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NM5507

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

1. QA: __QA__

Page: 1 of: 21

2.	X	Analysis	Check all that apply

Type of Analysis		Engineering
	X	Performance Assessment
		Scientific

Intended Use of Analysis		Input to Calculation
		Input to another Analysis or Model
	X	Input to Technical Document
	X	Input to other Technical Products

Describe use:

The results of this AMR serve as inputs to the Waste Package Degradation AMR analyses of localized corrosion of the 316NG waste package inner barrier.

3.	X	Model	Check all that apply

Type of Model		Conceptual Model	X	Abstraction Model
		Mathematical Model		System Model
		Process Model		

Intended Use of Model		Input to Calculation
		Input to another Model or Analysis
	X	Input to Technical Document
	X	Input to other Technical Products

Describe use:

The results of this AMR serve as inputs to the Waste Package Degradation AMR models of localized corrosion of the 316NG waste package inner barrier.

4. Title:

Abstraction of Models for Stainless Steel Structural Material Degradation

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

ANL-EBS-PA-000005 REV 00

6. Total Attachments:

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7. Attachment Numbers - No. of Pages in Each:

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9.	Checker	Jan Bostelman	*Robert MacKinnon for JB*	4/18/2000
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DTN: LL000201505924.122, LL991210605924.107, LL000320405924.146 used as input data.

DTN: MO0004SPASMA05.004 applies to output data.

For TSPA-SR

This document may contain citations to draft documents currently in development and all cited reference information will be completed and approved before completion and approval of this document.

Per Section 5.5.6 of AP-3.10Q, the responsible manager has determined that the subject AMR is not subject to AP-2.14Q review because the analysis does not affect a discipline or area other than the originating organization (Performance Assessment). The upstream supplier of inputs for this AMR (Joe Farmer, Waste Package Dept.) has worked closely with the originator of this AMR to ensure that inputs were used properly. The downstream user of the information resulting from this AMR is the Performance Assessment (PA) Dept., which is also the originating organization of this work. PA has made the decision to not take credit for the stainless steel inner barrier in the TSPA-SR. This approach is bounding and acceptable to the Waste Package Dept. Thus, the subject AMR does not provide direct input to the TSPA-SR and only provides a technical basis for better understanding the performance of the stainless-steel inner barrier. Therefore, no formal AP-2.14Q reviews were requested or determined to be necessary.

-3.10Q.4

Rev. 06/30/1999

Enclosure 15

2. Analysis or Model Title:	
Abstraction of Models for Stainless Steel Structural Material Degradation	
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4. Revision/Change No.	5. Description of Revision/Change
00	Initial Issue

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ACRONYMS

AMR	Analyses and Models Report
ASTM	American Society for Testing and Materials
CDF	Cumulative Distribution Function
CRWMS	Civilian Radioactive Waste Management System
DOE	Department of Energy
DTN	Data Tracking Number
EBS	Engineered Barrier System
HLW	High Level Waste
IRSR	Issue Resolution Status Report
KTI	Key Technical Issue
LA	License Application
MIC	Microbial-Induced Corrosion
MGR	Managed Geologic Repository
M&O	Management and Operating Contractor
NRC	Nuclear Regulatory Commission
PAO	Performance Assessment Operations
SAW	Simulated Acidified Water
SCC	Stress Corrosion Cracking
SCW	Simulated Concentrated Water
SNF	Spent Nuclear Fuel
SSW	Simulated Saturated Water
WP	Waste Package

1. PURPOSE

This analyses and models report (AMR) was conducted in response to written work direction (CRWMS M&O 1999a). The purpose and scope of this AMR is to review and analyze upstream process-level models (CRWMS M&O 2000) and information relevant to pitting and crevice corrosion degradation of waste package inner barrier (316NG) material, and to develop abstractions of the important processes in a form that is suitable for input to the WAPDEG analysis for long-term degradation of waste package inner barrier in the proposed repository. The abstracted models documented in this technical product are potentially important to the evaluation of principle factors for the post-closure safety case, particularly those related to performance of the waste package inner barrier. This analysis is limited to the use of 316NG as the material composing the waste package inner barrier. This analysis supports Performance Assessment Department (PAD) and its Engineered Barrier Performance Section in modeling waste package degradation.

2. QUALITY ASSURANCE

This analysis was prepared in accordance with the Civilian Radioactive Waste Management system (CRWMS) Management and Operating Contractor (M&O) Quality Assurance (QA) program. The information provided in this analysis will be used for evaluating the post-closure performance of the Monitored Geologic Repository (MGR) waste package and engineered barrier segment. The Performance Assessment Operations (PAO) responsible manager has evaluated the technical document development activity in accordance with QAP-2-0, *Conduct of Activities*. The QAP-2-0 activity evaluation (CRWMS M&O 1999b) has determined that the preparation and review of this technical document is subject to *Quality Assurance Requirements and Description* (DOE 2000) requirements. In accordance with AP-2.13Q, *Technical Product Development Plan*, a work plan was developed, issued, and utilized in the preparation of this document (CRWMS M&O 1999a). The documentation of this analysis is in accordance with the guidance given in AP-3.1Q, *Conduct of Performance Assessment*, and the directions found in AP-3.10Q, *Analyses and Models*. There is no determination of importance evaluation developed in accordance with NLP-2-0, *Determination of Importance Evaluations*, since the analysis does not involve any field activity.

3. COMPUTER SOFTWARE AND MODEL USAGE

3.1 COMPUTER SOFTWARE

A software routine, BBreg Version 1.0, is implemented in Mathcad 2000 Professional (see Attachment I for documentation and verification that the software routine provides correct results over the range of input parameters considered in this AMR). Mathcad 2000 Professional is commercially available software. This software is appropriate for this application as it offers all of the mathematical and graphical functionality necessary to perform and document the numerical manipulations used in this AMR. Mathcad 2000 Professional was executed on a DELL PowerEdge 2200 Workstation equipped with two Pentium II 266 MHz processors (CRWMS M&O tag 112371) in the Windows NT 4.0 operating system. Details of the Mathcad

2000 Professional numerical manipulations performed in support of this AMR are discussed throughout this analysis and included in Attachment I.

3.2 MODELS USED

One pre-existing model is referenced in this AMR. The conceptual model for general and localized corrosion initiation and propagation for the 316NG stainless steel waste package inner barrier is documented in the AMR on degradation of stainless steel (CRWMS M&O 2000, Section 6.11). The rate model for general and localized corrosion propagation is also referenced (CRWMS M&O 2000, Table 11 and Figure 12).

4. INPUTS

4.1 DATA AND PARAMETERS

Corrosion and critical electrochemical potential measurement data for 316L (analog for 316NG (see Assumption 5.1)) stainless steel were obtained (Table 2) at solution temperatures ranging from 30 to 120°C, chloride ion concentrations between 67 and 154,000 mg/L, and pH values between 2.7 and 10.2 (Table 3). This data is appropriate for its intended use as it was developed specifically for this use and potentially represents the range of expected waste package chemical exposure conditions in the proposed repository. The solution compositions are abbreviated as SCW (Simulated Concentrated Water), SAW (Simulated Acidified Water), and SSW (Simulated Saturated Water). Table 1 summarizes these data, data tracking numbers (DTNs), and Table numbers.

Table 1. Data and Parameters and Their Sources

Parameter	DTN	Table in this Document
Electrochemical potential measurements of 316L	LL000201505924.122 S00116_001	Table 2
SCW, SAW, and SSW Cl⁻ concentration and pH	LL000320405924.146	Table 3
Coefficients in expressions representing CDFs of 316L corrosion rates.	LL991210605924.107 S00114_001	Table 4

In Table 2, *Ecrit* is given by "Threshold Potential 1" (see CRWMS M&O 2000, Table 4 and Section 6.4.2 for explanation of potential nomenclature) for data collected in SCW and SSW solutions. For data collected in SAW solutions, *Ecrit* is given by "Repassivation Potential 3" (see Assumption 5.2). The last data row (in boldface) was not used in this analysis as it is clearly an outlier (see Assumption 5.3)

Table 2. Electrochemical Potential Measurements (DTN: LL000201505924.122) of 316L Stainless Steel in Solutions of Various Composition (see Table 3 in this AMR).

Solution	T (°C)	Ecorr (mV Ag/AgCl)	Ecrit (mV Ag/AgCl)
SCW	30	-181	422
SCW	60	-185	283
SCW	90	-263	135
SCW	60	-243	298
SCW	90	-294	179
SCW	30	-76	422
SCW	60	-260	263
SCW	90	-239	194
SAW	60	-267	1030
SAW	60	-363	1100
SAW	30	-227	1140
SAW	60	-286	1030
SAW	60	-294	1020
SAW	90	-353	304
SSW	100	-269	-123
SSW	120	-175	266
SSW	100	-295	-83
SSW	120	-208	-80
SSW	100	-259	-56
SSW	**100**	**-233**	**749**

The "target compositions" of the aqueous solutions used for corrosion testing are presented in Table 3. According to the discussion accompanying Table 1 in DTN: LL000320405924.146, actual compositions may vary significantly because of other experimental factors and pH values are estimates and will vary depending on other experimental conditions. For this reason, the solution compositions are referred to as "target compositions."

Table 3. Target Compositions of Solutions in which Corrosion Potential Measurements of 316L were made (DTN: LL000320405924.146).

Solution	T (°C)	Cl⁻ mg/L	pH
SCW	60, 90	6700	9.8 – 10.2
SAW	60, 90	24250	2.7
SSW	100	128000	5.5 – 7
SSW	120	154000	5.5 – 7

Note: These data have changed relative to previous revisions of this document due to changes in source data.

In the AMR (CRWMS M&O 2000) on degradation of stainless steel, various corrosion rate data were used to create a cumulative distribution functions (CDFs) of general and localized corrosion rates. These CDFs were presented as cumulative probability (in percent) as linear functions of the base 10 logarithm of general corrosion rate (μm/year), i.e.

$$CDF = b_o + b_1 \cdot \log(Rate) \qquad \text{(Eq. 1)}$$

One should note that Equation 1 has the form of a log-uniform distribution. In Table 4, the values of the coefficients b_o and b_1 for the various possible corrosion environments and modes are reproduced from Table 11 of the AMR on degradation of stainless steel (CRWMS M&O 2000).

Table 4. Coefficients in Expressions Representing CDFs of Corrosion Rates of 316NG Stainless Steel in "Atmospheric" and "Aqueous Phase" Environments (DTN: LL991210605924.107) (CRWMS M&O 2000, Table 11).

Environment	Mode	b_0	b_1
Atmospheric	General	259.11	108.29
Aqueous Phase	General	38.91	36.85
Aqueous Phase	Localized	-184.2	71.564

4.2 CRITERIA

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

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

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

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

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

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

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

Of these sub-issues, only sub-issues (1) and (2) are relevant to this analysis.

4.2.1 Acceptance Criteria Applicable To All Six Sub-Issues

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

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

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

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

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

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

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

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

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

4.2.2 Acceptance Criteria For Sub-Issue 1

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

(2)   The DOE shall identify the broad range of environmental conditions within the WP emplacement drifts that may promote the corrosion processes listed previously, taking

into account the possibility of irregular wet and dry cycles that may enhance the rate of container degradation (NRC 1999, Section 4.1.1).

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

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

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

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

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

4.2.3   Acceptance Criteria for Sub-Issue 2

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

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

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

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

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

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

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

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

4.3   CODES AND STANDARDS

The acceptance criteria listed above are consistent with the methodology described in the ASTM Standard Practice C-1174 for prediction of the long-term behavior of EBS components in a geologic repository (ASTM 1997).

5.   ASSUMPTIONS

None of the following assumptions require confirmation prior to the use of the parameters developed in this document.

5.1   Stainless steel 316L (for which alloy the experimental data was collected) is assumed to be an adequate analog for 316NG. This assumption is based on an identical assumption in the AMR on degradation of stainless steel from which the experimental data was obtained (CRWMS M&O 2000, Section 5.4). This assumption is used throughout this analysis. As most of the experimental data was collected for 316L stainless steel, "316L" shall be used throughout this analysis to refer to the experimental data, and "316NG" will be used to refer to the waste package inner barrier material localized corrosion initiation criteria and localized corrosion rates.

5.2   *Ecrit*, the critical potential for localized corrosion initiation, is given by "Threshold Potential 1" (see CRWMS M&O 2000, Table 3 and Section 6.4.2 for explanation of potential nomenclature) for data collected in SCW and SSW solutions, and by "Repassivation Potential 3" for data collected in SAW solutions. This assumption is based on the discussion and recommendations presented in the AMR on stainless steel

degradation (CRWMS M&O 2000, Section 6.4.2 and Table 4). This assumption is used throughout this analysis, but is most relevant to the calculations performed in Attachment I.

5.3 The last experimentally observed data point in Table 2 (in boldface, obtained from an SSW solution with $Ecorr = -233$ mV and $Ecrit = 749$ mV Ag/AgCl) was not part of the data set used in Attachment I to derive the 316NG localized corrosion initiation criteria. This data point was considered an outlier. The basis for this assumption is that this data point is an outlier as ($\Delta E = Ecrit - Ecorr$) for this data point is 982 mV, a value almost 4 times that for any other data point obtained in the same solution. This assumption is used in Attachment I in specifying the input data to the fitting procedure (the Dat matrix) (Attachment I, page I-2).

5.4 It is assumed that the difference in potential (ΔE) between $Ecrit$ and $Ecorr$ (the corrosion potential) can be modeled to vary linearly with temperature (in Kelvin), the logarithm in base 10 of the chloride concentration (in mol/L), and the pH of the solution in which the potentials were measured. An infinite number of other assumed functional forms are possible. The linear functional form was chosen because it was the simplest functional form that reflected the possibly important functional dependencies of the potential data. This assumption is based (in part) on assumptions used in the Analysis Model Report (AMR) on degradation of stainless steel (CRWMS M&O 2000, Section 6.4.3) where $Ecrit$ and $Ecorr$ are represented by regression equations based on the exposure temperature. Linear dependence of the potential difference on the logarithm in base 10 of the chloride concentration and solution pH is assumed based on the assumed temperature dependence. This assumption was used throughout Attachment I.

5.5 The error terms and model coefficients (the b_i's) for all regression models derived in Attachment I are assumed to be normally distributed. The basis for this assumption is the Central Limit Theorem (Steidinger, et. al., 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 not unreasonable 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. This assumption is used in Attachment I on page I-3 in formulating the EE(T, logCl, pH, z) function.

5.6 Chloride ion concentrations and pH values are supplied in Table 3 for SCW and SAW solutions at 60 and 90°C. $Ecrit$ and $Ecorr$ values are supplied at 30, 60, and 90°C in Table 2. It is assumed that the chloride ion concentrations and pH values at 60 and 90°C are appropriate for use at 30°C as well. The basis of this assumption is that it is reasonable and is expected to have little impact on the analysis results. This assumption is used throughout Attachment I.

5.7 The pH values of SCW, and SSW solutions are provided as ranges in Table 3. It is assumed that the median value of each pH value range is representative of the solution pH value. The basis of this assumption is that it is reasonable and is expected to have little impact on the analysis results. This assumption is used throughout Attachment I.

6. ANALYSIS/MODEL

6.1 CONCEPTUAL MODEL

The conceptual model for general and localized corrosion initiation and propagation for the 316NG stainless steel waste package inner barrier is documented in the Analysis Model Report (AMR) on degradation of stainless steel (CRWMS M&O 2000, Section 6.11). In summary, any corrosion degradation of the waste package inner barrier requires penetration of the waste package outer barrier. In the absence of dripping water, the 316NG stainless steel waste package inner barrier can only undergo general corrosion. The rate of the general corrosion is given by the general corrosion rate distribution in an "atmospheric" environment presented in Table 12 of the AMR on degradation of stainless steel (CRWMS M&O 2000). If aqueous phase corrosion can occur (only under dripping water conditions), the corrosion and critical potentials are used to determine whether the mode of attack is general corrosion only or general and localized corrosion together, i.e., only if the corrosion potential ($Ecorr$) exceeds the critical potential for localized corrosion initiation ($Ecrit$) can localized corrosion initiate. The distribution of "aqueous phase" general and localized corrosion rates presented in Table 12 of the AMR on degradation of stainless steel (CRWMS M&O 2000) will be used for the rate of general and localized corrosion of the 316NG stainless steel waste package inner barrier.

6.2 GENERAL CORROSION OF 316L

Corrosion degradation of the waste package inner barrier initiates upon penetration of the waste package outer barrier. In the absence of dripping water, the waste package inner barrier can only undergo general corrosion under "atmospheric" conditions. The rate of general corrosion under "atmospheric" conditions is given by a cumulative distribution function (CDF) represented by the functional form in Equation 1 with coefficients defined in Table 4.

$$CDF = 259.11 + 108.29 \cdot \log(Rate) \tag{Eq. 2}$$

The value of CDF in Equation 2 is equal to zero when Rate is equal to 4.05×10^{-6} mm/year and is equal to 100 when Rate is 3.39×10^{-5} mm/year. Note that $Rate$ in Equation 2 is in μm.

In the presence of dripping water, the waste package inner barrier can undergo general corrosion and potentially localized corrosion. The rate of general corrosion under "aqueous" conditions is given by a cumulative distribution function (CDF) represented by the functional form in Equation 1 with coefficients defined in Table 4.

$$CDF = 38.91 + 36.85 \cdot \log(Rate) \tag{Eq. 3}$$

The value of CDF in Equation 3 is equal to zero when $Rate$ is equal to 8.79×10^{-5} mm/year and is equal to 100 when $Rate$ is 4.55×10^{-2} mm/year. Note that $Rate$ in Equation 3 is in μm.

6.3 POTENTIAL DIFFERENCE-BASED LOCALIZED CORROSION INITIATION MODEL FOR 316NG STAINLESS STEEL

6.3.1 316NG Localized Corrosion Initiation Model Formulation

The data presented in Table 2 for 316L stainless steel was used to fit a function of absolute temperature, T, the base 10 logarithm of the chloride ion concentration, and solution pH to the potential difference (ΔE) between the critical potential for localized corrosion initiation, $Ecrit$, and the corrosion potential, $Ecorr$, i.e.,

$$\Delta E = b_0 + b_1 \cdot T + b_2 \cdot log(\ Cl^- \ ) + b_3 \cdot pH + \varepsilon \qquad \text{(Eq. 4)}$$

where b_0, b_1, b_2, and b_3 are constants determined from fitting to Equation 4 to the collected potential difference data (Table 2). The derivation of this regression equation is documented in detail in Attachment I. As discussed in Assumption 5.3, the last experimentally observed data point in Table 2 was not part of the data set used as it was considered to be an outlier. ε (referred to as the "error" variance or "residual" variance) is a term representing data variance not explained by the fitting procedure and has a normal distribution with a mean of zero (see Assumption 5.5). Linear regression gives the following estimates for the parameters in Equation 4: $b_0 = 2910$, $b_1 = -4.16$, $b_2 = -439$, and $b_3 = -133$. The covariance matrix, s, and correlation matrix, C, resulting from the fitting procedure was determined to be:

$$s = \begin{bmatrix} 471{,}000 & -1400 & 60{,}700 & 4{,}330 \\ -1400 & 4.24 & -193 & -17.0 \\ 60{,}700 & -193 & 15{,}900 & 1{,}410 \\ 4{,}330 & -17.0 & 1{,}410 & 275 \end{bmatrix} \quad C = \begin{bmatrix} 1.000 & -0.990 & 0.701 & 0.381 \\ -0.990 & 1.000 & -0.742 & -0.496 \\ 0.701 & -0.742 & 1.000 & 0.674 \\ 0.381 & -0.496 & 0.674 & 1.000 \end{bmatrix} \text{(Eq. 5)}$$

and the variance of ε determined from the linear regression fitting procedure is $27{,}600$.

As outlined in Section 6.1, localized corrosion can initiate when $Ecorr$ exceeds $Ecrit$. This is equivalent to the condition that the potential difference, $\Delta E = (Ecrit - Ecorr)$, is less than zero.

Figure 1 shows a plot of how the median potential difference (the top-most red-colored plane) varies with pH and absolute temperature at a chloride ion concentration of 3 mol/L. Also shown in Figure 1 is the -4σ confidence interval surface (the bottom-most blue-colored plane) and a zero plane (the semi-transparent gridded plane). Note that the -4σ confidence interval surface incorporates contributions from the median potential difference, the covariance of the regression coefficients, and the error variance term (see the EE function used in Attachment I, p. I-3).
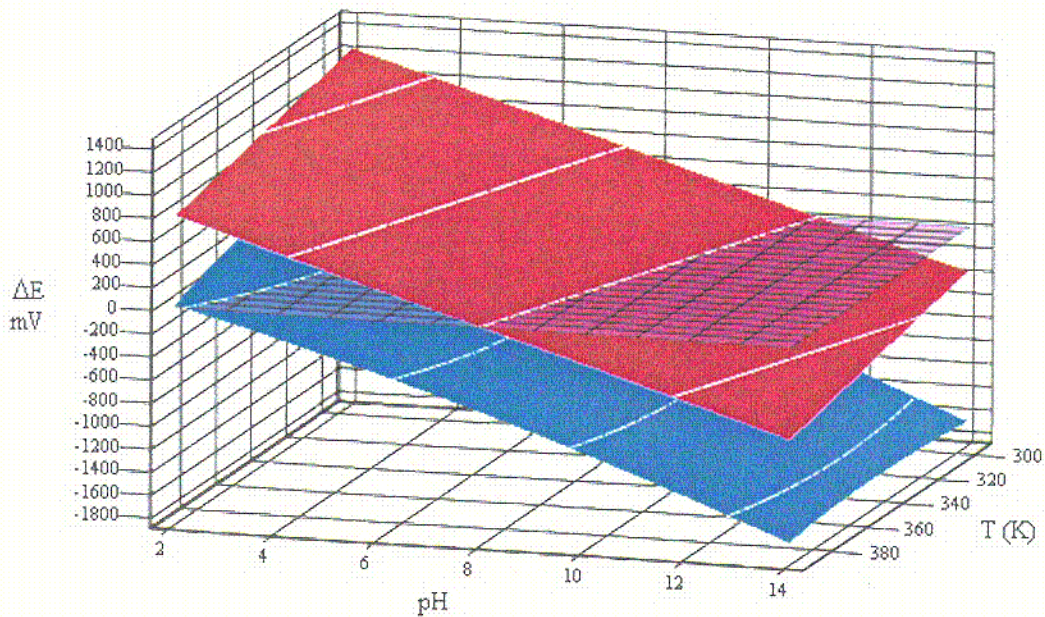
Figure 1.   Plot of the median ΔE and -4• confidence interval surfaces vs. pH and absolute temperature for 316NG stainless steel from Equation 4 using a chloride ion concentration of 3 mol/L

Figure 2 shows a plot of how the median potential difference (the top-most plane) varies with pH and base 10 logarithm of chloride ion concentration at an absolute temperature of 380 K. Also shown in Figure 2 is the -4• confidence interval surface (the bottom-most plane) and a zero plane (the semi-transparent gridded plane).
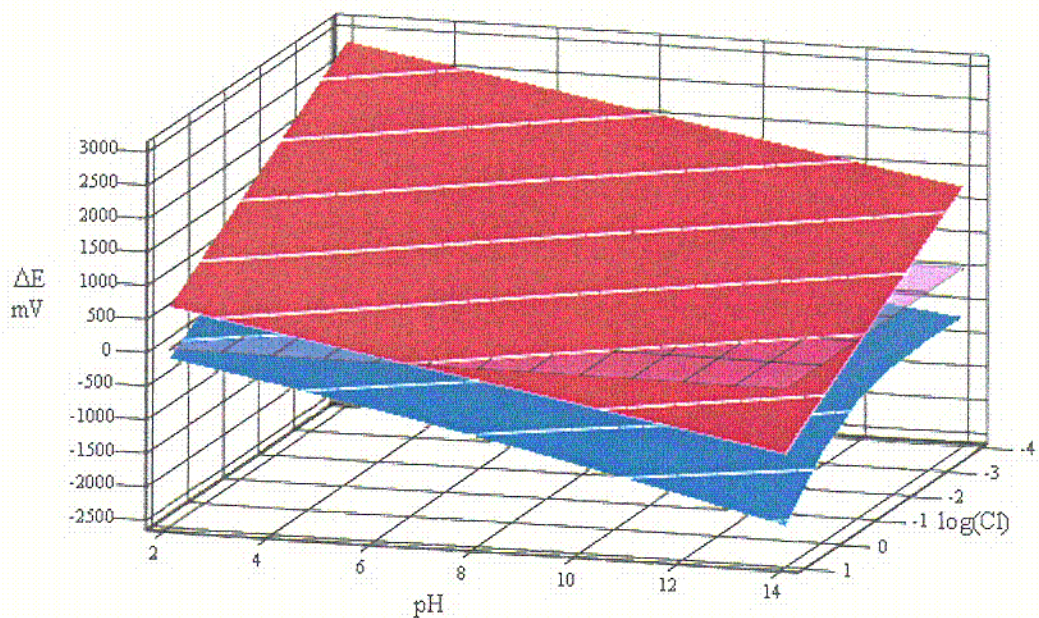

Figure 2.   Plot of the median ΔE and -4• confidence interval surfaces vs. pH and base 10 logarithm of chloride ion concentration for 316NG stainless steel using an absolute temperature of 380 K

C-1

ΔE median values decrease as pH, chloride concentration, and absolute temperature increases. It is concluded from Figure 1 and Figure 2 that localized corrosion initiation is probable at neutral pHs, temperatures below 380 K, and chloride concentrations in the range of 10^{-4} to 10 mol/L.

In Attachment I (p. I-3), "R Squared" for the regression equation (Equation 4) developed in Attachment I is determined to be 0.892. The closer R Squared is to unity, the more precisely the regression equation represents the data it was developed from. Since 0.892 is close to 1.0, it is concluded that the regression equation is a precise representation of the data from which it was developed. Accuracy refers to how well the data (and hence the regression equation developed from it) represents the actual process under consideration. The analyses presented in this document can in no way address this issue. Application of the regression equation developed in this analysis to exposure conditions that lie outside of those in which the data was collected is subject to uncertainty. Quantification of uncertainty is provided by the values of the covariance matrix, s (Equation 5), and the error variance, ε.

6.3.2 316NG Localized Corrosion Initiation Model Validation

The model validation criteria used in this section are based on comparison of the model results to experimental data to gain an appropriate level of confidence in the model. By far the strongest argument for the validity of the 316NG Localized Corrosion Initiation Model is the fact that it is based on fitting a surface (through linear regression techniques) to the experimental data presented in Table 2. The potential difference in Equation 4 is a function of absolute temperature, the base 10 logarithm of the chloride ion concentration, and solution pH. The method used to conduct the model validation is to demonstrate that the experimentally measured ΔE values are contained within the $\pm 4\sigma$ confidence intervals of the model. As shown in Table 5, the experimentally measured ΔE values are contained within the $\pm 4\sigma$ confidence intervals of the model, therefore, predictions based on this model are valid.

6.4 LOCALIZED CORROSION RATE OF 316NG

In the presence of dripping water, the waste package inner barrier can under go general corrosion and potentially localized corrosion. The rate of localized corrosion under "aqueous" conditions is given by a cumulative distribution function (CDF) represented by the functional form in Equation 1 with coefficients defined in Table 4.

$$CDF = -184.2 + 71.564 \cdot \log(Rate) \qquad \text{(Eq. 6)}$$

The value of CDF in Equation 6 is equal to zero when Rate is equal to 0.375 mm/year and is equal to 100 when Rate is 9.36 mm/year. Note that Rate in Equation 6 is in μm.

Table 5. Comparison of ΔE measured experimentally with the $\pm 4\sigma$ confidence intervals of the model.

Solution	T (°C)	ΔE Experimental (mV)	ΔE Model – 4σ (mV)	ΔE Model – 4σ (mV)
SCW	30	6.03e2	-1.27e2	1.39e3
SCW	60	4.68e2	-1.99e2	1.21e3
SCW	90	3.98e2	-3.56e2	1.12e3
SCW	60	5.41e2	-1.99e2	1.21e3
SCW	90	4.73e2	-3.56e2	1.12e3
SCW	30	4.98e2	-1.27e2	1.39e3
SCW	60	5.23e2	-1.99e2	1.21e3
SCW	90	4.33e2	-3.56e2	1.12e3
SAW	60	1.30e3	5.16e2	1.95e3
SAW	60	1.46e3	5.16e2	1.95e3
SAW	30	1.37e3	6.00e2	2.12e3
SAW	60	1.32e3	5.16e2	1.95e3
SAW	60	1.31e3	5.16e2	1.95e3
SAW	90	6.57e2	3.49e2	1.87e3
SSW	100	1.46e2	-4.49e2	1.00e3
SSW	120	4.41e2	-5.79e2	8.97e2
SSW	100	2.12e2	-4.49e2	1.00e3
SSW	120	1.28e2	-5.79e2	8.97e2
SSW	100	2.03e2	-4.49e2	1.00e3

7. CONCLUSIONS

7.1 GENERAL ANALYSIS CONCLUSIONS

In this document, general and localized corrosion of the waste package inner barrier (316NG) is analyzed. References were provided to other documents in which the TSPA-SR conceptual model for general and localized corrosion initiation and propagation is documented. Potential-based localized corrosion initiation threshold functions for 316NG stainless steel (based on data collected for 316L stainless steel (analog for 316NG, see Assumption 5.1)) were derived from the functional dependence of experimentally obtained electrochemical potential data on absolute temperature, pH, and the base 10 logarithm of chloride ion concentration. It was concluded that localized corrosion initiation is probable at neutral pHs, temperatures below 380 K, and chloride concentrations in the range of 10^{-4} to 10 mol/L. Any user of the 316NG Localized Corrosion Initiation Model should bear in mind that the model is based on measurements performed at solution temperatures ranging from 30 to 120°C, chloride ion concentrations between 67 and 154,000 mg/L, and pH values between 2.7 and 10.2 (Table 3). Extrapolation outside these ranges is subject to greater uncertainty. General corrosion rate distributions for 316NG stainless steel were analyzed and were found to be log-uniformly distributed with lower and upper bounds of 4.05×10^{-6} mm/year and 3.39×10^{-5} mm/year, respectively, under "atmospheric" conditions and

8.79x10^{-5} mm/year and 4.55x10^{-2} mm/year, respectively, under "aqueous" conditions. Localized corrosion rates distributions for 316NG stainless steel were analyzed and were found to be log-uniformly distributed with lower and upper bounds of 0.375 mm/year and 9.36 mm/year, respectively, under "aqueous" conditions.

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

The results of this analysis are based on data inputs tracked by DTNs: LL000201505924.122, LL991210605924.107, LL000320405924.146. DTN: LL991210605924.107 is unqualified, is tracked as Technical Product Output, and its status will be updated upon revision of the technical product that produced it (CRWMS M&O 2000). The results of this analysis are tracked by DTN: MO0004SPASMA05.004.

7.2 EVALUATION OF NRC IRSR CRITERIA

As this documentation contains only analysis of abstractions of process-level models, not all of the criteria spelled out in section 4.2 can be evaluated nor do they apply at this time.

For Section 4.2.1 (Acceptance Criteria Applicable To All Six Sub-Issues), criteria 2, 4, 7, 8, and 9 do not apply to this analysis. Criteria 1, 3, 5, and 6 were addressed in this analysis. Criteria 3 also requires further evaluation.

For Section 4.2.2 (Acceptance Criteria For Sub-Issue 1), criteria 2, 4, 5, and 7 do not apply to this analysis. Criteria 1, 3, and 6 were addressed in this analysis. Criteria 1, 3, and 6 require further evaluation.

For Section 4.2.3 (Acceptance Criteria for Sub-Issue 2), criteria 1, 4, 5, 6, and 8 do not apply to this analysis. Criteria 2, 3, and 7 require further evaluation.

8. INPUTS AND REFERENCES

8.1 DOCUMENTS CITED

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8.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER

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LL000320405924.146. Target Compositions Of Aqueous Solutions Used For Corrosion Testing. Submittal date: 03/22/2000.

LL991210605924.107. Degradation of Stainless Steel Structural Support For Waste Package. Submittal date: 01/11/2000.

9. ATTACHMENTS

Attachment	Title
I	316NG Stainless Steel Corrosion

Attachment I - 316NG Stainless Steel Corrosion

Software Routine: BBreg Version 1.0

In this attachment, the localized corrosion initiation criteria for 316NG stainless steel is derived. Electrochemical polarization data (see Section 4.1, Table 2) for 316L (analog for 316NG) stainless steel were used to fit a function of absolute temperature, T, the base 10 logarithm of the chloride ion concentration, and solution pH to the potential difference (ΔE) between the critical potential for localized corrosion initiation, *Ecrit*, and the corrosion potential, *Ecorr*.

Multiple regression function:

$$BBreg(rX, rY) := \begin{vmatrix} invrXX \leftarrow \left(rX^T \cdot rX\right)^{-1} \\[6pt] rb \leftarrow invrXX \cdot rX^T \cdot rY \\[6pt] r\sigma\epsilon2 \leftarrow \left| \dfrac{\left(rY^T \cdot rY - rb^T \cdot rX^T \cdot rY\right)}{(length(rY) - cols(rX))} \right| \\[6pt] r\Sigma \leftarrow r\sigma\epsilon2 \cdot invrXX \\[6pt] len \leftarrow length(rY) - 1 \\[6pt] SStot \leftarrow \displaystyle\sum_{i=0}^{len} \left(rY_i - mean(rY)\right)^2 \\[6pt] SSres \leftarrow \displaystyle\sum_{i=0}^{len} \left[rY_i - (rX \cdot rb)_i\right]^2 \\[6pt] SSreg \leftarrow \displaystyle\sum_{i=0}^{len} \left[(rX \cdot rb)_i - mean(rY)\right]^2 \\[6pt] Rsq \leftarrow \dfrac{SSreg}{SStot} \\[6pt] SS \leftarrow \left(r\sigma\epsilon2 \quad Rsq \quad SStot \quad SSres \quad SSreg\right) \\[6pt] \left(rb \quad r\Sigma \quad SS^T\right) \end{vmatrix}$$

- Regression coefficients (rb_i)

- Residual or error variance ($r\sigma\epsilon2$)

- Covariance matrix ($r\Sigma$)

- Sum of Squares total

- Sum of Squares residual

- Sum of Squares regression

- R Squared

- This function is used to fill a matrix, M, with r rows and c columns with a constant value, v. Note that matrix indices begin at zero and not one.

$$cmatrix(r, c, v) := \begin{vmatrix} \text{for } i \in 0 .. r - 1 \\ \quad \text{for } j \in 0 .. c - 1 \\ \qquad M_{i,j} \leftarrow v \\ M \end{vmatrix}$$

The field below allows for visual verfication that the cmatrix(r,c,v) function provides correct results and is therefore verfied.

$$cmatrix(3, 1, 1) = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

Cl- in mg/L converted to Cl- in mol/L by division by 35.453 g/mol (35,453 mg/mol) (Sargent-Welch Scientific Company 1979).

Ecrit for SCW is Threshold Potential 1
Ecrit for SAW is Repassivation Potential 3
Ecrit for SSW is Threshold Potential 1

$\Delta E = (Ecrit - Ecorr)$

The Dat matrix contains the 0 - 18 rows and 0 - 6 columns of numeric data.

Dat :=

		0	1	2	3	4	5	6
	Water	T	Ecorr	Ecrit	ΔE	Cl-	Cl-	pH
	Type	°C	mV vs. Ag/AgCl		mV	mg/L	mol/L	
0	SCW	30	-181	422	603	6700	1.89E-01	10.00
1	SCW	60	-185	283	468	6700	1.89E-01	10.00
2	SCW	90	-263	135	398	6700	1.89E-01	10.00
3	SCW	60	-243	298	541	6700	1.89E-01	10.00
4	SCW	90	-294	179	473	6700	1.89E-01	10.00
5	SCW	30	-76	422	498	6700	1.89E-01	10.00
6	SCW	60	-260	263	523	6700	1.89E-01	10.00
7	SCW	90	-239	194	433	6700	1.89E-01	10.00
8	SAW	60	-267	1030	1297	24250	6.84E-01	2.70
9	SAW	60	-363	1100	1463	24250	6.84E-01	2.70
10	SAW	30	-227	1140	1367	24250	6.84E-01	2.70
11	SAW	60	-286	1030	1316	24250	6.84E-01	2.70
12	SAW	60	-294	1020	1314	24250	6.84E-01	2.70
13	SAW	90	-353	304	657	24250	6.84E-01	2.70
14	SSW	100	-269	-123	146	128000	3.61E+00	6.25
15	SSW	120	-175	266	441	154000	4.34E+00	6.25
16	SSW	100	-295	-83	212	128000	3.61E+00	6.25
17	SSW	120	-208	-80	128	154000	4.34E+00	6.25
18	SSW	100	-259	-56	203	128000	3.61E+00	6.25

This is to fit $\quad \Delta E = rb_0 + rb_1 \cdot T + rb_2 \cdot \log(Cl) + rb_3 \cdot pH \qquad$ T is in Kelvin, Cl is in mol/L

$rY := Dat^{\langle 3 \rangle}$

This is a vector of $\Delta E = (Ecrit - Ecorr)$

$rX^{\langle 0 \rangle} := cmatrix(length(rY), 1, 1)$

This is column 0 of the data matrix, rX, it is composed of 1's and is used in obtaining the "intercept" of the model fit.

$rX^{\langle 1 \rangle} := Dat^{\langle 0 \rangle} + 273.15$

This is column 1 of the data matrix, rX, it is composed of temperatures in Kelvin (column 0 of the Dat matrix is temperature in °C).

$rX^{\langle 2 \rangle} := \log\left(Dat^{\langle 5 \rangle}\right)$

This is column 2 of the data matrix, rX, it is composed of base 10 logarithms of the solution chloride ion concentration (column 5 of the Dat matrix).

$rX^{\langle 3 \rangle} := \left(Dat^{\langle 6 \rangle}\right)$

This is column 3 of the data matrix, rX, it is composed of solution pHs (column 6 of the Dat matrix).

Linear regression was performed

$(b \quad s \quad SS) := BBreg(rX, rY)$

- Residual variance ($r\sigma\epsilon 2$)
- R Squared
- Sum of Squares total
- Sum of Squares residual
- Sum of Squares regression

- Regression coefficients (b_i)   - Covariance matrix

$$(b \quad s \quad SS) = \left[\begin{pmatrix} 2.91 \times 10^3 \\ -4.16 \\ -4.39 \times 10^2 \\ -1.33 \times 10^2 \end{pmatrix} \begin{pmatrix} 4.71 \times 10^5 & -1.40 \times 10^3 & 6.07 \times 10^4 & 4.33 \times 10^3 \\ -1.40 \times 10^3 & 4.24 & -1.93 \times 10^2 & -1.70 \times 10^1 \\ 6.07 \times 10^4 & -1.93 \times 10^2 & 1.59 \times 10^4 & 1.41 \times 10^3 \\ 4.33 \times 10^3 & -1.70 \times 10^1 & 1.41 \times 10^3 & 2.75 \times 10^2 \end{pmatrix} \begin{pmatrix} 2.76 \times 10^4 \\ 8.87 \times 10^{-1} \\ 3.67 \times 10^6 \\ 4.14 \times 10^5 \\ 3.25 \times 10^6 \end{pmatrix} \right]$$

The correlation matrix (Corr(i,j)) is determined from the covariance matrix, s:

$i := 0..3 \quad j := 0..3$

$$Corr_{i,j} := \frac{s_{j,i}}{\sqrt{s_{j,j}} \cdot \sqrt{s_{i,i}}} \qquad Corr = \begin{pmatrix} 1.000 & -0.990 & 0.701 & 0.381 \\ -0.990 & 1.000 & -0.742 & -0.496 \\ 0.701 & -0.742 & 1.000 & 0.674 \\ 0.381 & -0.496 & 0.674 & 1.000 \end{pmatrix}$$

EE(T,logCl,pH,z) is a function that evaluates ΔE using the temperature, T, in Kelvin, the base 10 logarithm of chloride ion concentration, the solution pH, a given z-value (number of standard deviations away from the median value, Xob), the residual variance, SS_0, and the covariance matrix, s.

$$EE(T, logCl, pH, z) := \left| \begin{array}{l} Xo \leftarrow (1 \quad T \quad logCl \quad pH) \\ \left[(Xo \cdot b) + z \cdot \sqrt{SS_0 + Xo \cdot s \cdot Xo^T}\right]_0 \end{array} \right.$$

$T := 20, 25..120 \qquad pH := 2..14 \qquad logCl := -4..1$
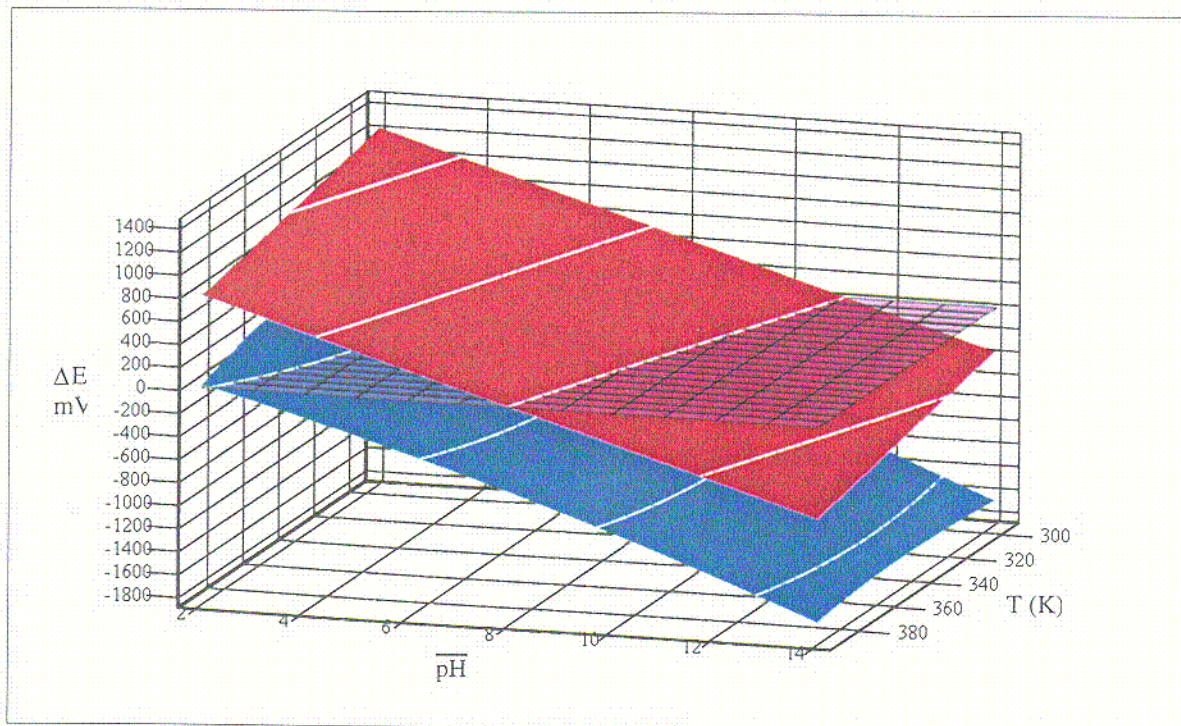
The following steps evaluate the EE function at various values of T and pH (stored in the TT and ppH matrices, respectively) and for a constant chloride ion concentration of 3 mol/L.

$$TT_{\frac{T-20}{5},pH-2} := T + 273.15 \qquad ppH_{\frac{T-20}{5},pH-2} := pH \qquad ZZ1_{\frac{T-20}{5},pH-2} := 0 \qquad \text{ZZ1 is a matrix of zero values}$$

$$Z1 := \overrightarrow{EE(TT,\log(3),ppH,0)}$$

Z1 is a matrix of median values of ΔE and Z1m4 is a matrix of -4σ confidence values of ΔE each evaluated at the various values stores in TT and ppH.

$$Z1m4 := \overrightarrow{EE(TT,\log(3),ppH,-4)}$$

$$(TT,ppH,Z1),(TT,ppH,Z1m4),(TT,ppH,ZZ1)$$

The following steps evaluate the EE function at various values of the base 10 logarithm of chloride ion concentration and pH (stored in the iCl and ipH matrices, respectively) for a constant temperature of 380 K.

$$iCl_{logCl+4,pH-1} := logCl \qquad ipH_{logCl+4,pH-1} := pH \qquad ZZ2_{logCl+4,pH-1} := 0 \qquad \text{ZZ2 is a matrix of zero values}$$

$$Z2 := \overrightarrow{EE(380,iCl,ipH,0)}$$

Z2 is a matrix of median values of ΔE and Z2m4 is a matrix of -4σ confidence values of ΔE each evaluated at the various values stores in iCl and ipH.

$$Z2m4 := \overrightarrow{EE(380,iCl,ipH,-4)}$$

C-2
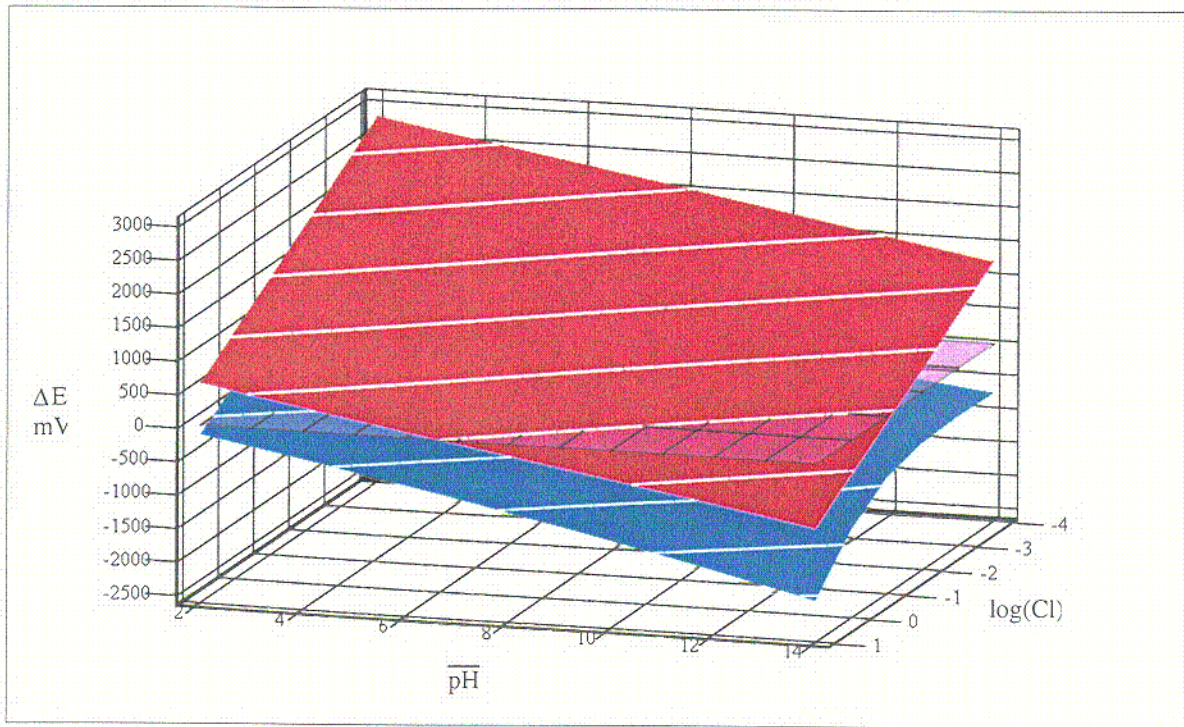
$(iCl, ipH, Z2), (iCl, ipH, Z2m4), (iCl, ipH, ZZ2)$

C-3

The results of the software routine documented in this Attachment are verified by numerical comparision of model outputs to model inputs. The manipulations below show that the computer outputs are accpetable for the current application and that the software routine is properly operating for the specified input parameters.

Here, for each experimental data point in the Dat matrix, the model ΔE values for the -4σ confidence surface are computed and stored in column one of the Diff matrix, i.e., Diff$^{\langle 1 \rangle}$:

$$\text{Diff}^{\langle 1 \rangle} := \overrightarrow{\left(\text{EE} \left(\text{Dat}^{\langle 0 \rangle} + 273.15, \log \left(\text{Dat}^{\langle 5 \rangle} \right), \text{Dat}^{\langle 6 \rangle}, -4 \right) \right)}$$

and the model ΔE values for the +4σ confidence surface are computed and stored in column two of the Diff matrix, i.e., Diff$^{\langle 2 \rangle}$:

$$\text{Diff}^{\langle 2 \rangle} := \overrightarrow{\left(\text{EE} \left(\text{Dat}^{\langle 0 \rangle} + 273.15, \log \left(\text{Dat}^{\langle 5 \rangle} \right), \text{Dat}^{\langle 6 \rangle}, 4 \right) \right)}$$

Diff$^{\langle 0 \rangle} := \text{Dat}^{\langle 3 \rangle}$ and the experimental ΔE values are stored in column zero of the Diff matrix, i.e., Diff$^{\langle 0 \rangle}$:

Diff =

	0	1	2
0	$6.03 \cdot 10^2$	$-1.27 \cdot 10^2$	$1.39 \cdot 10^3$
1	$4.68 \cdot 10^2$	$-1.99 \cdot 10^2$	$1.21 \cdot 10^3$
2	$3.98 \cdot 10^2$	$-3.56 \cdot 10^2$	$1.12 \cdot 10^3$
3	$5.41 \cdot 10^2$	$-1.99 \cdot 10^2$	$1.21 \cdot 10^3$
4	$4.73 \cdot 10^2$	$-3.56 \cdot 10^2$	$1.12 \cdot 10^3$
5	$4.98 \cdot 10^2$	$-1.27 \cdot 10^2$	$1.39 \cdot 10^3$
6	$5.23 \cdot 10^2$	$-1.99 \cdot 10^2$	$1.21 \cdot 10^3$
7	$4.33 \cdot 10^2$	$-3.56 \cdot 10^2$	$1.12 \cdot 10^3$
8	$1.30 \cdot 10^3$	$5.16 \cdot 10^2$	$1.95 \cdot 10^3$
9	$1.46 \cdot 10^3$	$5.16 \cdot 10^2$	$1.95 \cdot 10^3$
10	$1.37 \cdot 10^3$	$6.00 \cdot 10^2$	$2.12 \cdot 10^3$
11	$1.32 \cdot 10^3$	$5.16 \cdot 10^2$	$1.95 \cdot 10^3$
12	$1.31 \cdot 10^3$	$5.16 \cdot 10^2$	$1.95 \cdot 10^3$
13	$6.57 \cdot 10^2$	$3.49 \cdot 10^2$	$1.87 \cdot 10^3$
14	$1.46 \cdot 10^2$	$-4.49 \cdot 10^2$	$1.00 \cdot 10^3$
15	$4.41 \cdot 10^2$	$-5.79 \cdot 10^2$	$8.97 \cdot 10^2$
16	$2.12 \cdot 10^2$	$-4.49 \cdot 10^2$	$1.00 \cdot 10^3$
17	$1.28 \cdot 10^2$	$-5.79 \cdot 10^2$	$8.97 \cdot 10^2$
18	$2.03 \cdot 10^2$	$-4.49 \cdot 10^2$	$1.00 \cdot 10^3$