Equation 2-3	Mean $a_0 = 190.242$ Mean $a_1 = -3.008$ Mean $a_2 = -46.800$ Mean $a_3 = 535.625$ Mean $a_4 = 0.061$ Covariance matrix given in Equation 2-4 (SNL 2007 [DIRS 178519], Section 8) Uncertainty	Measurement	Entire distribution	N/A
Error term of crevice repassivation potential model Equation 2-3	Normal distribution with a mean of zero mV versus SSC and a standard deviation of 45.055 mV versus SSC	Model uncertainty	Entire distribution	N/A
Coefficients of long-term corrosion potential model, Equation 2-5	Mean $c_0 = 1051.219$ Mean $c_1 = -3.024$ Mean $c_2 = -155.976$ Mean $c_3 = -1352.040$ Mean $c_4 = 10.875$ Mean $c_5 = 137.856$ Mean $c_6 = -8.498$ Covariance matrix given in Equation 2-6 (SNL 2007 [DIRS 178519], Section 8)	Measurement	Entire distribution	N/A
Error term of long-term corrosion potential model Equation 2-5	Normal distribution with a mean of zero mV versus SSC and a standard deviation of 85.265 mV versus SSC	Model uncertainty	Entire distribution	N/A

Table 2-3. Summary of Localized Corrosion Model Output for WPOB (Continued)

Output Name	Output Description	Output Uncertainty		
		Source of Uncertainty	Uncertainty Distribution	Characteristic Values
Percentage of surface area affected by crevice corrosion	Uniform distribution: if maximum and minimum are of the same order of magnitude.  Log-uniform distribution: if maximum is greater than minimum by one order of magnitude or more.	Lack of knowledge	Entire distribution	Minimum: 0.05% of the waste package surface area Maximum: percentage of waste package area wetted by seepage

Source: As listed in Table 1-1.

The crevice corrosion initiation model is used exclusively for evaluating the long-term crevice corrosion susceptibility of the WPOB and is not intended for short-term transient behavior.

*General and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 6.4.5) evaluated the potential effects of MIC on localized corrosion. It was concluded that microbial activity will have no significant impact on localized corrosion of Alloy 22 under repository exposure conditions.

*General and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 6.4.6.1) also evaluated the effects of aging and phase instability on the corrosion behavior of Alloy 22. Although thermal aging was determined not to significantly increase the general corrosion rate of Alloy 22 under repository relevant aqueous conditions, aging could increase the localized corrosion susceptibility of Alloy 22 by increasing the corrosion potential (i.e.,  $E_{corr}$ ) of this material. However, Alloy 22 specimens had to be aged at temperatures well above those possible in the repository in order for these effects to be observed (e.g., 700°C for 173 hours). This is supported by *Aging and Phase Stability of Waste Package Outer Barrier* (BSC 2004 [DIRS 171924], Section 8), in which it was concluded that repository thermal hydrologic exposure conditions would not result in significant phase transformations in Alloy 22 base metal and welded material. Therefore, thermal aging is not expected to impact the localized corrosion behavior of Alloy 22 under repository exposure conditions.

The technical product outputs of the WPOB localized corrosion initiation model are documented in DTN: MO0703PAGENCOR.001 [DIRS 180663] and summarized in Table 2-3. Detailed information is contained in *General and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 8).

## 2.2.2 Localized Corrosion Propagation Model Implementation

The crevice corrosion penetration model (SNL 2007 [DIRS 178519], Section 6.4.4.7) assumes that, when it occurs, crevice corrosion propagates at a (time-independent) constant rate. This is a highly conservative assumption because it is known that the crevice corrosion rate decreases with time (SNL 2007 [DIRS 178519], Section 6.4.4.8).

The literature data for crevice corrosion of relevant alloys that were considered for the current crevice penetration rate model are for extremely corrosive conditions. Those extreme penetration rates found in the literature were used to bound crevice corrosion rates of Alloy 22 under repository conditions.

The technical product outputs of the WPOB localized corrosion propagation model are documented in DTN: MO0703PAGENCOR.001 [DIRS 180663] and summarized in Table 2-4. Detailed information is contained in *General and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 8).

Table 2-4. Summary of Localized Corrosion Propagation Model Output for WPOB

Output Name	Output Description	Output Uncertainty		
		Source of Uncertainty	Uncertainty Distribution	Characteristic Values
Crevice corrosion propagation rate	Log-uniform distribution	Conceptual model, data	Entire distribution	0 percentile = 12.7 $\mu\text{m}/\text{yr}$ 50 <sup>th</sup> percentile = 127 $\mu\text{m}/\text{yr}$ 100 <sup>th</sup> percentile = 1,270 $\mu\text{m}/\text{yr}$

Source: As listed in Table 1-1.

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### 3. PARAMETER VALUE UNCERTAINTY

Parameter value uncertainties relevant to the models included in this total system performance assessment (TSPA) data input package (TDIP) are discussed in Section 2. Section 2 also contains references to the appropriate sections of *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]) where uncertainty of the parameters is discussed.

#### 3.1 STATEMENT AND JUSTIFICATION OF UNCERTAINTY TREATMENT

Uncertainty treatments of the model parameters included in this TDIP are discussed in Section 2. Section 2 also contains references to the appropriate sections of *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]) where uncertainty of the parameters is discussed.

As mentioned in Section 2.1, the general corrosion model consists of two main parameters, the temperature-dependence term (i.e.,  $C_1$  parameter) and  $R_o$ . The temperature-dependence term is normally distributed with a mean of 4,905 K and a standard deviation of 1,413 K. This corresponds to an apparent activation energy of  $40.78 \pm 11.75$  kJ/mol.  $R_o$  is a Weibull distribution (with parameters given in Table 2-1) that was fit to the general corrosion rate distribution derived from weight-loss data of the five-year exposed crevice specimens. Microbially influenced corrosion (MIC) effects are applied when the relative humidity at the waste package surface is greater than a threshold relative humidity sampled from a uniform distribution between 75% and 90%. The variance in the MIC threshold relative humidity distribution is due to uncertainty. The MIC general corrosion enhancement factor is uniformly distributed between 1 and 2. The variance in this factor is due to spatial variability.

The crevice corrosion initiation model consists of submodels: the crevice repassivation potential submodel and the long-term corrosion potential submodel (see Section 2.2). The values of the regression coefficients of the crevice repassivation potential submodel and their uncertainties ( $\pm 1$  standard deviation) are determined to be:  $a_0 = 190.242 \pm 18.373$ ,  $a_1 = -3.008 \pm 0.225$ ,  $a_2 = -46.800 \pm 3.126$ ,  $a_3 = 535.625 \pm 26.140$ , and  $a_4 = 0.061 \pm 0.010$ . The variance of the submodel coefficients is calculated via a covariance matrix (Equation 2-4), and the entire variance is attributed to uncertainty (Table 1-1). The error term,  $\epsilon_{rcrev}$ , is a term representing data variance not explained by the fitting procedure and has a normal distribution with a mean of zero mV versus SSC and a standard deviation of 45.055 mV versus SSC. Variance in the error term,  $\epsilon_{rcrev}$ , is attributed to uncertainty. The estimated regression coefficients of the long-term corrosion model and their uncertainties ( $\pm 1$  standard deviation) are:  $c_0 = 1,051.219 \pm 119.774$ ,  $c_1 = -3.024 \pm 0.977$ ,  $c_2 = -155.976 \pm 11.495$ ,  $c_3 = -1,352.040 \pm 252.224$ ,  $c_4 = 10.875 \pm 1.890$ ,  $c_5 = 137.856 \pm 23.158$ , and  $c_6 = -8.498 \pm 0.801$ . The variance of the submodel is calculated via a covariance matrix (Equation 2-6), and the entire variance is attributed to uncertainty (Table 1-1). The error term,  $\epsilon_{corr}$ , is a term representing data variance not explained by the fitting procedure and has a normal distribution with a mean of zero mV versus SSC and a standard deviation of 85.265 mV versus SSC. Variance in the error term,  $\epsilon_{corr}$ , is attributed to uncertainty.

The crevice corrosion propagation rate is a log-uniform distribution with a 0 percentile value of 12.7  $\mu\text{m}/\text{yr}$ , a 50<sup>th</sup> percentile value of 127  $\mu\text{m}/\text{yr}$ , and a 100<sup>th</sup> percentile value of 1,270  $\mu\text{m}/\text{yr}$  (Table 1-1). Variation in this parameter values is attributed to uncertainty.

The minimum value of percentage of surface area affected by crevice corrosion is estimated to be 0.05% of the total waste package surface area. The maximum value is the waste package surface area contacted by seepage. Depending on the estimated maximum value, the distribution of the waste package area affected by crevice corrosion will be uniform or log-uniform.

### 3.2 QUANTIFICATION OF UNCERTAINTY

Table 1-1 contains tabulated information on the WPOB degradation process model parameters and their uncertainties. In addition, DTN: MO0703PAGENCOR.001 [DIRS 180663] and Section 8 of *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]) are controlled sources of tabulated information on the WPOB degradation process model parameters and the parameter uncertainties.

The long-term corrosion potential,  $E_{corr}$ , model is unchanged relative to the previous version of this TDIP. The crevice repassivation potential,  $E_{rcrev}$ , model differs from that in the previous version of this TDIP. Therefore, further discussion of the development of the crevice repassivation potential model is presented in this section.

#### 3.2.1 Analysis of Crevice Repassivation Potential Data

Table 3-1 summarizes the sources for the crevice repassivation potential data used to develop the new crevice repassivation potential model. Attachment I contains a detailed listing of the crevice repassivation potential data used to develop the new crevice repassivation potential model.

Table 3-1. Summary of All Input Data for Modeling the Crevice Repassivation Potential for the WPOB

Data Name	Data Source	DTN
Crevice Repassivation Potentials for Alloy 22	Waste Package Materials Testing	LL040902712251.119 [DIRS 173720] file: <i>Reduced Data Ahmet Yilmaz WBL 11Feb05.xls</i>
		LL050302312251.129 [DIRS 173921] file: <i>Mockup Developed RBR 21May05.xls</i>
		LL060603812251.164 [DIRS 178269] file: <i>Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls</i>
		LL060700312251.166 [DIRS 179385] file: <i>Rep Pot N06022 vs Temp 5M CaCl2 RBR 19Dec06.xls</i>
		LL060801812251.168 [DIRS 179386] file: <i>Rep Pot N06022 High Temp High NO3 RBR.xls</i>
		LL060803712251.170 [DIRS 179387] file: <i>Rep Pot N06022 vs Temp NaCl RBR 07Oct06.xls</i>

NOTE: See Attachment I for a detailed list of these data.

Each DTN listed in Table 3-1 contains listings of measured crevice repassivation potentials as well as posttest observations of the occurrence or absence of crevice corrosion or pitting corrosion. Only crevice repassivation potential data measured at exposure temperatures of 120°C or less and for which crevice corrosion or pitting corrosion was observed were used to develop the crevice repassivation potential model. Crevice repassivation potential data from specimens which had undergone high temperature aging treatments (e.g., 700°C for 173 hours) do not represent a repository relevant material condition and were not used for model development (SNL 2007 [DIRS 178519], Section 6.4.4). The crevice repassivation potentials for two specimens, DEA3130 (from DTN: LL060803712251.170 [DIRS 179387], file: *Rep Pot N06022 vs Temp NaCl RBR 07Oct06.xls*) and KE0416 (from DTN: LL060603812251.164 [DIRS 178269], file: *Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls*) will be used for model validation.

A number of measured crevice repassivation potentials were very high (greater than 550 mV versus SSC) and were not used in model development. These data are summarized in Table 3-2. Cyclic polarization curves for these samples typically showed very little hysteresis or negative hysteresis followed by a cross-over (crevice repassivation potential) at a very high value (e.g., Figure 3-1). Not using these high crevice repassivation potential values is conservative in that the mean crevice repassivation potential predicted by a model developed using these data would be higher than the mean crevice repassivation potential predicted by a model developed without the use of these data. However, use of these high crevice repassivation potential values would result in a larger variance in predicted values, i.e., the possibility of prediction of lower repassivation potentials at the extremes of the uncertainty band. Nonetheless, the crevice repassivation potential measurements that are considered for exclusion from model development are not representative of the crevice repassivation potential for Alloy 22 in the environments considered and, therefore, should not be used for model development.

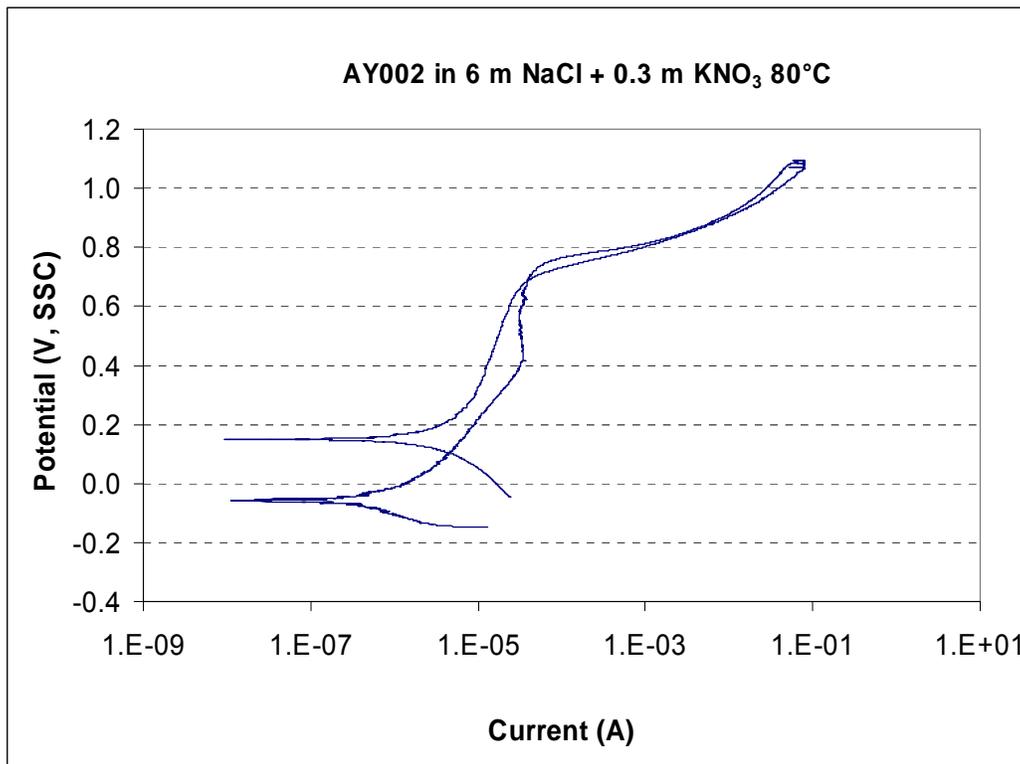
Table 3-2. Summary of Crevice Repassivation Potential Data Not Used for Modeling – Very High Values

DTN	Specimen ID	Specimen Type	Material Condition	Electrolyte	Type of Localized Corrosion	Temp. °C	E <sub>crev</sub> mV versus SSC
LL050302312251.129 [DIRS 173921] file: <i>Mockup Developed RBR 21May05.xls</i>	AY001	PCA	ASW – Mockup	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC	80	714
LL050302312251.129 [DIRS 173921] file: <i>Mockup Developed RBR 21May05.xls</i>	AY002	PCA	ASW – Mockup	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC	80	682
LL060803712251.170 [DIRS 179387] file: <i>Rep Pot N06022 vs Temp NaCl RBR 07Oct06.xls</i>	KE0622	PCA	ASW	0.0005 M NaCl	CC	60	867
LL060801812251.168 [DIRS 179386] file: <i>Rep Pot N06022 High Temp High NO3 RBR.xls</i>	KE0592	PCA	ASW	4 m KCl + 4 m NaCl + 0.4 m KNO <sub>3</sub> + 0.4 m NaNO <sub>3</sub>	CC	90	570

Table 3-2. Summary of Crevice Repassivation Potential Data Not Used for Modeling – Very High Values (Continued)

DTN	Specimen ID	Specimen Type	Material Condition	Electrolyte	Type of Localized Corrosion	Temp. °C	E <sub>crev</sub> mV versus SSC
LL060700312251.166 [DIRS 179385] file: <i>Rep Pot N06022 vs Temp 5M CaCl2 RBR 19Dec06.xls</i>	DEA3230	MCA	MA	5 M CaCl <sub>2</sub>	CC-II	45	568
LL060700312251.166 [DIRS 179385] file: <i>Rep Pot N06022 vs Temp 5M CaCl2 RBR 19Dec06.xls</i>	JE0115	MCA	ASW	5 M CaCl <sub>2</sub>	CC-II	45	570

NOTES: PCA = prism crevice assembly, MCA = multiple crevice assembly, ASW = as-welded, MA = mill-annealed, CC = crevice corrosion.



Source: DTN: LL050302312251.129 [DIRS 173921], file: *CPP AY002.xls*.

Figure 3-1. Cyclic Polarization Curve for Specimen AY002 Obtained in 6 m NaCl + 0.3 m KNO<sub>3</sub> at 80°C

In reference to the crevice repassivation potentials for specimens AY001 and AY002 (714 and 682 mV versus SSC, respectively), crevice repassivation potentials for specimens JE3313, JE3314, JE3217, and JE3228 in the same 6 m NaCl + 0.3 m KNO<sub>3</sub> solution at 80°C average about -103 mV versus SSC with a standard deviation of about 9 mV. Clearly the repassivation potentials for specimens AY001 and AY002 are significantly higher than similar measurements in the same exposure conditions. It should be noted that although specimens AY001 and AY002

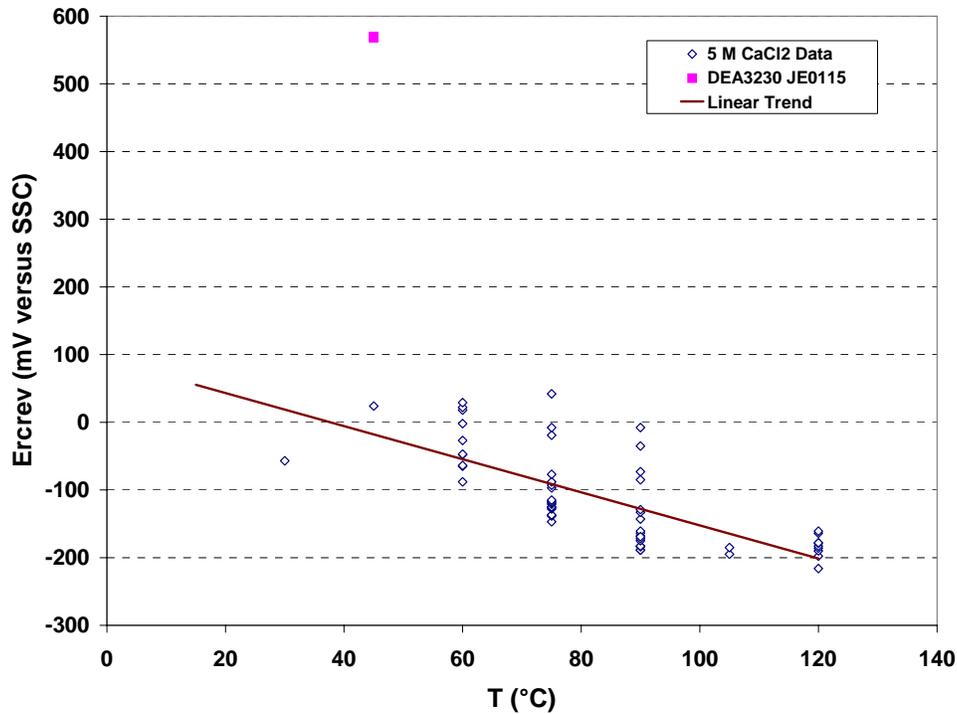
are from a waste package mockup study, it is not expected that this is the source of their high crevice repassivation potentials, as other specimens from the mockup study do not show this behavior (i.e., specimens AY005, AY006, AY007, AY008, AY009, AY010 in Attachment I). On these bases, the crevice repassivation potential of specimens AY001 and AY002 are not used for development of the crevice repassivation potential model.

In reference to specimen KE0622 exposed to 0.0005 M NaCl at 60°C with a crevice repassivation potential of 867 mV versus SSC, a second specimen KE0614 was also exposed to identical conditions and had a much lower crevice repassivation potential of 339 mV versus SSC. Furthermore, in DTN: LL060803712251.170 [DIRS 179387], file: *Rep Pot N06022 vs Temp NaCl RBR 07Oct06.xls*, a crevice repassivation potential of 312 mV versus SSC for specimen KE0601 was obtained in 0.0005 M NaCl at 60°C using a modified Tsujikawa-Hisamatsu electrochemical (THE) technique (see below). As discussed below, the THE method is believed to provide a more accurate measurement of the crevice repassivation potential than cyclic polarization. The very high crevice repassivation potential reported for specimen KE0622 may be due to transpassive dissolution or oxygen evolution and not repassivation. If this is true, the crevice repassivation potential reported for KE0622 may not be relevant to a repassivation process, and it would be inappropriate to include this value in the crevice repassivation potential model. Any crevice corrosion observed for this sample is likely due to an initiation phenomena that occurred under exposure conditions not relevant to the repository (e.g., a high potential was applied during the potentiodynamic experiment). On these bases, the crevice repassivation potential of specimen KE0622 is not used for development of the crevice repassivation potential model.

The THE method (DTN: LL040806212251.118 [DIRS 173722], file: LL040806212251.118 ReadMe.pdf) consists of ramping the potential at a scan rate of 0.167 mV/s until a peak current density is reached, typically on the order of 2  $\mu\text{A}/\text{cm}^2$ . Once this peak current value is achieved, it is maintained for a set period, usually two hours, to allow crevice corrosion to propagate in a controlled manner. After the designated galvanostatic period elapses, the potential is stepped downward (cathodically) in 10 mV increments. Each potential is held for two hours before transitioning to the next potentiostatic step. The most anodic potential at which no increase in current is observed is deemed the crevice repassivation potential. Since this is basically a potentiostatic method, the crevice repassivation potential obtained using this method is expected to be free from the influence of scan rates. Therefore, the crevice repassivation potential obtained using this technique should more accurately represent the crevice repassivation potential than does the crevice repassivation potential obtained using cyclic polarization technique. However, the repassivation potential data obtained using this technique was not used for model development because of the limited amount of data available.

In reference to specimen KE0592, a crevice repassivation potential of 570 mV versus SSC was measured in 4 m KCl + 4 m NaCl + 0.4 m KNO<sub>3</sub> + 0.4 m NaNO<sub>3</sub> at 90°C. Two other specimens, KE0688B and KE0579, were also exposed to the same solution and temperature. Crevice repassivation potential values of -82 mV and -80 mV versus SSC were obtained for KE0688B and KE0579, respectively. Clearly, the crevice repassivation potential value for specimen KE0592 is much higher than those of the specimens KE0688B and KE0579. On this basis, the crevice repassivation potential of specimen KE0592 is excluded from the data set used for developing the crevice repassivation potential model.

In reference to specimens DEA3230 and JE0115, crevice repassivation potential values of 568 mV and 570 mV versus SSC, respectively, were measured in 5 M CaCl<sub>2</sub> at 45°C. These values are much higher than the crevice repassivation potential of 24 mV versus SSC measured under the same exposure conditions for the specimen JE0114. In addition, the high crevice repassivation potential values for specimens DEA3230 and JE0115 are not consistent with the trend with temperature observed for the crevice repassivation potentials measured in 5 M CaCl<sub>2</sub> (Figure 3-2). On this basis, the crevice repassivation potentials of specimens DEA3230 and JE0115 are not used for development of the crevice repassivation potential model.



Source: DTN: LL060700312251.166 [DIRS 179385], file: *Rep Pot N06022 vs Temp 5M CaCl2 RBR 19Dec06.xls*.

Figure 3-2. Crevice Repassivation Potentials Measured in 5 M CaCl<sub>2</sub> at Various Temperatures

In addition to the data listed in Table 3-2, five other measured crevice repassivation potential values were considered outliers and, therefore, not used for developing the crevice repassivation potential model. These data are listed in Table 3-3.

Table 3-3. Summary of Crevice Repassivation Potential Data Not Used for Modeling – Outliers

DTN	Specimen ID	Specimen Type	Material Condition	Electrolyte	Type of Localized Corrosion	Temp. °C	E <sub>crev</sub> mV versus SSC
LL060803712251.170 [DIRS 179387] file: <i>Rep Pot N06022 vs Temp NaCl RBR 07Oct06.xls</i>	DEA3147	MCA	MA	1.25 M NaCl	LC	60	182
LL060803712251.170 [DIRS 179387] file: <i>Rep Pot N06022 vs Temp NaCl RBR 07Oct06.xls</i>	DEA3310	MCA	MA	4 M NaCl	CC	45	91
LL060603812251.164 [DIRS 178269] file: <i>Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls</i>	JE3213	MCA	ASW	1 m NaCl + 0.15 m KNO <sub>3</sub>	CC-II	80	290
LL060603812251.164 [DIRS 178269] file: <i>Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls</i>	DEA3386	MCA	MA	3.5 m NaCl + 0.525 m KNO <sub>3</sub>	CC	100	110
LL060603812251.164 [DIRS 178269] file: <i>Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls</i>	JE3211	MCA	ASW	3.5 m NaCl + 0.525 m KNO <sub>3</sub>	CC	60	268

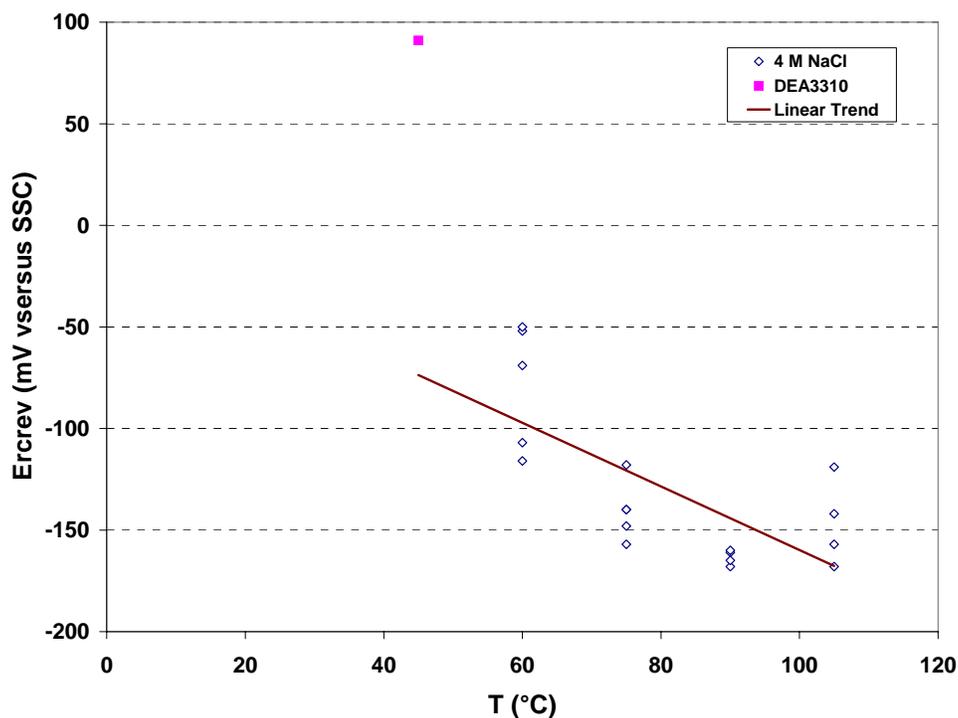
NOTES: MCA = multiple crevice assembly, MA = mill-annealed, ASW = as-welded, LC = localized corrosion, CC = crevice corrosion.

In reference to the specimen DEA3147, exposed to 1.25 M NaCl at 60°C, a crevice repassivation potential value of 182 mV versus SSC was observed. Two other specimens, DEA3267 and DEA3268, were also exposed to identical conditions and had much lower crevice repassivation potentials of 48 and 23 mV versus SSC, respectively. The observed crevice repassivation potential for specimen DEA3147 is about 150 mV higher than those for the specimens DEA3267 and DEA3268. The observed crevice repassivation potential for specimen DEA3147 is an anomalous experimental observation that is not representative of the crevice repassivation potential of Alloy 22 under these exposure conditions. Therefore, the crevice repassivation potential of specimen DEA3147 was not used for development of the crevice repassivation potential model.

In reference to the specimen DEA3310, exposed to 4 M NaCl at 45°C, the observed crevice repassivation potential value is not consistent with the trend with temperature observed for crevice repassivation potentials of other specimens measured in 4 M NaCl (Figure 3-3). The measured crevice repassivation potential of DEA3310 is about 150 mV greater than that expected from the trend. The observed crevice repassivation potential for specimen DEA3310 is

an anomalous experimental observation that is not representative of the crevice repassivation potential of Alloy 22 under these exposure conditions. Therefore, the crevice repassivation potential of specimen DEA3310 is not used for development of the crevice repassivation potential model.

It may be that the higher crevice repassivation potential obtained for specimen DEA3310 is related to the existence of a critical temperature for crevice corrosion initiation in 4 M NaCl solution. If this were the case, it would be expected that decreasing the temperature would result in a large increase in measured crevice repassivation potential. The model conservatively predicts behavior at the lower temperatures by extrapolating behavior from the higher temperatures.



Source: DTN: LL060803712251.170 [DIRS 179387], file: *Rep Pot N06022 vs Temp NaCl RBR 07Oct06.xls*.

Figure 3-3. Crevice Repassivation Potentials Measured in 4 M NaCl at Various Temperatures

In reference to the specimen JE3213, exposed to 1 m NaCl + 0.15 m KNO<sub>3</sub> at 80°C, a crevice repassivation potential of 290 mV versus SSC was observed using cyclic potentiodynamic polarization (CPP). The specimen KE0627, also exposed to an identical exposure condition, had a much lower crevice repassivation potential of 68 mV versus SSC based on CPP measurement (Attachment I). Based on CPP data, the repassivation potential value of specimen JE3213 is 222 mV higher than that of specimen KE0627. Another specimen KE0624 was exposed in 1 m NaCl + 0.15 m KNO<sub>3</sub> at 80°C, and its crevice repassivation potential was determined to be 19 mV versus SSC using the modified THE technique (DTN: LL060603812251.164 [DIRS 178269] (file: *Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls*). As mentioned above, the THE method is expected to provide a more accurate measurement of the crevice repassivation potential than does CPP technique. A comparison of this value with two other

values obtained under identical exposure condition using the CPP technique suggests that the crevice repassivation potential value of 290 mV for the specimen JE3213 is not representative of the crevice repassivation potential of Alloy 22 under these exposure conditions. Therefore, the crevice repassivation potential value of the specimen JE3213 was excluded from the dataset used for development of the crevice repassivation potential model.

In reference to specimen DEA3386 exposed to 3.5 m NaCl + 0.525 m KNO<sub>3</sub> at 100°C, a crevice repassivation potential of 110 mV versus SSC was obtained. Four additional specimens (JE1773, DEA3385, DEA3390, and JE3242) were also exposed to an identical set of exposure conditions and a negative repassivation potential value was observed for each specimen, as shown in Table 3-4. The average repassivation potential value for these four specimens is about -68 mV versus SSC with a standard deviation of about 44 mV. Clearly, the crevice repassivation potential of 110 mV versus SSC is significantly greater than would be expected based on the measured crevice repassivation potentials of these four samples. Furthermore, as seen in DTN: LL060603812251.164 [DIRS 178269], file: *Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls*, a crevice repassivation potential of -55 mV versus SSC for specimen KE0181, which was obtained in 3.5 m NaCl + 0.525 m KNO<sub>3</sub> at 100°C using the modified THE technique, is expected to provide a more accurate measurement of the crevice repassivation potential than cyclic polarization. On this basis, the observed crevice repassivation potential value of 110 mV for specimen DEA3386 is not representative of the crevice repassivation potential of Alloy 22 under these exposure conditions. Therefore, the crevice repassivation potential of specimen DEA3386 was not used for development of the crevice repassivation potential model.

Table 3-4. Summary of Crevice Repassivation Potential Data Used for Modeling in 3.5 m NaCl + 0.525 m KNO<sub>3</sub> at 100°C

DTN	Specimen ID	Specimen Type	Material Condition	Electrolyte	Type of Localized Corrosion	Temp. °C	E <sub>crev</sub> mV versus SSC
LL060603812251.164 [DIRS 178269], file: <i>Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls</i>	JE1773	MCA	ASW	3.5 m NaCl + 0.525 m KNO <sub>3</sub>	CC	100	-85
LL060603812251.164 [DIRS 178269], file: <i>Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls</i>	DEA3385	MCA	MA	3.5 m NaCl + 0.525 m KNO <sub>3</sub>	CC	100	-88
LL060603812251.164 [DIRS 178269], file: <i>Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls</i>	DEA3390	MCA	MA	3.5 m NaCl + 0.525 m KNO <sub>3</sub>	CC	100	-3

Table 3-4. Summary of Crevice Repassivation Potential Data Used for Modeling in 3.5 m NaCl + 0.525 m KNO<sub>3</sub> at 100°C (Continued)

DTN	Specimen ID	Specimen Type	Material Condition	Electrolyte	Type of Localized Corrosion	Temp. °C	E <sub>crev</sub> mV versus SSC
LL060603812251.164 [DIRS 178269], file: <i>Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls</i>	JE3242	MCA	ASW	3.5 m NaCl + 0.525 m KNO <sub>3</sub>	CC-II	100	-96

NOTES: MCA = multiple crevice assembly, ASW = as-welded, MA = mill-annealed, CC = crevice corrosion.

In reference to specimen JE3211, exposed to 3.5 m NaCl + 0.525 m KNO<sub>3</sub> at 60°C, a crevice repassivation potential of 268 mV versus SSC was obtained. It is seen from Table 3-4 that the minimum crevice repassivation potential measured in 3.5 m NaCl + 0.525 m KNO<sub>3</sub> at 100°C by cyclic polarization is -96 mV versus SSC. For specimen KE0629, exposed in 3.5 m NaCl + 0.525 m KNO<sub>3</sub> at 80°C, a crevice repassivation potential value of 3 mV versus SSC was obtained using the modified THE technique (DTN: LL060603812251.164 [DIRS 178269], file: *Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls*). This indicates that a reasonable value of the crevice repassivation potential for a specimen, such as JE3211, exposed to 3.5 m NaCl + 0.525 m KNO<sub>3</sub> at 60°C would be about 100 mV versus SSC, i.e., an increase of about 100 mV for every 20°C decrease temperature. However, specimen JE3211 had a crevice repassivation potential of 268 mV versus SSC, which is much higher than expected. On this basis, the measured crevice repassivation potential value of 268 mV for specimen JE3211 was considered not representative of the crevice repassivation potential of Alloy 22 under these exposure conditions and, therefore, was not used for developing the crevice repassivation potential model.

### 3.2.2 Development of the Crevice Repassivation Potential Model

Crevice corrosion of the WPOB initiates when the long-term corrosion potential ( $E_{corr}$ ) is equal to or greater than a critical potential ( $E_{critical}$ ), that is,  $\Delta E (= E_{critical} - E_{corr}) \leq 0$ . The crevice corrosion initiation model uses the crevice repassivation potential ( $E_{crev}$ ) as the critical potential. The **crevice repassivation potential model** ( $E_{crev}$ ) is expressed as follows:

$$E_{crev} = a_o + a_1 T + a_2 \ln[Cl^-] + a_3 \frac{[NO_3^-]}{[Cl^-]} + a_4 T \cdot [Cl^-] + \varepsilon_{crev} \quad (\text{Eq. 3-1})$$

where  $a_o$ ,  $a_1$ ,  $a_2$ ,  $a_3$ , and  $a_4$  are coefficients of the model parameters,  $T$  is the temperature (°C),  $[Cl^-]$  is the molal ( $m$ , moles/kg water) chloride ion concentration,  $[NO_3^-]$  is the molal nitrate ion concentration, and  $\varepsilon_{crev}$  is the error term.

The crevice repassivation potential data in Attachment I were fit to the functional form in Equation 3-1. The mean values of the coefficients of the model parameters from the fitting were determined to be:  $a_o = 183.686 \pm 21.587$ ,  $a_1 = -2.919 \pm 0.265$ ,  $a_2 = -46.109 \pm 3.675$ ,

$a_3 = 580.849 \pm 29.974$ , and  $a_4 = 0.057 \pm 0.012$ . The variance of the model coefficients is calculated via a covariance matrix:

$$\Sigma = \begin{pmatrix} 4.660E+002 & -5.394E+000 & -1.278E+001 & 1.207E+002 & 4.865E-002 \\ -5.394E+000 & 7.005E-002 & 1.268E-001 & -1.756E+000 & -1.141E-003 \\ -1.278E+001 & 1.268E-001 & 1.350E+001 & 1.955E+000 & -2.827E-002 \\ 1.207E+002 & -1.756E+000 & 1.955E+000 & 8.984E+002 & -3.456E-002 \\ 4.865E-002 & -1.141E-003 & -2.827E-002 & -3.456E-002 & 1.395E-004 \end{pmatrix} \quad (\text{Eq. 3-2})$$

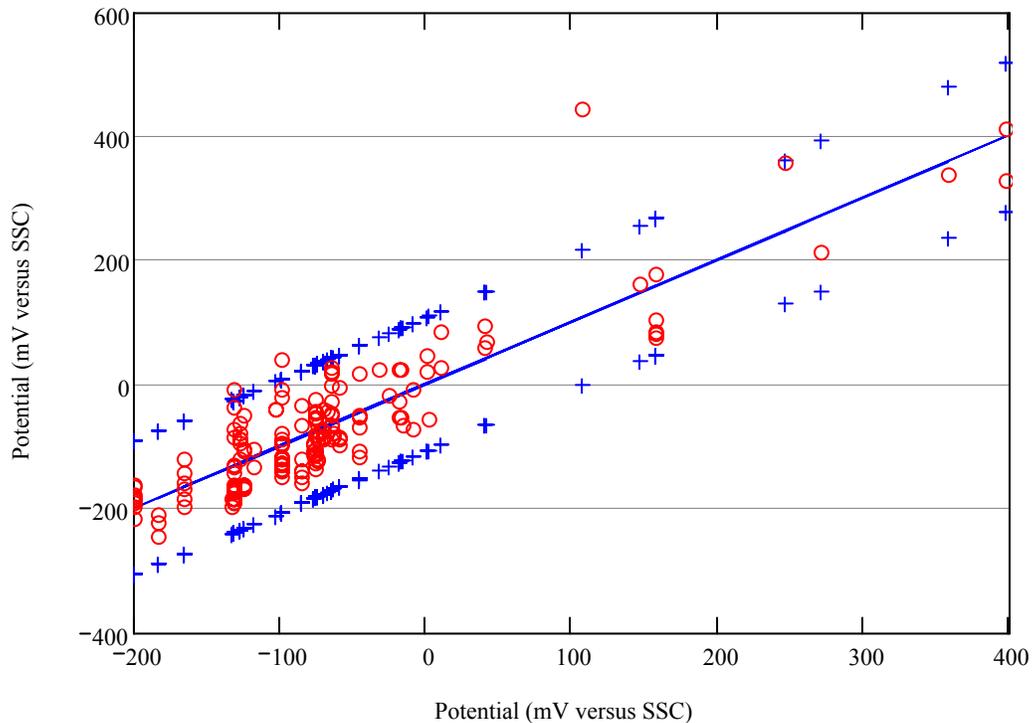
The error term,  $\varepsilon_{rrev}$ , is represents data variance not explained by the fitting procedure and has a normal distribution with a mean of zero mV versus SSC and a standard deviation of 52.993 mV versus SSC.

Figure 3-4 shows model predictions versus experimental data for the crevice repassivation potential of the waste package outer barrier. The horizontal axis is the crevice repassivation potential predicted by the model while the vertical axis is either the measured repassivation potential for the measured data points represented by circles, or the  $\pm 2$  standard deviation prediction intervals represented by plus signs, or the mean model prediction represented by the solid line. As can be seen from the figure, one measured crevice repassivation potential lies substantially above the +2 standard deviation prediction interval, i.e., the crevice repassivation potential model predicts a substantially less positive crevice repassivation potential for this specimen. The specimen is KE0572, from DTN: LL060801812251.168 [DIRS 179386], file: *Rep Pot N06022 High Temp High NO3 RBR.xls*, with a measured crevice repassivation potential of 446 mV versus SSC obtained in a 4 m KCl + 4 m NaCl + 2 m KNO<sub>3</sub> + 2 m NaNO<sub>3</sub> solution with 0.0001 m HCl added. The mean predicted crevice repassivation potential value from the crevice repassivation potential model is 108 mV versus SSC, and the +2 standard deviation prediction interval for this composition is 217 mV versus SSC. The crevice repassivation potential for specimen KE0572 is clearly an outlier and was removed from the data set used to model the crevice repassivation potential. Two other data points lie just outside of the +2 standard deviation prediction bound and are conservatively under-predicted (i.e., predicted crevice repassivation values are lower than these measured values).

The remaining crevice repassivation potential data were refit to the functional form in Equation 3-1. The mean values of the coefficients of the model parameters from the fitting were determined to be:  $a_0 = 190.242 \pm 18.373$ ,  $a_1 = -3.008 \pm 0.225$ ,  $a_2 = -46.800 \pm 3.126$ ,  $a_3 = 535.625 \pm 26.140$ , and  $a_4 = 0.061 \pm 0.010$ . The variance of the model coefficients is calculated via a covariance matrix (Equation 3-3), and the entire variance is due to uncertainty. Equation 3-3 is the covariance matrix mentioned in Table 1-1. The model coefficients are sampled from a multivariate normal distribution with the above-mentioned mean values consistent with the covariance matrix given in Equation 3-3.

$$r\Sigma = \begin{pmatrix} 3.376E+002 & -3.909E+000 & -9.310E+000 & 8.236E+001 & 3.559E-002 \\ -3.909E+000 & 5.077E-002 & 9.271E-002 & -1.202E+000 & -8.308E-004 \\ -9.310E+000 & 9.271E-002 & 9.770E+000 & 1.930E+000 & -2.048E-002 \\ 8.236E+001 & -1.202E+000 & 1.930E+000 & 6.833E+002 & -2.790E-002 \\ 3.559E-002 & -8.308E-004 & -2.048E-002 & -2.790E-002 & 1.011E-004 \end{pmatrix} \quad (\text{Eq. 3-3})$$

The error term,  $\varepsilon_{rcrev}$ , represents data variance not explained by the fitting procedure and has a normal distribution with a mean of zero mV versus SSC and a standard deviation of 45.055 mV SSC. Variance in the error term,  $\varepsilon_{rcrev}$ , is attributed to uncertainty (DTN: MO0703PAGENCOR.001 [DIRS 180663], file: *LC\_Initiation.pdf*).

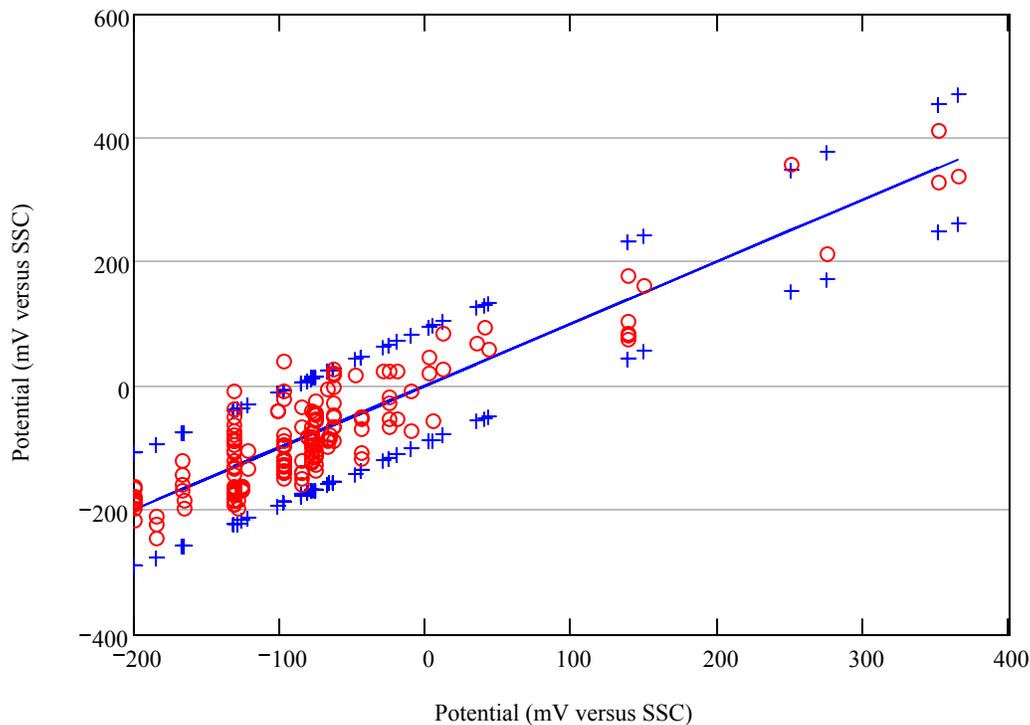


Sources: DTN: LL040902712251.119 [DIRS 173720], file: *Reduced Data Ahmet Yilmaz WBL 11Feb05.xls*  
 DTN: LL050302312251.129 [DIRS 173921], file: *Mockup Developed RBR 21May05.xls*  
 DTN: LL060603812251.164 [DIRS 178269], file: *Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls*  
 DTN: LL060700312251.166 [DIRS 179385], file: *Rep Pot N06022 vs Temp 5M CaCl2 RBR 19Dec06.xls*  
 DTN: LL060801812251.168 [DIRS 179386], file: *Rep Pot N06022 High Temp High NO3 RBR.xls*  
 DTN: LL060803712251.170 [DIRS 179387], file: *Rep Pot N06022 vs Temp NaCl RBR 07Oct06.xls*.

NOTE: Model predictions are displayed with  $\pm 2$  standard deviation prediction interval represented by blue plus signs.

Figure 3-4. Model Predictions and Experimental Data for the Crevice Repassivation Potential of the WPOB

Figure 3-5 shows model predictions versus experimental data for the crevice repassivation potential of the WPOB. The horizontal axis is the crevice repassivation potential predicted by the model while the vertical axis is either the measured repassivation potential for the measured data points represented by circles, or the  $\pm 2$  standard deviation prediction intervals represented by plus signs, or the mean model prediction represented by the solid line. As can be seen from the figure, all measured crevice repassivation potential data used to develop the crevice repassivation potential model lie within the  $\pm 2$  standard deviation prediction interval of the crevice repassivation potential model or are conservatively under-predicted by the crevice repassivation potential model.



Sources: DTN: LL040902712251.119 [DIRS 173720], file: *Reduced Data Ahmet Yilmaz WBL 11Feb05.xls*  
DTN: LL050302312251.129 [DIRS 173921], file: *Mockup Developed RBR 21May05.xls*  
DTN: LL060603812251.164 [DIRS 178269], file: *Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls*  
DTN: LL060700312251.166 [DIRS 179385], file: *Rep Pot N06022 vs Temp 5M CaCl2 RBR 19Dec06.xls*  
DTN: LL060801812251.168 [DIRS 179386], file: *Rep Pot N06022 High Temp High NO3 RBR.xls*  
DTN: LL060803712251.170 [DIRS 179387], file: *Rep Pot N06022 vs Temp NaCl RBR 07Oct06.xls*.

NOTE: Model predictions are displayed with  $\pm 2$  standard deviation prediction interval represented by blue plus signs.

Figure 3-5. Model Predictions and Experimental Data for the Crevice Repassivation Potential of the WPOB

### 3.2.3 Comparison of Crevice Repassivation Potential and Long-Term Corrosion Potential Model Results with Observations from the Long-Term Corrosion Potential Experiments

To build further confidence in the long-term corrosion potential and crevice repassivation potential models, a summary of observations from the long-term corrosion potential experiments was produced (Table 3-5). Table 3-5 contains the solution chemistry, immersion time, cell number, the number of creviced geometry specimens exposed, the number of creviced specimens observed to undergo crevice corrosion (column labeled CC), the number of rod geometry specimens exposed, the number of rod geometry specimens observed to undergo pitting corrosion (column labeled PC), and the mean and lower and upper bounding values of  $\Delta E = E_{rcrev} - E_{corr}$ . The lower bounding value of  $\Delta E$  is obtained by subtracting the upper bounding value of  $E_{corr}$  (the +2 standard deviation prediction bound of the *unconstrained* long-term corrosion potential model) from the lower bounding value of  $E_{rcrev}$  (the -2 standard deviation prediction bound of the *unconstrained* crevice repassivation potential model). The upper bounding value of  $\Delta E$  is obtained by subtracting the lower bounding value of  $E_{corr}$  (the -2 standard deviation prediction bound of the *unconstrained* long-term corrosion potential model) from the upper bounding value of  $E_{rcrev}$  (the +2 standard deviation prediction bound of the *unconstrained* crevice repassivation potential model). If  $\Delta E$  is negative then crevice corrosion initiation is predicted to occur.

Examination of Table 3-5 reveals that the crevice corrosion initiation model is consistent with or conservative relative to the long-term corrosion test results. For example, Cells 32 and 33 contain 5m CaCl<sub>2</sub> + 5m Ca(NO<sub>3</sub>)<sub>2</sub> at 100°C and 120°C, respectively. Each cell contained four creviced geometry specimens and two rod (boldly exposed) specimens. No localized corrosion (neither crevice nor pitting) was initiated during about 730 days of exposure. The crevice corrosion initiation model, i.e.,  $\Delta E$ , predicts that crevice corrosion should have initiated for over 50% of specimens at 120°C (the mean  $\Delta E$  is negative) and for less than 50% of the specimens exposed at 100°C. Neither crevice corrosion nor pitting corrosion was observed, indicating that the crevice corrosion initiation model is conservative (or crevice corrosion could initiate for longer exposure times). For 5 M CaCl<sub>2</sub> + 0.5 M Ca(NO<sub>3</sub>)<sub>2</sub> at 90°C (Cells 15 and 21), crevice corrosion was observed on six out of six creviced geometry specimens, and pitting corrosion was observed on one out of 12 rods. The crevice corrosion initiation model predicts that crevice corrosion should initiate for virtually all creviced specimens in agreement with these observations.

The crevice corrosion initiation model is conservative with respect to the observations in simulated acidified water (SAW) (Cells 1, 2, 7-2, 9, and 17), the crevice repassivation potential model is likely very conservative as no localized corrosion has been observed (although only rod specimens were exposed) and yet the crevice corrosion initiation model indicates that crevice corrosion initiation is very likely. The crevice corrosion initiation model is consistent with experimental observations obtained in basic saturated water (BSW), simulated dilute water (SDW), and simulated concentrated water (SCW) solutions (Cells 3, 4, 5, 6, 7-1, 16, and 19) in that crevice corrosion initiation was not observed for specimens exposed to these media and the predicted crevice repassivation potentials are positive (i.e., no crevice corrosion initiation is predicted) for these exposure conditions. The comparisons in Table 3-5 indicate that the crevice

corrosion initiation model is consistent with or conservative relative to the long-term corrosion test results.

This favorable comparison between the crevice corrosion initiation model ( $\Delta E = E_{rcrev} - E_{corr}$ ) and the long-term corrosion potential test observations also adds confidence in the use of the crevice corrosion initiation model implementation criteria discussed in Section 2.2.1.

Table 3-5. Summary of Long-Term Corrosion Test Cell Data

Solution	Immersion Days	Cell #	Temp. (°C)	Crevised Geometry	CC	Rod Geometry	PC	Modeled $\Delta E$		
								Lower Bound	Mean	Upper Bound
5m CaCl <sub>2</sub> + 5m Ca(NO <sub>3</sub> ) <sub>2</sub>	723	33	120	4	0	2	0	-398	-116	166
5m CaCl <sub>2</sub> + 5m Ca(NO <sub>3</sub> ) <sub>2</sub>	729	32	100	4	0	2	0	-184	93	370
3.5m NaCl + 0.175m KNO <sub>3</sub> + 0.7m MgSO <sub>4</sub>	735	31	80	4	2	2	0	-227	38	303
1M NaCl + 0.15M KNO <sub>3</sub>	741	30	90	4	0	2	0	-202	62	325
1M NaCl + 0.15M KNO <sub>3</sub>	749	29	75	4	0	2	0	-185	80	344
5M CaCl <sub>2</sub>	650	28	90	4	4	2	0	-466	-201	63
3.5m NaCl + 0.175m KNO <sub>3</sub>	252	25	100	4	0	0	0	-225	39	304
3.5m NaCl + 0.525m KNO <sub>3</sub>	256	24	100	4	0	0	0	-223	41	305
6m NaCl + 0.9m KNO <sub>3</sub>	265	23	100	4	2	0	0	-236	28	291
6m NaCl + 0.3m KNO <sub>3</sub>	280	22	100	4	0	0	0	-239	26	290
5M CaCl <sub>2</sub> + 0.5M Ca(NO <sub>3</sub> ) <sub>2</sub>	463	21	90	6	6	6	0	-597	-332	-66
5M CaCl <sub>2</sub>	497	20	120	6	6	6	0	-462	-191	79
BSW	256	19	105	0	0	8	0	15	284	554
4M NaCl	328	18	90	0	0	6	0	-233	31	295
SAW w/o Silicate	375	17	90	0	0	6	0	-485	-216	52
SCW	394	16	90	0	0	6	0	124	394	665
5M CaCl <sub>2</sub> + 0.5M Ca(NO <sub>3</sub> ) <sub>2</sub>	693	15	90	0	0	6	1	-597	-332	-66
5M CaCl <sub>2</sub> + 0.05M Ca(NO <sub>3</sub> ) <sub>2</sub>	704	14	90	0	0	6	1	-458	-194	70
1M CaCl <sub>2</sub> + 1M Ca(NO <sub>3</sub> ) <sub>2</sub>	622	13	90	0	0	6	0	-93	186	465
4.5 years LTCTF SAW	834	10	90	0	0	8	0	-435	-168	98
SAW	876	9	90	0	0	8	0	-587	-322	-57
SAW - LTCTF Vessel 26	846	7-2	25	0	0	3	0	-178	106	390
SDW - LTCTF Vessel 30	1089	6	90	0	0	2	0	18	304	590
SDW - LTCTF Vessel 29	1089	5	60	0	0	2	0	107	393	678
BSW	729	4	105	1	0	1	0	15	284	554
SCW - LTCTF Vessel 28	1089	3	90	0	0	2	0	101	373	646
SAW - LTCTF Vessel 26	1102	2	90	0	0	2	0	-435	-168	98
SAW - LTCTF Vessel 25	1089	1	60	0	0	2	0	-312	-42	228
<b>Data below is from cells not used for long-term corrosion potential model development</b>										
1m NaCl + 0.05m KNO <sub>3</sub>	223	27	100	4	0	0	0	-218	47	312
1m NaCl + 0.15m KNO <sub>3</sub>	230	26	100	4	0	0	0	-217	47	312
5 M CaCl <sub>2</sub>	894	8	120	0	0	5	5	-462	-191	79
SCW - LTCTF Vessel 27	218	7-1	60	0	0	2	0	281	559	837

Source: DTN: LL060900512251.177 [DIRS 178271], file: *Summary Ecorr Cells 1-36 29Sep06.xls*.

NOTES: Variations in solution composition (e.g., between the SAW solution compositions in Cells, 2, 9, 10, and 17) can lead to variations in the calculated  $\Delta E$  values. Details of the cell solution compositions can be found in DTN: MO0703PAGENCOR.001 [DIRS 180663], file: *EcorrRawData3.xls*.

BSW = basic saturated water, SAW = simulated acidified water, SCW = simulated concentrated water, SDW = simulated dilute water, LTCTF = Long-Term Corrosion Testing Facility, CC = crevice corrosion, PC = pitting corrosion.

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## 4. DIRECT INPUTS

This section documents all input data used for WPOB degradation process model development. This section also documents the direct inputs based on properly justified assumptions. The name, the qualification status, and a brief description of the software used for computation or calculation are also documented in this section.

### 4.1 PARAMETERS/DATA

Table 1-1 lists the sources for the relevant TSPA input parameters as well as their locations within technical products (a TSPA roadmap). Direct input data and assumptions used in the WPOB degradation process model development are documented in the remainder of this section.

#### 4.1.1 Direct Input Data

Table 4-1 lists the input data that provided direct feeds to WPOB degradation model development and identifies the DTNs and specific sources of the data. Additional details of the input data (a direct-input roadmap) are described in Section 4 of *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]).

Table 4-1. Summary of All Input Data for WPOB Degradation Analyses and Modeling

Data Name	Data Source/DTN
Oxide Layer on Alloy 22 Formed in Air	LL030406412251.045 [DIRS 163469], file: TDMS_TS444Q_data.doc
Oxide Layer on Alloy 22 Formed in Mixed Salt Environment	Andresen et al. 2003 [DIRS 170360], Section 3.0, Figures 3-8 through 3-11 and Figure 3-13
Calculated Pitzer pH and Molalities of Solutions Used in Various Electrochemical Tests	DTN: LL060904312251.186 [DIRS 178283], files: <i>AtmCO2GetEQData.xls</i> and <i>NoCO2GetEQData.xls</i>
Alloy 22 Weight-Loss Data of Crevice and Weight-Loss Specimens After Five Year Exposure in the LTCTF	LL030412512251.057 [DIRS 163712] file: C22 5 Year Coupon Corrosion Rates 4-14-03.xls
Polarization Resistance Data for Temperature Dependence	LL060900812251.180 [DIRS 178409] files: <i>175PRFitv2.xls</i> , <i>176PRFit.xls</i> , <i>179PRFit.xls</i> , and <i>187PRFit.xls</i>
Long-Term Open-Circuit Potential Measurement Data in Various Solutions at Different Temperatures	LL060900512251.177 [DIRS 178271] file: <i>Summary Ecorr Cells 1-36 29Sep06.xls</i> LL060901312251.181 [DIRS 178299] file: <i>Cell-1-partI.xls</i> , <i>Cell-1-partII.xls</i> , <i>Cell-2-partI.xls</i> , <i>Cell-2-partII.xls</i> , <i>Cell-3-partI.xls</i> , <i>Cell-3-partII.xls</i> , <i>Cell-5-partI.xls</i> , <i>Cell-5-partII.xls</i> , <i>Cell-6-partI.xls</i> , <i>Cell-6-partII.xls</i> , <i>Cell-7-2nd.xls</i> , <i>Cell-9.xls</i> , and <i>Cell-10.xls</i> . LL060901412251.182 [DIRS 178300], file: <i>Cell-13.xls</i> , <i>Cell-14.xls</i> , <i>Cell-15.xls</i> , and <i>Cell-28.xls</i>
Alteration of Corrosion Rates Associated with Microbial Activity	LL991203505924.094 [DIRS 138343] file: <i>SEP table S99502_001</i>

Table 4-1. Summary of All Input Data for WPOB Degradation Analyses and Modeling (Continued)

Data Name	Data Source/DTN
Relative Humidity Threshold for MIC	BSC 2004 [DIRS 169991], Section 7.1
Crevice Repassivation Potentials for Alloy 22	LL040902712251.119 [DIRS 173720] file: <i>Reduced Data Ahmet Yilmaz WBL 11Feb05.xls</i> LL050302312251.129 [DIRS 173921] file: <i>Mockup Developed RBR 21May05.xls</i> LL060603812251.164 [DIRS 178269] file: <i>Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls</i> LL060700312251.166 [DIRS 179385] file: <i>Rep Pot N06022 vs Temp 5M CaCl2 RBR 19Dec06.xls</i> LL060801812251.168 [DIRS 179386] file: <i>Rep Pot N06022 High Temp High NO3 RBR.xls</i> LL060803712251.170 [DIRS 179387] file: <i>Rep Pot N06022 vs Temp NaCl RBR 07Oct06.xls</i> See Attachment I
Density of Alloy 22	Haynes International 1997 [DIRS 100896], p. 13
Equivalent Weight of Alloy 22	ASTM G 102-89 1989 [DIRS 163908], Table 1
Universal Gas Constant	Lide 1991 [DIRS 131202], inside rear cover
Weibull shape estimator unbiasing factor	ASTM C 1239-06A. 2006 [DIRS 178286], Table 1
Alloy 22 Corrosion Rate in 10% Ferric Chloride Solution	Haynes International 1997 [DIRS 100897], p. 8
Alloy 22 Corrosion Rates in Concentrated Hydrochloric Acid	Haynes International 1997 [DIRS 100896], p. 12
Data Used to Determine Minimum Creviced Area	LB0503DUSTPCAP.001 [DIRS 173259], file: <i>Capil_Bundle.xls</i> SNL 2007 [DIRS 179394], Table 4-2 SNL 2007 [DIRS 179354], Table 4-3

Data from Haynes International (1997 [DIRS 100896] and 1997 [DIRS 100897]) are considered established fact according to SCI-PRO-004, *Managing Technical Product Inputs*, as they are numerical data from a primary source for the specific type of data. Similarly, data from ASTM G 102-89 (1989 [DIRS 163908]), ASTM C 1239-06A (2006 [DIRS 178286]), and Lide (1991 [DIRS 131202]) are also considered established fact because they are sources scientists would use in their standard work practices. Data from Andresen et al. (2003 [DIRS 170360]) are considered qualified data because these data are information received from a vendor or supplier such as analysis, characteristics or properties of materials, etc., that are acquired data collected under an approved QA program that meets the requirements of 10 CFR 63 (2005 [DIRS 173273]).

### 4.1.2 Assumptions

The following assumptions were used as direct inputs in the WPOB degradation process model development:

- The general corrosion rate of Alloy 22, at a given temperature, was assumed constant (i.e., time independent) (SNL 2007 [DIRS 178519], Section 5.2). This assumption is considered conservative because the general corrosion rate of metals and alloys tend to decrease with time.
- Although localized corrosion can be either pitting corrosion on boldly exposed surfaces or crevice corrosion, which takes place in occluded regions, the only form of localized corrosion was assumed to be crevice corrosion (SNL 2007 [DIRS 178519], Section 5.3). Crevice corrosion is considered to have the lowest barrier to initiation, and therefore this assumption is bounding and conservative.
- The error terms and model coefficients for the localized corrosion initiation regression models are assumed to be normally distributed. The basis for this assumption is the Central Limit Theorem (Stedinger et al. 1993 [DIRS 105941], p. 18.11), which states that “. . . if a random variable  $X$  is the sum of  $n$  independent and identically distributed random variables with finite variance, then with increasing  $n$  the distribution of  $X$  becomes normal regardless of the distribution of the original random variables.” It is reasonable to assume that the fitting coefficients and error variance arise from a sum of many independent and (at least nearly) identically distributed random processes with finite variances.
- The crevice corrosion of the WPOB was assumed to propagate at a (time-independent) constant rate (SNL 2007 [DIRS 178519], Section 5.4). This assumption is conservative because it is known that localized corrosion rates decrease with time (SNL 2007 [DIRS 178519], Section 5.4).
- The crevice corrosion data of the WPOB material (Alloy 22) that were generated in fully immersed conditions were assumed to be applicable to the crevice corrosion processes of the waste package in contact with thin water films (under porous layers of dust and mineral precipitates) having the same water chemistry as the fully immersed condition (SNL 2007 [DIRS 178519], Section 5.5). Under immersed conditions, the metal is in contact with a practically unlimited reservoir of corrosive solution. In contrast, the crevice corrosion behavior under thin film condition will be reactant-limited. In both cases only a limited amount of solution is necessary to form a stagnant boundary layer in the creviced region. This assumption is considered to be reasonable and realistic.
- The corrosion behavior of the stress-mitigated (low plasticity burnished) outer lid closure weld region is assumed not to differ significantly from the corrosion behavior of a closure-lid weld region that had not undergone stress-mitigation (SNL 2007 [DIRS 178519], Section 5.6). This assumption is based on comparisons of the general and localized corrosion characteristics of stress-mitigated and nonstress-mitigated

specimens (SNL 2007 [DIRS 178519], Section 5.6). This assumption is considered to be reasonable and realistic.

Proper justification for the use of these assumptions in the model development was provided in Section 5 of *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]).

## 4.2 NON-PARAMETER INFORMATION

The formulas, algorithms, and implementation guidance for implementation of the WPOB general corrosion model are discussed in Section 2.1, and in Section 8.2 of the WPOB model report (SNL 2007 [DIRS 178519]). Further details related to the development of formulas, algorithms, and implementation guidance for implementation of the WPOB general corrosion model are discussed in Section 6.4.3 of the WPOB model report (SNL 2007 [DIRS 178519]).

The formulas, algorithms, and implementation guidance for implementation of the WPOB localized corrosion model are discussed above in Section 2.2, and in Section 8.3 of the WPOB model report (SNL 2007 [DIRS 178519]). Further details related to the development of formulas, algorithms, and implementation guidance for implementation of the WPOB general corrosion model are discussed in Section 6.4.4 of the WPOB model report (SNL 2007 [DIRS 178519]).

## 4.3 SOFTWARE

No unqualified software has been used in the preparation of this TDIP and *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]). Microsoft Excel 97 SR-2, bundled with Microsoft Office 1997, is a commercial off-the-shelf software program used in this report. The Excel computations performed in this report use only standard built-in functions and are documented in sufficient detail to allow an independent technical reviewer to reproduce or verify the results by visual inspection or hand calculation without recourse to the originator (SNL 2007 [DIRS 178519], Sections 6.4.3 to 6.4.6) or to the Excel files included in DTN: MO0703PAGENCOR.001 [DIRS 180663]. The calculation results are not dependent upon the use of this particular software. Therefore, use of this software is not subject to IM-PRO-003, *Software Management*. Microsoft Excel 97 SR-2 is appropriate for this application as it offers the mathematical and graphical functionality necessary to perform and document the numerical manipulations used in this report. Microsoft Excel 97 SR-2 was executed on an Optiplex GX260 Workstation (SNL tag S884914, located in the Summerlin offices, Las Vegas, Nevada) equipped with the Windows 2000 operating system.

Mathcad version 13.0 is a commercial off-the-shelf software program used in this TDIP and the WPOB general corrosion and localized corrosion model report (SNL 2007 [DIRS 178519]). The Mathcad computations performed in this report use only standard functions and are documented in sufficient detail to allow an independent technical reviewer to reproduce or verify the results by visual inspection or hand calculation without recourse to the originator (SNL 2007 [DIRS 178519], Sections 6.4.3 to 6.4.4) or to the Mathcad worksheet files included in DTN: MO0703PAGENCOR.001 [DIRS 180663]. The calculation results are not dependent upon the use of this particular software. Therefore, use of this software is not subject to

IM-PRO-003. This software is appropriate for this application as it offers the mathematical and graphical functionality necessary to perform and document the numerical manipulations used in this report. Mathcad version 13.0 was executed on a computer (SNL tag S884914, located in the Summerlin offices, Las Vegas, Nevada) equipped with the Windows 2000 operating system.

S-PLUS 2000 Professional Release 2 is a commercial off-the-shelf software program used in the development of this report and the WPOB general corrosion and localized corrosion model report (SNL 2007 [DIRS 178519]). The S-PLUS computations performed in this report use only standard functions and are documented in sufficient detail to allow an independent technical reviewer to reproduce or verify the results by visual inspection or hand calculation without recourse to the originator (SNL 2007 [DIRS 178519], Section 6.4.3) or to DTN: MO0703PAGENCOR.001 [DIRS 180663]. The calculation results are not dependent upon the use of this particular software. Therefore, use of this software is not subject to IM-PRO-003. This software is appropriate for this application as it offers the mathematical and graphical functionality necessary to perform and document the numerical manipulations used in this report. S-PLUS 2000 Professional Release 2 was executed on a computer (SNL tag S884301, located in the Summerlin offices, Las Vegas, Nevada) equipped with the Windows XP operating system. These software and their use are also discussed in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 3).

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## 5. JUSTIFICATION

*General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]) was developed under the Yucca Mountain Quality Assurance (QA) program and was subject to *Quality Assurance Requirements and Description* (QARD) (DOE 2006 [DIRS 177092]) requirements. All waste package configurations have been determined to be important for waste isolation in accordance with LS-PRO-0203, *Q-List and Classification of Structures, Systems, and Components*. *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]) is being prepared in accordance with SCI-PRO-006, *Models*, and *Technical Work Plan for Postclosure Engineered Barrier Degradation Modeling* (SNL 2007 [DIRS 178849]).

The inputs to *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* model report (SNL 2007 [DIRS 178519]) will be documented according to SCI-PRO-004, *Managing Technical Product Inputs*. The methods used to control the electronic management of data as required by IM-PRO-002, *Control of the Electronic Management of Information*, will be accomplished in accordance with the TWP (SNL 2007 [DIRS 178849]). Models documented in this TDIP were developed using accepted standard modeling techniques and will be validated in accordance with the relevant sections of SCI-PRO-006 in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]). Uncertainties resulting from measured data and application of models will be evaluated, propagated and included in specification of outputs. Since the model inputs will be obtained from controlled and/or qualified sources, and the mathematical models will be validated per applicable quality assurance procedures, the output parameters provided to TSPA will be adequate for their intended use as inputs into the TSPA model for the prediction of long-term corrosion behavior of the WPOB.

### 5.1 DESCRIPTION AND JUSTIFICATION OF PROCESS MODELS AND/OR ABSTRACTIONS

This section identifies the process models whose outputs will be used as inputs into the TSPA model. Names and brief discussion on the relevant waste package degradation process models and their TSPA implementation/justification are provided in Sections 2.1 and 2.2. Justification for the process models and/or abstractions is also provided in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Sections 6 and 7).

### 5.2 TSPA OR PROCESS-LEVEL MODEL INPUT

Inputs from *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]) into TSPA model will be based on the waste package degradation process model outputs as discussed in Sections 5.2.1 and 5.2.2.

#### 5.2.1 General Corrosion Model Outputs

WPOB general corrosion model output parameters, which are used as inputs into the TSPA model, are listed in Tables 1-1 and 2-2. As documented in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Sections 6.4.3, 7, and 8), this model and its parameters were developed using inputs obtained from controlled and/or qualified sources, and the mathematical model was validated per applicable quality assurance

procedures (see Section 5.3). Therefore, the WPOB general corrosion model and its parameter values and associated uncertainties are adequate for their intended use as inputs into the TSPA model for the prediction of long-term general corrosion behavior of the waste package outer barrier.

### **5.2.2 Localized Corrosion Model Outputs**

WPOB localized corrosion model output parameters, which are to be used as inputs into the TSPA model, are listed in Table 1-1, Table 2-3, and Table 2-4. As documented in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Sections 6.4.4, 7, and 8), the WPOB localized corrosion models and their parameters were developed using inputs from controlled and/or qualified sources, and the mathematical models were validated per applicable quality assurance procedures (see Section 5.3). Therefore, the waste package outer barrier localized corrosion models and their parameter values and associated uncertainties are adequate for their intended use as inputs into the TSPA model for the prediction of long-term localized corrosion behavior of the waste package outer barrier.

## **5.3 DESCRIPTION AND JUSTIFICATION OF MODEL VALIDATION**

Models described in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]) are expected to adequately predict general and localized corrosion processes of the WPOB under the exposure conditions expected in the repository for the entire regulatory period (SNL 2007 [DIRS 178519]). The unusually long-term application makes it difficult to validate these models in the usual way (i.e., by comparison of model predicted values with those observed experimentally for the whole range of service time). Consequently, these models will be validated by justifying the input parameter values used and comparing these parameters and model predictions to available peer-reviewed literature and qualified YMP data. As mentioned in SCI-PRO-002, *Planning For Science Activities*, and as stated in the TWP for waste package modeling (SNL 2007 [DIRS 178849], Section 2.3.1), the required level of confidence (i.e., the level of validation) in the WPOB degradation process models is the highest, which is Level II according to SCI-PRO-002. The required level of confidence in the WPOB general and localized corrosion models will be obtained by building confidence in the methods used to develop the models and by corroborating or validating the model output values with those available in the peer reviewed scientific literature (SNL 2007 [DIRS 178519], Section 7). It may be noted that there is no model discussed in this TDIP that requires additional model validation beyond what will be provided in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]).

### **5.3.1 Confidence Building during Model Development to Establish Scientific Basis and Accuracy for Intended Use**

The inputs to the general and localized corrosion models for the WPOB have all been obtained from qualified sources (SNL 2007 [DIRS 178519], Section 4.1). All model assumptions have been properly justified (SNL 2007 [DIRS 178519], Section 5). Detailed discussion about model concepts along with discussion of initial and boundary conditions are also provided, and the waste package degradation models and ranges of application are discussed in SNL (2007 [DIRS 178519], Sections 1.2, 6, and 8). Uncertainties associated with the WPOB's capabilities and the

impact of uncertainties on the model results are documented in Sections 6.4.3, 6.4.4, 6.4.5 and 8 of *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]).

### **5.3.2 Postdevelopment Activities for Confidence Building in Models by Demonstrating Accuracy of the Models for their Intended Use**

According to Attachment 3 of SCI-PRO-002, a Level II validation requires model predictions to be corroborated by at least two postdevelopment model validation methods described in Section 6.3.2 of SCI-PRO-006. The postdevelopment model validation methods, as described in Section 6.3.2 of SCI-PRO-006, include:

- Corroboration of model results with data acquired from the laboratory, field experiments, analog studies, or other relevant observations, not previously used to develop or calibrate the model.
- Corroboration of model results with relevant information published in refereed journals or literature provided that data used to develop and calibrate a model shall not be used to validate a model.
- Corroboration of model results with other model results obtained from the implementation of other independent mathematical models developed for similar or comparable intended use/purpose.

In light of these model validation options, four postdevelopment model validation activities were documented in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Section 7) to ensure that the required level of confidence in these models for their stated purposes has been achieved. These activities were:

Activity One: Show that the modeled propagation rates of general corrosion and localized corrosion of the waste package are reasonable and consistent with rates determined by alternative techniques or alternative models for the conditions expected in the repository.

Activity Two: Show that the modeled propagation rates of general corrosion and localized corrosion of the waste package are reasonable and consistent with rates from literature data and natural or industrial analogues of relevant corrosion resistant alloys for the conditions expected in the repository.

Activity Three: Show that the response of the correlations for  $E_{corr}$  and  $E_{critical}$  of the waste package are reasonable and consistent with literature data on relevant corrosion resistant alloys and available analogues for the conditions expected in the repository.

Activity Four: Show that the response of the correlations for  $E_{corr}$  and  $E_{critical}$  of the waste package are consistent with other alternative models for localized corrosion initiation for the conditions expected in the repository.

The criterion for satisfying these four validation activities is that the corroborating data must match reasonably well with the model predictions, and any deviation from this criterion must be properly justified (SNL 2007 [DIRS 178849], Section 2.3.1).

The validation activities mentioned above were performed to fulfill the model validation requirements of the governing procedure SCI-PRO-006 (Section 6.3.2) and the TWP (SNL 2007 [DIRS 178849], Section 2.3.1). Detailed descriptions of the validation of the WPOB general and localized corrosion models are documented Section 7 of *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]).

#### **5.4 MODEL AND/OR ANALYSIS OUTPUT AND RATIONALE**

WPOB general corrosion and localized corrosion model outputs are reported in Sections 2.1 (see Tables 2-1 and 2-2) and 2.2 (see Tables 2-3 and 2-4), respectively. Additionally, Section 8 of *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519]) and DTN: MO0703PAGENCOR.001 [DIRS 180663] are controlled sources of WPOB degradation process model outputs.

As documented in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (SNL 2007 [DIRS 178519], Sections 6.4.3, 6.4.4, 7, and 8), the WPOB degradation models and their parameters were developed using inputs from controlled and/or qualified sources, and the developed mathematical models were validated per applicable quality assurance procedures (see Sections 5.2 and 5.3). Therefore, the WPOB degradation models and their parameter values and associated uncertainties are adequate for their intended use as inputs into the TSPA model for the prediction of long-term corrosion behavior of the waste package outer barrier.

## 6. REFERENCES

### 6.1 DOCUMENTS CITED

- 170360 Andresen, P.L.; Kim, Y.J.; Emigh, P.W.; Catlin, G.M.; and Martiniano, P.J. 2003. *GE GRC Final Report*. BSC PO 2450-100-PO-10508. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20040520.0076.
- 171924 BSC (Bechtel SAIC Company) 2004. *Aging and Phase Stability of Waste Package Outer Barrier*. ANL-EBS-MD-000002 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041005.0003.
- 169991 BSC 2004. *Evaluation of Potential Impacts of Microbial Activities on Drift Chemistry*. ANL-EBS-MD-000038 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041118.0005; DOC.20050505.0001; DOC.20050609.0001.
- 169996 BSC 2004. *WAPDEG Analysis of Waste Package and Drip Shield Degradation*. ANL-EBS-PA-000001 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041004.0005.
- 173944 BSC 2005. *Multiscale Thermohydrologic Model*. ANL-EBS-MD-000049 REV 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20050711.0001.
- 171452 Dunn, D.S.; Cragolino, G.A.; Pan, Y.M.; and Tang, L.T. 2004. "Effect of Fabrication Processes on Alloy 22 Corrosion Resistance." *Corrosion/2004, 59th Annual Conference & Exposition, March 28-April 1, 2004, New Orleans*. Paper No. 04698. Houston, Texas: NACE International. TIC: 255943.
- 178104 Dunn, D.S.; Pensado, O.; Pan, Y.-M.; Pabalan, R.T.; Yang, L.; He, X.; and Chiang, K.T. 2005. *Passive and Localized Corrosion of Alloy 22 - Modeling and Experiments*. CNWRA 2005-02. San Antonio, Texas: Center for Nuclear Waste Regulatory Analyses. ACC: LLR.20070305.0002.
- 100897 Haynes International 1997. *Hastelloy Alloy C-276*. Haynes International Product Brochure. Kokomo, Indiana: Haynes International. TIC: 238832.
- 100896 Haynes International 1997. *Hastelloy C-22 Alloy*. Kokomo, Indiana: Haynes International. TIC: 238121.
- 173259 LB0503DUSTPCAP.001. ECRB Dust Pore Diameter Distribution and Capillary Pressure Characteristic Curves. Submittal date: 3/25/2005.
- 131202 Lide, D.R., ed. 1991. *CRC Handbook of Chemistry and Physics*. 72nd Edition. Boca Raton, Florida: CRC Press. TIC: 3595.

- 163469 LL030406412251.045. Transmission Electron Microscopy (TEM) Images of Oxide Film on Air-Oxidized Alloy 22 (UNS N06022) Samples Aged at 550C. Submittal date: 04/11/2003.
- 163712 LL030412512251.057. LTCTF Corrosion Rate Calculations for Five-Year Exposed Alloy C22 Specimens Cleaned Under TIP-CM-51. Submittal date: 05/28/2003.
- 173722 LL040806212251.118. Crevice Repassivation Potential (CRP) of Alloy 22 Determined by the Tsujikawa-Hisamatsu Electrochemical (THE) Method. Submittal date: 03/23/2005.
- 173720 LL040902712251.119. Corrosion Rate and Potential Parameter Data Taken From Cyclic Potentiodynamic Polarization (CPP) Curves for Laser Peened, Burnished, and As-Welded Alloy 22 Specimens. Submittal date: 02/15/2005.
- 173921 LL050302312251.129. Electrochemical Behavior of Alloy 22 Specimens Prepared from a Mockup Container. Submittal date: 05/24/2005.
- 178269 LL060603812251.164. Compilation of Crevice Repassivation Potentials for Alloy 22 in NaCl + KNO<sub>3</sub> - Developed. Submittal date: 09/11/2006.
- 179385 LL060700312251.166. Compilation of Crevice Repassivation Potentials for Alloy 22 in 5 M CaCl<sub>2</sub> - Developed. Submittal date: 12/19/2006.
- 179386 LL060801812251.168. Compilation of Crevice Repassivation Potentials for Alloy 22 in High Temperature High Nitrate Solutions - Developed. Submittal date: 01/16/2007.
- 179387 LL060803712251.170. Compilation of Crevice Repassivation Potentials for Alloy 22 in NaCl Solutions - Developed. Submittal date: 12/19/2006.
- 178271 LL060900512251.177. Long-Term Corrosion Potentials (E<sub>corr</sub>) of Alloy 22 in 37 Different Solutions - Developed. Submittal date: 11/01/2006.
- 178409 LL060900812251.180. Effect of Temperature on the Polarization Resistance of Alloy 22 - Developed. Submittal date: 11/06/2006.
- 178299 LL060901312251.181. Long-Term Open Circuit Potentials of Alloy 22 in Multi-Ionic Solutions (SAW, SDW, SCW and BSW) - 13 Cells - Acquired. Submittal date: 10/19/2006.
- 178300 LL060901412251.182. Long-Term Open Circuit Potentials of Alloy 22 in CaCl<sub>2</sub> and Ca(NO<sub>3</sub>)<sub>2</sub> Based Solutions - 7 Cells - Acquired. Submittal date: 10/21/2006.
- 178283 LL060904312251.186. Modeling of Pitzer pH for Selected E<sub>corr</sub> Test Solutions. Submittal date: 11/02/2006.

- 138343 LL991203505924.094. Approach and Supporting Data for MIC Modeling. Submittal date: 12/13/1999.
- 167921 Lloyd, A.C.; Shoesmith, D.W.; McIntyre, N.S.; and Noël, J.J. 2003. "Effects of Temperature and Potential on the Passive Corrosion Properties of Alloys C22 and C276." *Journal of the Electrochemical Society*, 150, (4), B120-B130. [New York, New York]: Electrochemical Society. TIC: 255963.
- 180663 MO0703PAGENCOR.001. Output from General Corrosion and Localized Corrosion of Waste Package Outer Barrier 2007 Second Version. Submittal date: 05/03/2007.
- 178519 SNL (Sandia National Laboratories) 2007. *General Corrosion and Localized Corrosion of Waste Package Outer Barrier*. ANL-EBS-MD-000003 REV 03. Las Vegas, Nevada: Sandia National Laboratories.
- 178849 SNL 2007. *Technical Work Plan for Postclosure Engineered Barrier Degradation Modeling*. TWP-EBS-MD-000020 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070216.0001.
- 179320 SNL 2007. *Technical Work Plan for: Total System Performance Assessment (TSPA) Parameter Selection and Documentation with TSPA Data Input Package (TDIP)*. TWP-MGR-PA-000044 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070116.0002.
- 179354 SNL 2007. *Total System Performance Assessment Data Input Package for Requirements Analysis for EBS In-Drift Configuration*. TDR-TDIP-ES-000010 REV 00. Las Vegas, Nevada: Sandia National Laboratories.
- 179394 SNL 2007. *Total System Performance Assessment Data Input Package for Requirements Analysis for TAD Canister and Related Waste Package Overpack Physical Attributes Basis for Performance Assessment*. TDR-TDIP-ES-000006 REV 00. Las Vegas, Nevada: Sandia National Laboratories.
- 105941 Stedinger, J.R.; Vogel, R.M.; and Foufoula-Georgiou, E. 1993. "Frequency Analysis of Extreme Events." Chapter 18 of *Handbook of Hydrology*. Maidment, D.R., ed. New York, New York: McGraw-Hill. TIC: 236568.
- 174800 Wong, L.L.; Lian, T.; Fix, D.V.; Sutton, M.; and Rebak, R.B. 2004. "Surface Analysis of Alloy 22 Coupons Exposed for Five Years to Concentrated Ground Waters." *Corrosion/2004, 59th Annual Conference & Exposition, March 28 - April 1, 2004, New Orleans*. Paper No. 04701. Houston, Texas: NACE International. TIC: 255943.

## 6.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

- 173273 10 CFR 63. 2005. Energy: Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada. ACC: MOL.20050405.0118.
- 178286 ASTM C 1239-06A. 2006. *Standard Practice for Reporting Uniaxial Strength Data and Estimating Weibull Distribution Parameters for Advanced Ceramics*. West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 258790.
- 163908 ASTM G 102-89 (Reapproved 1999). 1989. *Standard Practice for Calculation of Corrosion Rates and Related Information from Electrochemical Measurements*. West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 249897.
- 177092 DOE (U.S. Department of Energy) 2006. *Quality Assurance Requirements and Description*. DOE/RW-0333P, Rev. 18. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20060602.0001.

IM-PRO-002, Rev. 0, ICN 0. *Control of the Electronic Management of Information*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20060927.0023.

IM-PRO-003, Rev. 2, ICN 0. *Software Management*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20070228.0002.

LS-PRO-001, Rev. 2, ICN 0. *Technical Reports*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20070115.0001.

LS-PRO-0203, Rev. 2, ICN 0. *Q-List and Classification of Structures, Systems, and Components*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20060927.0016.

SCI-PRO-002, Rev. 2, ICN 0. *Planning for Science Activities*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20070320.0001.

SCI-PRO-004, Rev. 2, ICN 0. *Managing Technical Product Inputs*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20070410.0002.

SCI-PRO-006, Rev. 2, ICN 0. *Models*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20070420.0001.

**ATTACHMENT I**

**CREVICE REPASSIVATION POTENTIAL DATA USED IN MODEL DEVELOPMENT**



Table I-1. Data Used in Development of Crevice Repassivation Potential Model

Source DTN	Specimen ID	Sample Type	Material Condition	Electrolyte	Type of LC	Temperature (°C)	Calculated Pitzer pH	[Cl] molal	[NO <sub>3</sub> ] molal	NO <sub>3</sub> /Cl molal ratio	E <sub>crev</sub> (mV vs. SSC)
LL060803712251.170 [DIRS 179387]	KE0614	PCA	ASW	0.0005 M NaCl	CC	60	6.51	5.00E-04	0.00	0.00	339
LL060803712251.170 [DIRS 179387]	KE0117	PCA	ASW	0.0005 M NaCl	CC	90	6.21	5.00E-04	0.00	0.00	214
LL060803712251.170 [DIRS 179387]	KE0618	PCA	ASW	0.005 M NaCl	CC	60	6.51	5.80E-03	0.00	0.00	359
LL060803712251.170 [DIRS 179387]	KE0617	PCA	ASW	0.05 M NaCl	CC	60	6.51	0.05	0.00	0.00	161
LL060803712251.170 [DIRS 179387]	KE0610	PCA	ASW	0.5 M NaCl	CC	60	6.45	0.51	0.00	0.00	61
LL060803712251.170 [DIRS 179387]	JE3321	MCA	MA	1 M NaCl	CC	60	6.45	1.02	0.00	0.00	84
LL060803712251.170 [DIRS 179387]	JE3322	MCA	MA	1 M NaCl	CC	60	6.45	1.02	0.00	0.00	28
LL060803712251.170 [DIRS 179387]	DEA3129	MCA	MA	1 M NaCl	CC	90	6.16	1.02	0.00	0.00	-24
LL060803712251.170 [DIRS 179387]	JE3324	MCA	MA	1 M NaCl	CC	90	6.16	1.02	0.00	0.00	-126
LL060803712251.170 [DIRS 179387]	JE3328	MCA	MA	1 M NaCl	CC	90	6.16	1.02	0.00	0.00	-109
LL060803712251.170 [DIRS 179387]	DEA3262	MCA	MA	1 M NaCl	CC	90	6.16	1.02	0.00	0.00	-42
LL040902712251.119 [DIRS 173720]	W6	PCA	ASW	1 M NaCl	CC	90	6.16	1.02	0.00	0.00	-104
LL040902712251.119 [DIRS 173720]	B3	PCA	ASW - LPB	1 M NaCl	CC	90	6.16	1.02	0.00	0.00	-134
LL040902712251.119 [DIRS 173720]	P5	PCA	ASW - LSP	1 M NaCl	CC	90	6.16	1.02	0.00	0.00	-114
LL060803712251.170 [DIRS 179387]	DEA3263	MCA	MA	1 M NaCl	CC	90	6.16	1.02	0.00	0.00	-45
LL050302312251.129 [DIRS 173921]	AY009	PCA	ASW - Mockup	1 M NaCl	CC	90	6.16	1.02	0.00	0.00	-54
LL050302312251.129 [DIRS 173921]	AY010	PCA	ASW - Mockup	1 M NaCl	CC	90	6.16	1.02	0.00	0.00	-52
LL060803712251.170 [DIRS 179387]	DEA3267	MCA	MA	1.25 M NaCl	LC	60	6.44	1.29	0.00	0.00	48

Source DTN	Specimen ID	Sample Type	Material Condition	Electrolyte	Type of LC	Temperature (°C)	Calculated Pitzer pH	[Cl] molal	[NO <sub>3</sub> ] molal	NO <sub>3</sub> /Cl molal ratio	E <sub>rev</sub> (mV vs. SSC)
LL060803712251.170 [DIRS 179387]	DEA3268	MCA	MA	1.25 M NaCl	LC	60	6.44	1.29	0.00	0.00	23
LL060803712251.170 [DIRS 179387]	DEA3271	MCA	MA	1.25 M NaCl	CC	90	6.14	1.29	0.00	0.00	-33
LL060803712251.170 [DIRS 179387]	DEA3269	MCA	MA	1.25 M NaCl	CC	90	6.14	1.29	0.00	0.00	-65
LL060803712251.170 [DIRS 179387]	KE0612	PCA	ASW	4 M NaCl	CC	60	6.25	4.40	0.00	0.00	-52
LL060803712251.170 [DIRS 179387]	DEA3296	MCA	MA	4 M NaCl	CC	60	6.25	4.40	0.00	0.00	-116
LL060803712251.170 [DIRS 179387]	DEA3297	MCA	MA	4 M NaCl	CC	60	6.25	4.40	0.00	0.00	-107
LL060803712251.170 [DIRS 179387]	DEA3298	MCA	MA	4 M NaCl	CC-II	60	6.25	4.40	0.00	0.00	-50
LL060803712251.170 [DIRS 179387]	DEA3299	MCA	MA	4 M NaCl	CC-II	60	6.25	4.40	0.00	0.00	-69
LL060803712251.170 [DIRS 179387]	DEA3304	MCA	MA	4 M NaCl	CC	75	6.10	4.40	0.00	0.00	-140
LL060803712251.170 [DIRS 179387]	DEA3305	MCA	MA	4 M NaCl	CC	75	6.10	4.40	0.00	0.00	-140
LL060803712251.170 [DIRS 179387]	DEA3307	MCA	MA	4 M NaCl	CC	75	6.10	4.40	0.00	0.00	-157
LL060803712251.170 [DIRS 179387]	KE0710	PCA	MA	4 M NaCl	CC	75	6.10	4.40	0.00	0.00	-118
LL060803712251.170 [DIRS 179387]	DEA3306	MCA	MA	4 M NaCl	CC-II	75	6.10	4.40	0.00	0.00	-148
LL060803712251.170 [DIRS 179387]	DEA3300	MCA	MA	4 M NaCl	CC	90	5.97	4.40	0.00	0.00	-161
LL060803712251.170 [DIRS 179387]	DEA3301	MCA	MA	4 M NaCl	CC	90	5.97	4.40	0.00	0.00	-168
LL060803712251.170 [DIRS 179387]	DEA3302	MCA	MA	4 M NaCl	CC	90	5.97	4.40	0.00	0.00	-160
LL060803712251.170 [DIRS 179387]	DEA3303	MCA	MA	4 M NaCl	CC	90	5.97	4.40	0.00	0.00	-165
LL060803712251.170 [DIRS 179387]	DEA3312	MCA	MA	4 M NaCl	CC	105	5.85	4.40	0.00	0.00	-157
LL060803712251.170 [DIRS 179387]	DEA3313	MCA	MA	4 M NaCl	CC	105	5.85	4.40	0.00	0.00	-168

Source DTN	Specimen ID	Sample Type	Material Condition	Electrolyte	Type of LC	Temperature (°C)	Calculated Pitzer pH	[Cl] molal	[NO <sub>3</sub> ] molal	NO <sub>3</sub> /Cl molal ratio	E <sub>rev</sub> (mV vs. SSC)
LL060803712251.170 [DIRS 179387]	DEA3314	MCA	MA	4 M NaCl	CC	105	5.85	4.40	0.00	0.00	-119
LL060803712251.170 [DIRS 179387]	DEA3315	MCA	MA	4 M NaCl	CC	105	5.85	4.40	0.00	0.00	-142
LL060801812251.168 [DIRS 179386]	KE0571	PCA	ASW	3 m KCl + 3 m NaCl + 3 m KNO <sub>3</sub> + 3 m NaNO <sub>3</sub> (+ 0.0001 m HCl)	CC-II	110	3.19	6.00	6.00	1.00	330
LL060801812251.168 [DIRS 179386]	KE0575	PCA	ASW	3 m KCl + 3 m NaCl + 3 m KNO <sub>3</sub> + 3 m NaNO <sub>3</sub> (+ 0.0001 m HCl)	CC-II	110	3.19	6.00	6.00	1.00	413
LL060801812251.168 [DIRS 179386]	KE0588	PCA	ASW	4 m CaCl <sub>2</sub>	CC	110	4.41	8.00	0.00	0.00	-243
LL060801812251.168 [DIRS 179386]	KE0689	PCA	ASW	4 m KCl + 4 m NaCl	CC	110	5.76	8.00	0.00	0.00	-223
LL060801812251.168 [DIRS 179386]	KE0691	PCA	ASW	4 m KCl + 4 m NaCl	CC	110	5.76	8.00	0.00	0.00	-210
LL060801812251.168 [DIRS 179386]	KE0688B	PCA	ASW	4 m KCl + 4 m NaCl + 0.4 m KNO <sub>3</sub> + 0.4 m NaNO <sub>3</sub>	CC	90	5.89	8.00	0.80	0.10	-82
LL060801812251.168 [DIRS 179386]	KE0579	PCA	ASW	4 m KCl + 4 m NaCl + 0.4 m KNO <sub>3</sub> + 0.4 m NaNO <sub>3</sub>	CC	90	5.89	8.00	0.80	0.10	-80
LL060801812251.168 [DIRS 179386]	KE0687	PCA	ASW	4 m KCl + 4 m NaCl + 0.4 m KNO <sub>3</sub> + 0.4 m NaNO <sub>3</sub>	CC	110	5.76	8.00	0.80	0.10	-50
LL060801812251.168 [DIRS 179386]	KE0692	PCA	ASW	4 m KCl + 4 m NaCl + 0.4 m KNO <sub>3</sub> + 0.4 m NaNO <sub>3</sub>	CC	110	5.76	8.00	0.80	0.10	-103
LL060801812251.168 [DIRS 179386]	KE0573	PCA	ASW	4 m KCl + 4 m NaCl + 0.4 m KNO <sub>3</sub> + 0.4 m NaNO <sub>3</sub> (+ 0.0001 m HCl)	CC	110	3.36	8.00	0.80	0.10	-106
LL060801812251.168 [DIRS 179386]	KE0589	PCA	ASW	4 m KCl + 4 m NaCl + 0.8 m KNO <sub>3</sub> + 0.8 m NaNO <sub>3</sub>	CC	110	5.76	8.00	1.60	0.20	-44
LL060801812251.168 [DIRS 179386]	KE0572	PCA	ASW	4 m KCl + 4 m NaCl + 2 m KNO <sub>3</sub> + 2 m NaNO <sub>3</sub> (+ 0.0001 m HCl)	CC-II	110	3.09	8.00	4.00	0.50	446
LL060700312251.166 [DIRS 179385]	JE1647	MCA	ASW	5 M CaCl <sub>2</sub>	CC	30	4.55	11.99	0.00	0.00	-57
LL060700312251.166 [DIRS 179385]	KE0381	PCA	ASW	5 M CaCl <sub>2</sub>	CC	60	4.20	11.99	0.00	0.00	-65
LL060700312251.166 [DIRS 179385]	KE0380	PCA	ASW	5 M CaCl <sub>2</sub>	CC	60	4.20	11.99	0.00	0.00	-64
LL060700312251.166 [DIRS 179385]	JE0114	MCA	ASW	5 M CaCl <sub>2</sub>	CC-II	45	4.36	11.99	0.00	0.00	24

Source DTN	Specimen ID	Sample Type	Material Condition	Electrolyte	Type of LC	Temperature (°C)	Calculated Pitzer pH	[Cl] molal	[NO <sub>3</sub> ] molal	NO <sub>3</sub> /Cl molal ratio	E <sub>rev</sub> (mV vs. SSC)
LL060700312251.166 [DIRS 179385]	JE0112	MCA	ASW	5 M CaCl <sub>2</sub>	CC-II	60	4.20	11.99	0.00	0.00	-88
LL060700312251.166 [DIRS 179385]	JE0113	MCA	ASW	5 M CaCl <sub>2</sub>	CC-II	60	4.20	11.99	0.00	0.00	-48
LL060700312251.166 [DIRS 179385]	JE0111	MCA	ASW	5 M CaCl <sub>2</sub>	CC-II	60	4.20	11.99	0.00	0.00	-47
LL060700312251.166 [DIRS 179385]	DEA3295	MCA	MA	5 M CaCl <sub>2</sub>	CC-II	60	4.20	11.99	0.00	0.00	18
LL060700312251.166 [DIRS 179385]	DEA3294	MCA	MA	5 M CaCl <sub>2</sub>	CC-II	60	4.20	11.99	0.00	0.00	22
LL060700312251.166 [DIRS 179385]	DEA3226	MCA	MA	5 M CaCl <sub>2</sub>	LC	60	4.20	11.99	0.00	0.00	-27
LL060700312251.166 [DIRS 179385]	DEA3224	MCA	MA	5 M CaCl <sub>2</sub>	LC	60	4.20	11.99	0.00	0.00	-2
LL060700312251.166 [DIRS 179385]	DEA3225	MCA	MA	5 M CaCl <sub>2</sub>	LC	60	4.20	11.99	0.00	0.00	29
LL060700312251.166 [DIRS 179385]	DEA3228	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-147
LL060700312251.166 [DIRS 179385]	DEA3233	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-138
LL060700312251.166 [DIRS 179385]	KE0383	PCA	ASW	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-138
LL060700312251.166 [DIRS 179385]	KE0382	PCA	ASW	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-137
LL060700312251.166 [DIRS 179385]	DEA3278	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-128
LL060700312251.166 [DIRS 179385]	JE0040	MCA	ASW	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-126
LL060700312251.166 [DIRS 179385]	JE0042	MCA	ASW	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-125
LL060700312251.166 [DIRS 179385]	DEA3281	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-121
LL060700312251.166 [DIRS 179385]	DEA3238	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-119
LL060700312251.166 [DIRS 179385]	JE0041	MCA	ASW	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-117
LL060700312251.166 [DIRS 179385]	DEA3221	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-115

Source DTN	Specimen ID	Sample Type	Material Condition	Electrolyte	Type of LC	Temperature (°C)	Calculated Pitzer pH	[Cl] molal	[NO <sub>3</sub> ] molal	NO <sub>3</sub> /Cl molal ratio	E <sub>rev</sub> (mV vs. SSC)
LL060700312251.166 [DIRS 179385]	DEA3220	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-97
LL060700312251.166 [DIRS 179385]	DEA3279	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-93
LL060700312251.166 [DIRS 179385]	DEA3222	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-88
LL060700312251.166 [DIRS 179385]	DEA3223	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-77
LL060700312251.166 [DIRS 179385]	DEA3260	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-19
LL060700312251.166 [DIRS 179385]	DEA3280	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	-8
LL060700312251.166 [DIRS 179385]	DEA3261	MCA	MA	5 M CaCl <sub>2</sub>	LC	75	4.08	11.99	0.00	0.00	42
LL060700312251.166 [DIRS 179385]	JE0037	MCA	ASW	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-189
LL060700312251.166 [DIRS 179385]	KE0701	PCA	MA	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-189
LL060700312251.166 [DIRS 179385]	KE0373	PCA	ASW	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-184
LL060700312251.166 [DIRS 179385]	DEA3216	MCA	MA	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-183
LL060700312251.166 [DIRS 179385]	DEA3376	MCA	MA	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-183
LL060700312251.166 [DIRS 179385]	JE0039	MCA	ASW	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-175
LL060700312251.166 [DIRS 179385]	KE0374	PCA	ASW	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-172
LL060700312251.166 [DIRS 179385]	KE0702	PCA	MA	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-168
LL060700312251.166 [DIRS 179385]	JE1635	MCA	ASW	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-164
LL060700312251.166 [DIRS 179385]	JE0038	MCA	ASW	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-161
LL060700312251.166 [DIRS 179385]	DEA3219	MCA	MA	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-143
LL060700312251.166 [DIRS 179385]	DEA3218	MCA	MA	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-133

Source DTN	Specimen ID	Sample Type	Material Condition	Electrolyte	Type of LC	Temperature (°C)	Calculated Pitzer pH	[Cl] molal	[NO <sub>3</sub> ] molal	NO <sub>3</sub> /Cl molal ratio	E <sub>rev</sub> (mV vs. SSC)
LL060700312251.166 [DIRS 179385]	DEA3217	MCA	MA	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-129
LL060700312251.166 [DIRS 179385]	DEA3176	MCA	MA	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-85
LL060700312251.166 [DIRS 179385]	DEA3388	MCA	MA	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-35
LL060700312251.166 [DIRS 179385]	DEA3177	MCA	MA	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-8
LL050302312251.129 [DIRS 173921]	AY007	PCA	ASW - Mockup	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-73
LL050302312251.129 [DIRS 173921]	AY008	PCA	ASW - Mockup	5 M CaCl <sub>2</sub>	LC	90	4.00	11.99	0.00	0.00	-169
LL060700312251.166 [DIRS 179385]	DEA3167	MCA	MA	5 M CaCl <sub>2</sub>	LC	105	3.95	11.99	0.00	0.00	-195
LL060700312251.166 [DIRS 179385]	DEA3168	MCA	MA	5 M CaCl <sub>2</sub>	LC	105	3.95	11.99	0.00	0.00	-185
LL060700312251.166 [DIRS 179385]	DEA3235	MCA	MA	5 M CaCl <sub>2</sub>	LC	120	3.93	11.99	0.00	0.00	-216
LL060700312251.166 [DIRS 179385]	DEA3237	MCA	MA	5 M CaCl <sub>2</sub>	LC	120	3.93	11.99	0.00	0.00	-198
LL060700312251.166 [DIRS 179385]	KE0384	PCA	ASW	5 M CaCl <sub>2</sub>	LC	120	3.93	11.99	0.00	0.00	-190
LL060700312251.166 [DIRS 179385]	KE0385	PCA	ASW	5 M CaCl <sub>2</sub>	LC	120	3.93	11.99	0.00	0.00	-186
LL060700312251.166 [DIRS 179385]	JE0036	MCA	ASW	5 M CaCl <sub>2</sub>	LC	120	3.93	11.99	0.00	0.00	-183
LL060700312251.166 [DIRS 179385]	JE0035	MCA	ASW	5 M CaCl <sub>2</sub>	LC	120	3.93	11.99	0.00	0.00	-179
LL060700312251.166 [DIRS 179385]	DEA3236	MCA	MA	5 M CaCl <sub>2</sub>	LC	120	3.93	11.99	0.00	0.00	-178
LL060700312251.166 [DIRS 179385]	DEA3234	MCA	MA	5 M CaCl <sub>2</sub>	LC	120	3.93	11.99	0.00	0.00	-164
LL060700312251.166 [DIRS 179385]	JE0034	MCA	ASW	5 M CaCl <sub>2</sub>	LC	120	3.93	11.99	0.00	0.00	-161
LL060801812251.168 [DIRS 179386]	JE3463	MCA	ASW	10 m CaCl <sub>2</sub>	LC	100	3.67	20.00	0.00	0.00	-197
LL060801812251.168 [DIRS 179386]	JE3464	MCA	ASW	10 m CaCl <sub>2</sub>	LC	100	3.67	20.00	0.00	0.00	-183

Source DTN	Specimen ID	Sample Type	Material Condition	Electrolyte	Type of LC	Temperature (°C)	Calculated Pitzer pH	[Cl] molal	[NO <sub>3</sub> ] molal	NO <sub>3</sub> /Cl molal ratio	E <sub>rev</sub> (mV vs. SSC)
LL060603812251.164 [DIRS 178269]	JE3209	MCA	ASW	1 m NaCl + 0.05 m KNO <sub>3</sub>	CC-II	60	6.45	1.00	0.05	0.05	94
LL060603812251.164 [DIRS 178269]	JE3244	MCA	ASW	1 m NaCl + 0.05 m KNO <sub>3</sub>	CC	80	6.25	1.00	0.05	0.05	25
LL060603812251.164 [DIRS 178269]	JE3227	MCA	ASW	1 m NaCl + 0.05 m KNO <sub>3</sub>	CC-II	80	6.25	1.00	0.05	0.05	-52
LL060603812251.164 [DIRS 178269]	JE3225	MCA	ASW	1 m NaCl + 0.05 m KNO <sub>3</sub>	CC	100	6.08	1.00	0.05	0.05	-118
LL060603812251.164 [DIRS 178269]	JE3236	MCA	ASW	1 m NaCl + 0.05 m KNO <sub>3</sub>	CC	100	6.08	1.00	0.05	0.05	-122
LL060603812251.164 [DIRS 178269]	KE0356	PCA	ASW	1 m NaCl + 0.05 m KNO <sub>3</sub>	CC	100	6.08	1.00	0.05	0.05	-86
LL060603812251.164 [DIRS 178269]	KE0360	PCA	ASW	1 m NaCl + 0.05 m KNO <sub>3</sub>	CC	100	6.08	1.00	0.05	0.05	-81
LL060603812251.164 [DIRS 178269]	KE0361	PCA	ASW	1 m NaCl + 0.05 m KNO <sub>3</sub>	CC	100	6.08	1.00	0.05	0.05	-64
LL060603812251.164 [DIRS 178269]	KE0627	PCA	ASW	1 m NaCl + 0.15 m KNO <sub>3</sub>	CC	80	6.25	1.00	0.15	0.15	68
LL060603812251.164 [DIRS 178269]	JE3237	MCA	ASW	1 m NaCl + 0.15 m KNO <sub>3</sub>	CC-II	100	6.08	1.00	0.15	0.15	-65
LL060603812251.164 [DIRS 178269]	JE1771	MCA	ASW	3.5 m NaCl + 0.175 m KNO <sub>3</sub>	CC-II	60	6.30	3.50	0.175	0.05	-6
LL060603812251.164 [DIRS 178269]	JE3204	MCA	ASW	3.5 m NaCl + 0.175 m KNO <sub>3</sub>	CC-II	60	6.30	3.50	0.175	0.05	-73
LL060603812251.164 [DIRS 178269]	JE3232	MCA	ASW	3.5 m NaCl + 0.175 m KNO <sub>3</sub>	CC	80	6.10	3.50	0.175	0.05	-77
LL060603812251.164 [DIRS 178269]	JE3234	MCA	ASW	3.5 m NaCl + 0.175 m KNO <sub>3</sub>	CC	80	6.10	3.50	0.175	0.05	-85
LL060603812251.164 [DIRS 178269]	JE3221	MCA	ASW	3.5 m NaCl + 0.175 m KNO <sub>3</sub>	CC	100	5.94	3.50	0.175	0.05	-132
LL060603812251.164 [DIRS 178269]	JE3239	MCA	ASW	3.5 m NaCl + 0.175 m KNO <sub>3</sub>	CC	100	5.94	3.50	0.175	0.05	-104
LL060603812251.164 [DIRS 178269]	JE1773	MCA	ASW	3.5 m NaCl + 0.525 m KNO <sub>3</sub>	CC	100	5.94	3.50	0.525	0.15	-85
LL060603812251.164 [DIRS 178269]	DEA3385	MCA	MA	3.5 m NaCl + 0.525 m KNO <sub>3</sub>	CC	100	5.94	3.50	0.525	0.15	-88
LL060603812251.164 [DIRS 178269]	DEA3390	MCA	MA	3.5 m NaCl + 0.525 m KNO <sub>3</sub>	CC	100	5.94	3.50	0.525	0.15	-3

Source DTN	Specimen ID	Sample Type	Material Condition	Electrolyte	Type of LC	Temperature (°C)	Calculated Pitzer pH	[Cl] molal	[NO <sub>3</sub> ] molal	NO <sub>3</sub> /Cl molal ratio	E <sub>rev</sub> (mV vs. SSC)
LL060603812251.164 [DIRS 178269]	JE3242	MCA	ASW	3.5 m NaCl + 0.525 m KNO <sub>3</sub>	CC-II	100	5.94	3.50	0.525	0.15	-96
LL060603812251.164 [DIRS 178269]	JE3210	MCA	ASW	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC-II	60	6.15	6.00	0.3	0.05	-18
LL060603812251.164 [DIRS 178269]	JE3313	MCA	MA	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC	80	5.96	6.00	0.3	0.05	-114
LL060603812251.164 [DIRS 178269]	JE3314	MCA	MA	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC	80	5.96	6.00	0.3	0.05	-107
LL060603812251.164 [DIRS 178269]	JE3217	MCA	ASW	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC-II	80	5.96	6.00	0.3	0.05	-95
LL060603812251.164 [DIRS 178269]	JE3228	MCA	ASW	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC-II	80	5.96	6.00	0.3	0.05	-97
LL060603812251.164 [DIRS 178269]	JE3201	MCA	ASW	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC	100	5.80	6.00	0.3	0.05	-88
LL060603812251.164 [DIRS 178269]	JE3223	MCA	ASW	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC	100	5.80	6.00	0.3	0.05	-120
LL060603812251.164 [DIRS 178269]	KE0358	PCA	ASW	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC	100	5.80	6.00	0.3	0.05	-93
LL060603812251.164 [DIRS 178269]	KE0359	PCA	ASW	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC	100	5.80	6.00	0.3	0.05	-61
LL060603812251.164 [DIRS 178269]	JE3315	MCA	MA	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC	100	5.80	6.00	0.3	0.05	-88
LL060603812251.164 [DIRS 178269]	JE3316	MCA	MA	6 m NaCl + 0.3 m KNO <sub>3</sub>	CC	100	5.80	6.00	0.3	0.05	-79
LL060603812251.164 [DIRS 178269]	JE3317	MCA	MA	6 m NaCl + 0.9 m KNO <sub>3</sub>	CC	80	5.97	6.00	0.90	0.15	-52
LL060603812251.164 [DIRS 178269]	JE3318	MCA	MA	6 m NaCl + 0.9 m KNO <sub>3</sub>	CC	80	5.97	6.00	0.90	0.15	-27
LL060603812251.164 [DIRS 178269]	JE3203	MCA	ASW	6 m NaCl + 0.9 m KNO <sub>3</sub>	CC-II	80	5.97	6.00	0.90	0.15	26
LL060603812251.164 [DIRS 178269]	JE3319	MCA	MA	6 m NaCl + 0.9 m KNO <sub>3</sub>	CC	100	5.81	6.00	0.90	0.15	-85
LL060603812251.164 [DIRS 178269]	JE3320	MCA	MA	6 m NaCl + 0.9 m KNO <sub>3</sub>	CC	100	5.81	6.00	0.90	0.15	-89
LL060603812251.164 [DIRS 178269]	JE3215	MCA	ASW	6 m NaCl + 0.9 m KNO <sub>3</sub>	CC-II	100	5.81	6.00	0.90	0.15	-85
LL060603812251.164 [DIRS 178269]	JE3240	MCA	ASW	6 m NaCl + 0.9 m KNO <sub>3</sub>	CC-II	100	5.81	6.00	0.90	0.15	-39

Source DTN	Specimen ID	Sample Type	Material Condition	Electrolyte	Type of LC	Temperature (°C)	Calculated Pitzer pH	[Cl] molal	[NO <sub>3</sub> ] molal	NO <sub>3</sub> /Cl molal ratio	E <sub>rev</sub> (mV vs. SSC)
LL050302312251.129 [DIRS 173921]	AY005	PCA	ASW - Mockup	6 m NaCl + 0.9 m KNO <sub>3</sub>	CC	100	5.81	6.00	0.90	0.15	-75
LL050302312251.129 [DIRS 173921]	AY006	PCA	ASW - Mockup	6 m NaCl + 0.9 m KNO <sub>3</sub>	CC	100	5.81	6.00	0.90	0.15	-74
LL060801812251.168 [DIRS 179386]	JE3284	MCA	ASW	10 m CaCl <sub>2</sub> + 0.5 m Ca(NO <sub>3</sub> ) <sub>2</sub>	LC	100	3.89	20.00	1.00	0.05	-41
LL060801812251.168 [DIRS 179386]	JE3270	MCA	ASW	10 m CaCl <sub>2</sub> + 0.5 m Ca(NO <sub>3</sub> ) <sub>2</sub>	LC	100	3.89	20.00	1.00	0.05	-39
LL060801812251.168 [DIRS 179386]	JE3285	MCA	ASW	10 m CaCl <sub>2</sub> + 1.5 m Ca(NO <sub>3</sub> ) <sub>2</sub>	LC	100	4.38	20.00	3.00	0.15	18
LL060801812251.168 [DIRS 179386]	KE0369	PCA	ASW	10 m CaCl <sub>2</sub> + 5 m Ca(NO <sub>3</sub> ) <sub>2</sub>	LC	100	5.39	20.00	10.00	0.50	76
LL060801812251.168 [DIRS 179386]	KE0371	PCA	ASW	10 m CaCl <sub>2</sub> + 5 m Ca(NO <sub>3</sub> ) <sub>2</sub>	LC	100	5.39	20.00	10.00	0.50	83
LL060801812251.168 [DIRS 179386]	KE0370	PCA	ASW	10 m CaCl <sub>2</sub> + 5 m Ca(NO <sub>3</sub> ) <sub>2</sub>	LC	100	5.39	20.00	10.00	0.50	87
LL060801812251.168 [DIRS 179386]	JE3286	MCA	ASW	10 m CaCl <sub>2</sub> + 5 m Ca(NO <sub>3</sub> ) <sub>2</sub>	LC	100	5.39	20.00	10.00	0.50	105
LL060801812251.168 [DIRS 179386]	KE0372	PCA	ASW	10 m CaCl <sub>2</sub> + 5 m Ca(NO <sub>3</sub> ) <sub>2</sub>	LC	100	5.39	20.00	10.00	0.50	179

Sources: Calculated Pitzer pH and chloride and nitrate ion concentration values are from DTN: LL060904312251.186 [DIRS 178283], file: *NoCO2GetEQData.xls*  
 All other columns are from DTN: LL040902712251.119 [DIRS 173720], file: *Reduced Data Ahmet Yilmaz WBL 11Feb05.xls*,  
 DTN: LL050302312251.129 [DIRS 173921], file: *Mockup Developed RBR 21May05.xls*,  
 DTN: LL060603812251.164 [DIRS 178269], file: *Rep Pot N06022 vs Temp NaCl + KNO3 60-100C RBR 07Aug06.xls*,  
 DTN: LL060700312251.166 [DIRS 179385], file: *Rep Pot N06022 vs Temp 5M CaCl2 RBR 19Dec06.xls*,  
 DTN: LL060801812251.168 [DIRS 179386], file: *Rep Pot N06022 High Temp High NO3 RBR.xls*, and  
 DTN: LL060803712251.170 [DIRS 179387], file: *Rep Pot N06022 vs Temp NaCl RBR 07Oct06.xls* as noted in column 1.

NOTES: 1. Samples W6, B3, and P5 were verified to have crevice corrosion in DTN: LL040902712251.119 [DIRS 173720] file: *05606 Rebak.pdf*.  
 2. DTN: LL050302312251.129 [DIRS 173921], file: *Mockup Developed RBR 21May05.xls*, indicates that specimens were prepared from mockup containers using hockey pucks removed from the longitudinal weld. Therefore, specimens AY005, AY006, AY007, AY008, AY009, and AY010 are as-welded.  
 ASW = as-welded, CC = crevice corrosion, LC = localized corrosion, MA = mill-annealed, MCA = multiple crevice assembly, PCA = prism crevice assembly.

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