

**OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET**

1. QA: QA
Page: 1 of 43

Complete Only Applicable Items

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In-Package Chemistry Abstraction

5. Document Identifier (including Rev. No. and Change No., if applicable):
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**OFFICE OF CIVILIAN RADIOACTIVE WASTE
MANAGEMENT
ANALYSIS/MODEL REVISION RECORD**
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4. Revision/Change No.

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Initial Issue
The entire abstraction model was revised to reflect updated inputs/outputs from the feed process model AMR.

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LIST OF ACRONYMS

AMR	Analysis Model Report
CC	cladding coverage
co-disposal	co-disposal waste package
CFR	Code of Federal Regulations
CRWMS	Civilian Radioactive Waste Management System
CSNF	commercial spent nuclear fuel
DIE	Determination of Importance Evaluation
DOE	U. S. Department of Energy
EBS	Engineered Barrier System
FEPs	Features, Events, and Processes
GDR	Glass Dissolution Rate
IRSR	issue resolution status report
KTI	key technical issue
M&O	Management and Operating
MIC	Microbial Induced Corrosion
NFE	near-field environment
NRC	U.S. Nuclear Regulatory Commission
NTS	Nevada Test Site
OCRWM	Office of Civilian Radioactive Waste Management
PA(O)	Performance Assessment (Operations)
Q	water flux through the WP
QA	Quality Assurance
QAP	Quality Administrative Procedure(s)

QARD	Quality Assurance Requirements and Description for the Civilian Radioactive Waste Management Program
THC	thermal-hydrologic-chemical
TPO	technical product output
TSPA	Total-System Performance Assessment
TWP	technical work plan
WF	waste form
WP	waste package
YMP	Yucca Mountain Site Characterization Project

1. PURPOSE

The purpose of this analysis-model report (AMR), as directed by the Technical Work Plan (TWP) (CRWMS M&O 2000b) is to develop the in-package (waste package) chemistry abstraction model using updated technical product output (TPO) (DTN: SN0009T0811199.008) information. The processes included in this model are seepage interaction with the waste form (WF) and waste package (WP) materials and the resulting fluid chemistry. The output of this abstraction will be response surface of pH (as a function of time, water flux (Q) through the WP, metal corrosion rate, and fuel exposure) for the commercial spent nuclear fuel (CSNF) packages. For the Department of Energy (DOE) co-disposal packages the pH will be set to fixed ranges as determined from the process models output. For both CSNF and co-disposal packages the Eh and total carbonate are calculated based on thermodynamic relations relating them to pH. The parameters of ionic strength, chloride, and fluoride will be set to fixed ranges based on the output of the process model.

This abstraction is planned to be used as input to the TSPA where the relationships developed herein should be linked to the principle factors of waste form degradation, radionuclide solubilities, waste package degradation, cladding degradation, and colloid generation.

2. QUALITY ASSURANCE

An activity evaluation (CRWMS M&O 2000b, Enclosure 3), which was prepared per AP-2.21Q, *Quality Determinations and Planning for Scientific, Engineering, and Regulatory Compliance Activities*, determined that the Quality Assurance (QA) program applies to the activity under which this analysis was developed. This analysis does not affect any items on the Q-List (YMP 2000). Control of electronic management of data as required by AP-SV.1Q, *Control of the Electronic Management of Information*, was accomplished in accordance with the controls specified by CRWMS M&O (2000b, Enclosure 5). The preparation of this analysis did not require classification of items in accordance with QAP-2-3, *Classification of Permanent Items*.

3. COMPUTER SOFTWARE AND MODEL USAGE

3.1 COMPUTER SOFTWARE

Two software packages were used in abstracting the results of the in-package process model results, these included Microsoft's Excel 97 SR-2, and SigmaPlot for Windows Version 4.01, both of which are classified as commercially available software. Excel was used for data manipulation and plotting and SigmaPlot was used to perform regression analysis of the data in generation of the response surfaces. Neither macros nor software routines were developed for either Excel or SigmaPlot for the abstraction rendering use of these software packages as

exempt. The regression analysis performed using SigmaPlot is a menu driven function within SigmaPlot, and, therefore, does not constitute a single use routine. Further discussion of the use of these packages is provided in Section 6. Both of these software packages were installed on a Duke Engineering and Services Inc. Dell OptiPlex GXa, serial number DES0070033, Pentium II 266 MHz processor, running Microsoft NT 4.0.

4. INPUTS

All of the input for the in-package abstraction was taken directly from the CD-ROM containing the output files (DTN: SN0009T0811199.008) from the following document: *In-Package Chemistry for Waste Forms* (CRWMS M&O 2000a).

4.1 DATA AND PARAMETERS

Data used in the abstraction were comprised of two groups; 1) Input parameters used as constraints in the in-package process models (CRWMS M&O 2000a) and 2) EQ6 output of time dependent aqueous concentration data, also from the in-package process models (CRWMS M&O 2000a, DTN: SN0009T0811199.008). Both of these data types were documented in the *In-Package Chemistry for Waste Forms* (CRWMS M&O 2000a).

4.1.1 Process Model Input Constraints

Process model input constraints included parameters that were uncertain and therefore, suited over a range of values to provide a range of bounding chemistry for the in-package environment. The parameter ranges and rationale for selecting them is discussed in the *In-Package Chemistry for Waste Forms* (CRWMS M&O 2000a). These parameters included water flux through the waste package and the corrosion rates of the waste package materials. In addition, for the CSNF packages the fraction of fuel exposed was also varied and for the co-disposal packages the rate of glass dissolution was varied. Combined with the results of the EQ3/6 simulations these parameters allowed multi-dimensional response surfaces to be created where the three variables were independent.

The values of the model input constraints and their accompanying EQ6 file names are summarized in Table 1. The information in Table 1 is input to both the process models and the abstraction.

Table 1. EQ6 input files and corresponding independent variable values (from CRWMS M&O 2000a, DTN: SN0009T0811199.008)

EQ6 file name (*6I)	Water Flux (l/yr)	Fuel Exposure (Percent)	WP Materials Corrosion Rate ¹
CSNF_10	0.15	10	1

Table 1 continued			
EQ6 file name (*6I)	Water Flux (l/yr)	Fuel Exposure (Percent)	WP Materials Corrosion Rate ¹
CSNF_11	1.5	10	1
CSNF_12	15	10	1
CSNF_20	0.15	1	1
CSNF_21	1.5	1	1
CSNF_22	15	1	1
CSNF_10L	0.15	10	0.1
CSNF_11L	1.5	10	0.1
CSNF_12L	15	10	0.1
CSNF_20L	0.15	1	0.1
CSNF_21L	1.5	1	0.1
CSNF_22L	15	1	0.1
FFTF_00	0.15	N/A	N/A
FFTF_01	1.5	N/A	N/A
FFTF_02	15	N/A	N/A
Fermi_00	0.15	N/A	N/A
Fermi_01	1.5	N/A	N/A
Fermi_02	15	N/A	N/A

1 – relative WP materials corrosion rates, 1= base case, and 0.1 = base case/10. Base Case Rates: Al-alloy = 2.535E-13, A516 carbon steel = 1.7976E-11, 316SS = 5.05648E-13, 316SS/B = 1.169E-13 (mol/cm²*s), (Section 6.1.1).

4.1.2 In-Package Output Chemistry

The aqueous geochemistry of the in-package environment for both the CSNF and co-disposal packages is documented in the *In-Package Chemistry for Waste Forms* (CRWMS M&O 2000a), all of the input parameters required for the abstraction were taken from this report and from the data CD-ROM (DTN: SN0009T0811199.008). The time dependent parameters required for the abstraction included: pH, Eh, ionic strength, total aqueous carbonate, chloride, and fluoride.

4.2 CRITERIA

Programmatic requirements for this document are listed in the TWP (CRWMS M&O 2000b). That the TWP specifies that this document and all analyses described herein must adhere to the requirements of AP-3.10Q, *Analyses and Models*, and must address applicable NRC issue resolution status report (IRSR) criteria (NRC 1999).

Below is a summary of the applicable NRC review methods and acceptance criteria outlined in the issue resolution status report (IRSR) that apply to model development for the following near-field environment (NFE) key technical issue (KTI) sub-issue effects: (a) coupled thermal-hydrologic-chemical processes on the waste package chemical environment, (b) coupled

thermal-hydrologic-chemical (THC) processes on the chemical environment for radionuclide release, and (c) coupled THC processes on radionuclide transport through engineered and natural barriers (NRC 1999).

4.2.1 NRC IRSR Criteria

Evaluations of the criteria are discussed in Section 7.3.

4.2.1.1 Data and Model Justification Acceptance Criteria

1. Consider both temporal and spatial variations in conditions affecting coupled THC effects on the chemical environment for radionuclide release. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
2. Evaluation of coupled THC processes shall consider site characteristics in establishing initial and boundary conditions for conceptual models and simulations of coupled processes that may affect the chemical environment for radionuclide release. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
3. Sufficient data shall be collected on the characteristics of the natural system and engineered materials, such as the type, quantity, and reactivity of materials, in establishing initial and boundary conditions for conceptual models and simulations of THC coupled processes that may affect the chemical environment for radionuclide release. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
4. A nutrient and energy inventory calculation should be used to determine the potential for microbial activity that could impact the waste package (WP) chemical environment. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
5. Should microbial activity be sufficient to allow microbial influenced corrosion (MIC) of the WP, then the time-history of temperature, humidity, and dripping should be used to constrain the probability for MIC. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
6. Sensitivity and uncertainty analyses (including consideration of alternative conceptual models) shall be used to determine whether additional new data are needed to better define ranges of input parameters. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
7. If the testing program for coupled THC processes on the chemical environment for radionuclide release from the engineered barrier system is not complete at the time of license application, or if sensitivity and uncertainty analyses indicate that additional data are needed, specific plans to acquire the necessary information as part of the

performance confirmation program shall be identified. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

4.2.1.2 Data Uncertainty and Verification Acceptance Criteria

1. Reasonable or conservative ranges of parameters or functional relations were used to determine effects of coupled THC processes on the chemical environment for radionuclide release. Parameter values, assumed ranges, probability distributions, and bounding assumptions shall be technically defensible and reasonably account for uncertainties. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
2. Uncertainty in data due to both temporal and spatial variations in conditions affecting coupled THC effects on the chemical environment for radionuclide release shall be considered. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
3. Evaluation of coupled THC processes shall consider the uncertainties in the characteristics of the natural system and engineered materials, such as the type, quantity, and reactivity of materials, in establishing initial and boundary conditions for conceptual models and simulations of THC coupled processes that may affect the chemical environment for radionuclide release. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
4. The initial conditions, boundary conditions, and computational domain used in sensitivity analysis involving coupled THC effects on the chemical environment for radionuclide release shall be consistent with available data. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
5. A performance confirmation program shall be developed to assess whether the natural system and engineered materials are functioning as intended and anticipated with regard to coupled THC effects on the chemical environment for radionuclide release from the engineered barrier system (EBS). [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

4.2.1.3 Model Uncertainty Acceptance Criteria

1. Appropriate models, tests, and analyses shall be used that are sensitive to the THC couplings under consideration for both natural and engineered systems as described in the following examples. The effects of THC coupled processes that may occur in the natural setting or due to interactions with engineered materials or their alteration products include: (i) Thermohydrologic (TH) effects on gas and water chemistry; (ii) hydrothermally driven geochemical reactions, such as zeolitization of volcanic glass; (iii) dehydration of hydrous phases liberating moisture; (iv) effects of microbial processes; and (v) changes in water chemistry that may result from interactions

between cementitious or WP, materials and groundwater, which, in turn, may affect the chemical environment for radionuclide release. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

2. Alternative modeling approaches consistent with available data and current scientific understanding shall be investigated, and their results and limitations shall be appropriately considered. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
3. A reasonable description of the mathematical models included in analyses of coupled THC effects on the chemical environment for radionuclide release shall be provided. The description should include a discussion of alternative modeling approaches not considered in its final analysis and the limitations and uncertainties of the chosen model. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

4.2.1.4 Model Verification Acceptance Criteria

1. The mathematical models for coupled THC effects on the chemical environment for radionuclide release shall be consistent with conceptual models based on inferences about the near-field environment, field data and natural alteration observed at the site, and expected engineered materials. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
2. Accepted and well-documented procedures shall be adopted to construct and test the numerical models used to simulate coupled THC effects on the chemical environment for radionuclide release. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]
3. Abstracted models for coupled THC effects on the chemical environment for radionuclide release shall be based on the same assumptions and approximations shown to be appropriate for closely analogous natural or experimental systems. Abstracted model results shall be verified through comparison to outputs of detailed process models and empirical observations. Abstracted model results shall be compared with different mathematical models to judge robustness of results. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

4.2.2 YMP Features, Events and Processes (FEPs)

This AMR being an abstraction is not subject to FEPs in the sense that the abstraction is a mathematical simplification of the process model results. A discussion of the FEPs that may impact the in-package chemistry is covered in the *In-Package Chemistry for Waste Forms* (CRWMS M&O 2000a).

4.3 CODES AND STANDARDS

4.3.1 Codes

This AMR was prepared to comply with the DOE interim guidance (Dyer 1999) which directs the use of the proposed NRC high-level waste rule, 10 CFR 63 (64 FR 8640). Relevant requirements for performance assessment from Section 114 of proposed 10 CFR 63 (64 FR 8640) are: “Any performance assessment used to demonstrate compliance with Sec. 113(b) shall: (a) Include data related to the geology, hydrology, and geochemistry used to define parameters and conceptual models used in the assessment. (b) Account for uncertainties and variabilities in parameter values and provide the technical basis for parameter ranges, probability distributions, or bounding values used in the performance assessment. (g) Provide the technical basis for models used in the performance assessment such as comparisons made with outputs of detailed process-level models.

4.3.2 Standards

ASTM C 1174-97 (1998) *Standard Practice for Prediction of the Long-Term Behavior of Materials, Including Waste Forms, Used in Engineered Barrier Systems (EBS) for Geological Disposal of High-Level Radioactive Waste* was used as guidance in the preparation of this abstraction model.

5. ASSUMPTIONS

- 5.1 The system pH can be used as an indicator for changes in the chemistry of the system, i.e., changes in pH are indicative of changes in fluid chemistry. The basis for this assumption is that pH is the “master” chemical variable, i.e., based on the principles of chemical equilibria, pH controls the total carbonate concentration at a constant carbon dioxide fugacity, and the electron activity (Eh) at constant oxygen fugacity. This assumption is applied to all of Section 6, and does not require confirmation.
- 5.2 The term water flux (Q) with regard to this AMR refers to the total flux of water flowing through an individual waste package. The basis for this assumption is that water that does not flow through the WP will not react with the WP or its contents, therefore, only the water that flows through the WP is considered. This assumption is used in Section 6, and does not require confirmation.
- 5.3 The time frame used in this abstraction begins at the time that a waste package first breaches. The basis for this assumption is that prior to breach there is no possibility for reaction of the WP or its contents with water. This assumption is used in Section 6, and does not require confirmation.

6. ANALYSIS/MODEL

The abstraction of the in-package chemistry seeks to simplify the detailed complex time dependent chemistry into blocks of time where realistic conservative assumptions have been used to bound the chemistry. This step allowed the generation of multi-dimensional response surfaces for in-package chemical parameters that can be directly implemented in the TSPA. Thus, the *In-Package Chemistry Abstraction* is appropriate for assessing the principle factors of radionuclide concentration limits and colloid stability in WP effluent.

The discussion that follows outlines the chemical parameters that are considered in the abstraction and the method/reasoning used in the abstraction for both the CSNF and the co-disposal.

6.1 ABSTRACTION OF pH

The chemical parameter pH constitutes the most important in-package chemical parameter. The reasons are two-fold, first it is the one parameter that is used by all of the sub-models to the in-package chemistry, and second, it can be used to calculate the solution total carbonate and the system Eh.

The pH abstraction uses two different methods depending on the waste package type (CSNF or co-disposal). The CSNF abstraction employs the use of response surfaces/lines and distributions where pH is a function of time, WP corrosion rate, water flux, and fuel exposure. In the case of the co-disposal packages a distribution of pH is used to describe the pH – time profile.

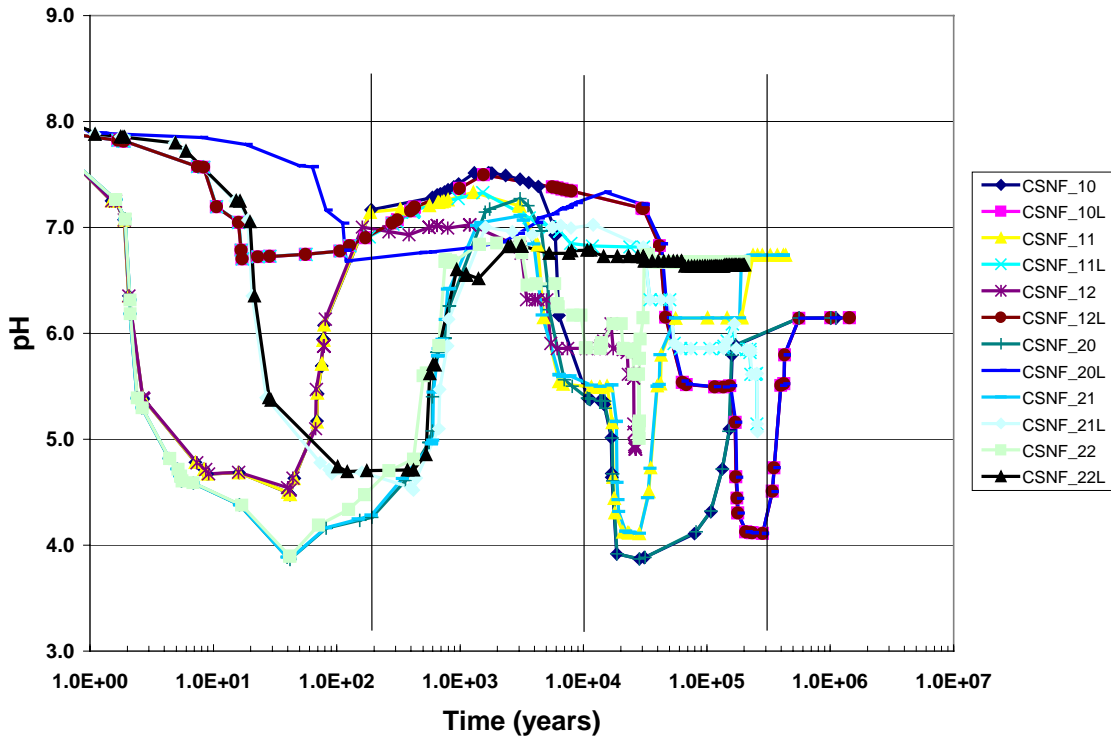


Figure 1. pH versus time for the CSNF waste packages (from CRWMS M&O 2000a, DTN: SN0009T0811199.008).

6.1.1 CSNF pH Abstraction

Figure 1 shows the pH time history of the in-package fluids for CSNF waste packages. The vertical black lines drawn on Figure 1 delineates the time break down for the pH abstraction. Table 2 lists the time periods and the criteria used in the pH abstraction.

Table 2. Criteria used to define the pH for each abstracted time period.

Time Period (years post WP breach)	pH Criteria ¹
0 – 200	Minimum
200 – 10,000	Average
10,000 – 300,000	Minimum
300,000 - 1000000	Stabilized ²

- 1 – pH criteria is the value used for each scenario to generate a point on the response surface
- 2 – When the in-package pH achieves a constant value – no further reaction.

The time discretization was based on the observed trends in pH. The guiding criterion was that all of the pH – time histories had to achieve either a minimum or a maximum pH value during a particular interval. Although this method only provides a rough discretization of the pH – time history it still honors the overall observed pH trends in the data.

The choice of what pH criteria to apply per time period was guided by the principle of “realistic conservatism”. An explanation comparing this approach to a purely conservative approach is warranted. The purely conservative approach would assume that the pH inside of a WP is always going to maximize the dissolved concentration of radionuclides. For example, if the solubility limiting phase for a particular radionuclide is highly soluble at low values of pH, then a purely conservative approach would be to use the absolute minimum pH, for the entire pH – time series, attained for a particular water flux/fuel exposure/corrosion rate scenario and use it in the generation of a response surface. However, applying realistic conservatism, the pH – time series is divided into segments and based on the observed pH trend(s) during each segment a judgement is made as to what pH criteria (minimum, maximum, or average) best represent the observed pH during a particular time period. In other words, the application of realistic conservatism was the approach taken to make the abstraction more closely adhere to the output from the process model.

Response surfaces/lines were generated for each of the four time periods using the pH criteria listed in Table 2. The results are eight matrices of values (Tables 3 – 9), which in turn were used to generate four response surfaces, two response lines, and one pH distribution for each of the four time periods. Note that the minimum and average pH values reported in Tables 3 – 8 were calculated in EXCEL using either the “MIN” or “AVERAGE” intrinsic function, respectively, for the pH values in given time period. The stabilized pH in Table 9 was determined by inspection, as was the minimum and maximum listed in Table 9. The information contained in Tables 3 – 9 were directly copied from the EXCEL spreadsheet “CSNF_ABSTRACTION.XLS”, DTN: MO0011SPAIPC37.002.

The pH values for each flux/fuel exposure/corrosion scenario representing each time period were compiled into eight matrices such that a response surface or line could be generated in SigmaPlot. For 3-dimensional response surfaces three data columns were specified in SigmaPlot (x = water flux, y = fuel exposure, and z = pH) and the regression wizard was used to fit a 3-dimensional plane to the data. The output consisted of the coefficients of the equation of the plane and various goodness-of-fit statistical parameters (Attachment I), and contained in the SigmaPlot file “CSNF_SURFACE.JNB”, DTN: MO0011SPAIPC37.002. It was necessary to generate two matrices for each time period, one representing the “base case” WP corrosion rates ($\text{mol}/\text{cm}^2 \cdot \text{s}$), and a second representing the “low” WP corrosion rates. The waste package was modeled as being composed of four component metal alloys where the dissolution rate of each alloy was simultaneously decreased by an order of magnitude compared to the “base case” for

sensitivity analyses (CRWMS M&O 2000a). Therefore, the absolute value(s) of the corrosion rates were not used, and, in fact, are unimportant to the abstraction. The approach taken was to lump the change in WP dissolution rates together into “base case” and “low” corrosion rate groups, such that two response surfaces were created, one for low WP corrosion rates and the other for base case WP corrosion rates. The axes of the three dimensional surfaces were x = water flux, y = fuel exposure, and z = pH. It is the region between the pH response surfaces that should be sampled in the TSPA. Similarly, for 2-dimensional response lines two data columns were specified in SigmaPlot (x = water flux and y = pH) and the regression wizard was used to fit a linear relationship to the data (“CSNF_SURFACE.JNB”, DTN: MO0011SPAIPC37.002).

Table 3. CSNF matrix for base case WP corrosion rates for the 0 to 200 year time frame (from CRWMS M&O 2000a, DTN: SN0009T0811199.008).

EQ6 input file (*.6i)	Water Flux(l/yr)	Fuel Exposure	Minimum pH
CSNF_10	0.15	0.1	4.48
CSNF_11	1.5	0.1	4.48
CSNF_12	15	0.1	4.52
CSNF_20	0.15	0.01	3.87
CSNF_21	1.5	0.01	3.87
CSNF_22	15	0.01	3.90

Table 4. CSNF matrix for low WP corrosion rates for the 0 to 200 year time frame (from CRWMS M&O 2000a, DTN: SN0009T0811199.008).

EQ6 input file (*.6i)	Water Flux(l/yr)	Fuel Exposure	Minimum pH
CSNF_10L	0.15	0.1	6.70
CSNF_11L	1.5	0.1	6.70
CSNF_12L	15	0.1	6.70
CSNF_20L	0.15	0.01	6.68
CSNF_21L	1.5	0.01	4.67
CSNF_22L	15	0.01	4.70

Table 5. CSNF matrix for base case WP corrosion rates for the 200 to 10,000 year time frame (from CRWMS M&O 2000a, DTN: SN0009T0811199.008).

EQ6 input file (*.6i)	Water Flux(l/yr)	Fuel Exposure	Average pH
CSNF_10	0.15	0.1	7.26
CSNF_11	1.5	0.1	6.89
CSNF_12	15	0.1	6.62
CSNF_20	0.15	0.01	6.07
CSNF_21	1.5	0.01	5.95
CSNF_22	15	0.01	6.26

Table 6. CSNF matrix for low WP corrosion rates for the 200 to 10,000 year time frame (from CRWMS M&O 2000a, DTN: SN0009T0811199.008).

EQ6 input file (*.6i)	Water Flux(l/yr)	Fuel Exposure	Average pH
CSNF_10L	0.15	0.1	7.27
CSNF_11L	1.5	0.1	7.09
CSNF_12L	15	0.1	7.27
CSNF_20L	0.15	0.01	7.04
CSNF_21L	1.5	0.01	6.12
CSNF_22L	15	0.01	6.05

Table 7. CSNF matrix for base case WP corrosion rates for the 10,000 to 300,000 year time frame (from CRWMS M&O 2000a, DTN: SN0009T0811199.008).

EQ6 input file (*.6i)	Water Flux(l/yr)	Average pH
CSNF_10	0.15	3.87
CSNF_11	1.5	4.11
CSNF_12	15	4.91
CSNF_20	0.15	3.87
CSNF_21	1.5	4.11
CSNF_22	15	5.01

Table 8. CSNF matrix for low WP corrosion rates for the 10,000 to 300,000 year time frame (from CRWMS M&O 2000a, DTN: SN0009T0811199.008).

EQ6 input file (*.6i)	Water Flux(l/yr)	Average pH
CSNF_10L	0.15	4.11
CSNF_11L	1.5	5.15
CSNF_12L	15	4.11
CSNF_20L	0.15	4.11
CSNF_21L	1.5	5.07
CSNF_22L	15	6.63

Table 9. CSNF matrix for base case and low WP corrosion rates for the 300,000 to 1E6 year time frame (from CRWMS M&O 2000a, DTN: SN0009T0811199.008).

EQ6 input file (*.6i)	Water Flux(l/yr)	Stabilized pH
CSNF_10	0.15	6.14
CSNF_11	1.5	6.74
CSNF_12	15	N/A

Table 9 continued		
EQ6 input file (*.6i)	Water Flux(l/yr)	Stabilized pH
CSNF_20	0.15	6.15
CSNF_21	1.5	6.74
CSNF_22	15	6.74
CSNF_10L	0.15	6.15
CSNF_11L	1.5	N/A
CSNF_12L	15	6.15
CSNF_20L	0.15	6.15
CSNF_21L	1.5	N/A
CSNF_22L	15	6.65
	Minimum	6.14
	Maximum	6.74

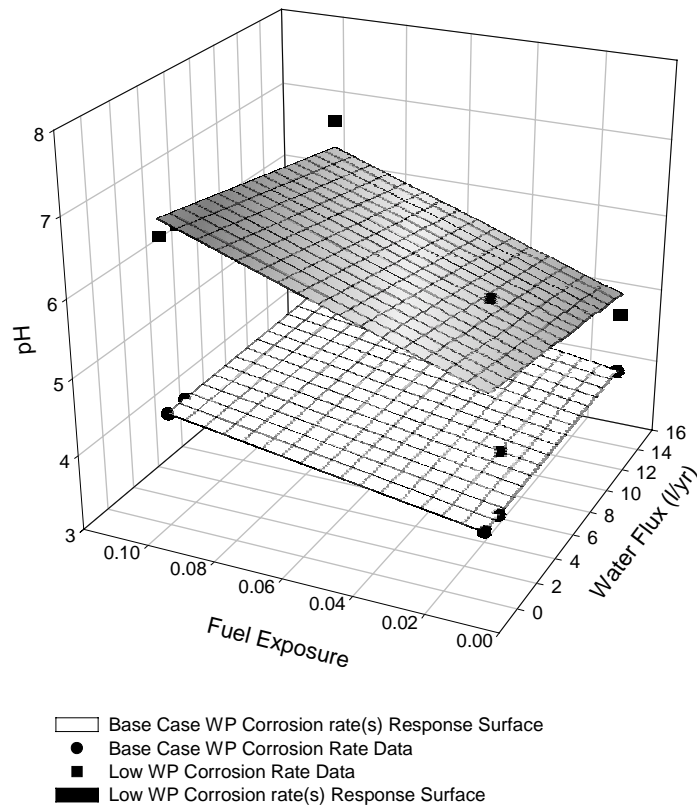


Figure 2. Response surface of pH for CSNF waste packages for the 0 to 200 year post-breach (DTN: MO0011SPAIPC37.002).

Figures 2 and 3 depict the response surfaces for the 0 to 200 year and 200 to 10,000 year time periods, respectively. The values of the coefficients for the response surface equations and the correlation coefficients are provided in Table 10.

Note that the timing of depletion of the CSNF is inversely proportional to the surface area of the exposed fuel. In other words, as the value of fuel exposure increases the duration for complete dissolution of the fuel decreases. The rate of fuel dissolution is also dependent on the pH and the dissolved carbonate concentration, however, to a much smaller degree compared to the surface area term. Therefore, when the fuel depletes there is no longer any dependency of the in-package chemistry on the fuel exposure parameter. Inspection of the EQ6 output information reveals that the CSNF is completely depleted in approximately 7000 years for the 1-percent exposure cases and in approximately 200 years for the 100-percent exposure cases. The implications of this with regard to the abstraction is that at times greater than 10,000 years the pH will depend only on the water flux through the WP and not on water flux and fuel exposure together. Therefore, for times greater than 10,000 years pH is a function of water flux and WP corrosion rate and as such may be described by two lines rather than two planes. Figure 4 shows the lines that describe pH as a function of water flux for the 10,000 to 300,000 year period, and Table 11 provides the coefficients for the equation of the line and the correlation information.

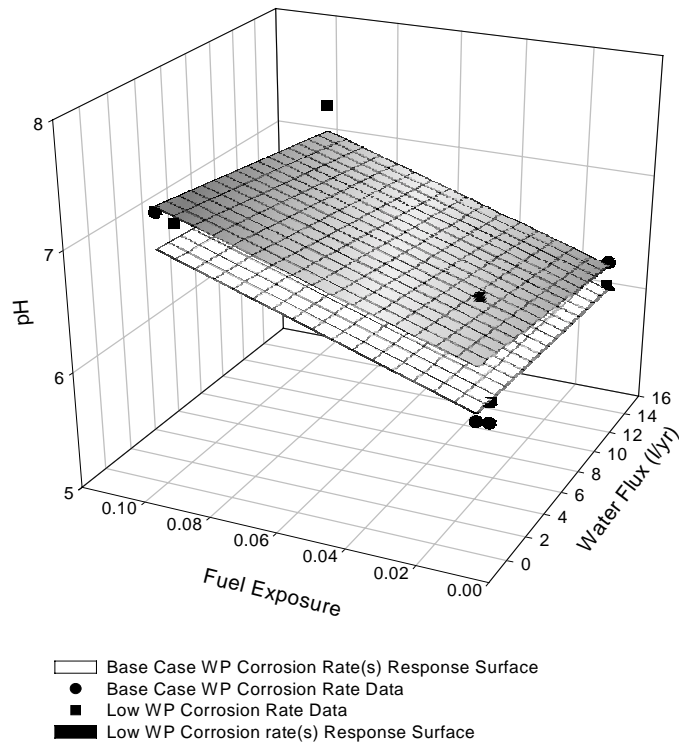


Figure 3. Response surfaces of pH for CSNF waste packages for the 200 to 10,000 year post-breach period (DTN: MO0011SPAIPC37.002).

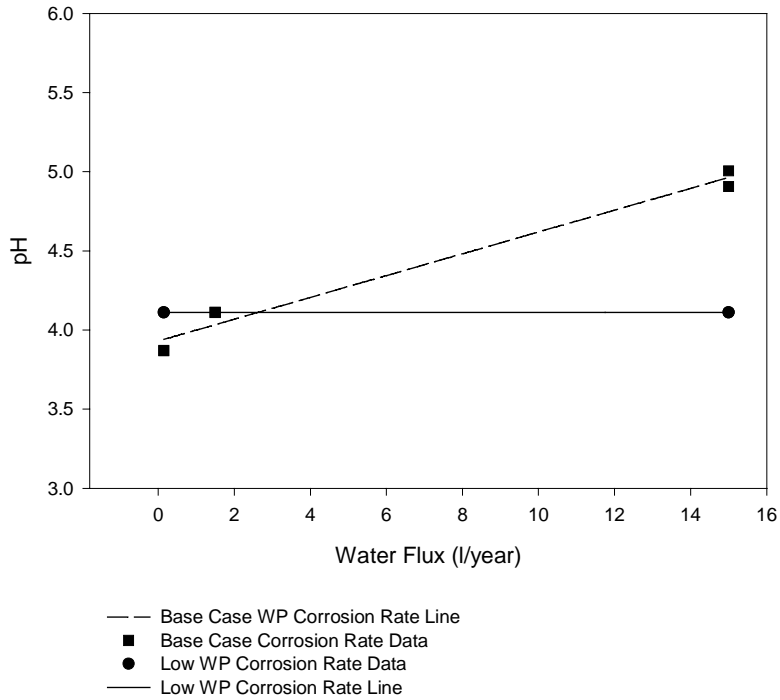


Figure 4. Response lines of pH for CSNF waste packages for the 10,000 to 300,000 year post-breach period (DTN: MO0011SPAIPC37.002).

At times greater than 300,000 years all of the waste package components are nearly depleted and the in-package chemistry tends toward stabilization. The stabilized pH value for each modeled scenario was used in the abstraction. Inspection of the stabilized pH values (Table 9 and Figure 5) reveals there is no systematic variation of pH with water flux, therefore, a uniform distribution of pH is suggested for use in the TSPA using the minimum and maximum pH values as the bounds on the distribution (Table 11).

Table 10. TSPA input pH input parameters for the response surfaces from 0 to 10,000 years.

$Z^1 = y_0 + ax + by$				
Case	y_0	a	b	Correlation Coefficient
0 – 200 years, base case corrosion rate	3.7950	0.0025	6.8296	0.99989944
0 – 200 years, low corrosion rate	5.4198	-0.0394	15.0214	0.76519908
200 – 10,000 years, base case corrosion rate	6.0496	-0.0084	9.1963	0.90134342
200 – 10,000 years, low corrosion rate	6.4146	-0.0180	8.9477	0.81242016

Z = pH, x = water flux (l/yr), y = Fuel Exposure (fractional value), y_0 , a, and b are coefficients of the equation
 1 - A range of +/- 1 pH unit should be applied to all calculated pH values.

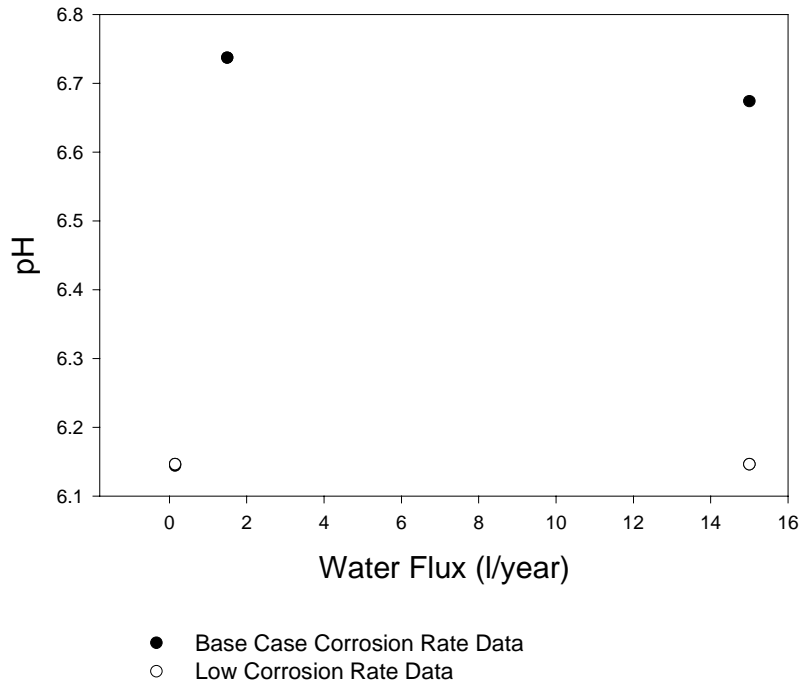


Figure 5. pH for CSNF waste packages for the 300,000 to 1E6 year post-breach period (DTN: MO0011SPAIPC37.002).

Table 11. TSPA input pH input parameters for 10,000 to 1E6 years.

$Y' = mx + b$, where $y = \text{pH}$, $x = \text{water flux}$	m	b	Correlation Coefficient
10,000 – 300K years, base case corrosion rate	0.0689	3.9306	0.98967427
10,000 – 300K years, low corrosion rate	0.0	4.11	1.0
Distribution	Minimum	Maximum	Distribution Type
300K – 1E6 years, base case corrosion rate	6.14	6.74	Uniform
300K – 1E6 years, low corrosion rate			

1 - A range of +/- 1 pH unit should be applied to all calculated pH values.

To avoid calculating pH values out of the range of those observed from the process modeling (Figure 1) it was necessary to define pH ranges for each abstracted time period and set limits on the independent parameters. The pH criteria for each time period was determined by taking the minimum and maximum for each period and adjusting that value by one pH unit, down for the minimum and up for the maximum, to reflect the uncertainty in the pH. The limits on the independent parameters were then hand calculated such that the pH criteria were not violated for any combination of the independent parameters that fall within the defined range. Table 12 provides the parameter limits and the pH criteria. Note that there is no process model output that reflects the zero water flux scenario, rather the minimum water flux of 0.0 l/yr/wp in Table 12

allows calculation of the pH for packages which do not receive any seepage with the caveat that future process modeling may change the zero-flux pH abstraction.

Table 12. Parameter limits for CSNF response surfaces.

Case	Minimum Water Flux (l/yr/WP)	Maximum Water Flux (l/yr/WP)	Minimum Fuel Exposure	Maximum Fuel Exposure	pH Criteria	
					Min	Max
0 - 200 years, base case corrosion rate	0.0	65	0.0001	0.25	2.9	9.0
0 - 200 years, low corrosion rate	0.0	65	0.0001	0.25	2.9	9.0
200 - 10,000 years, base case corrosion rate	0.0	150	0.0	0.23	3.5	8.5
200 - 10,000 years, low corrosion rate	0.0	150	0.0	0.23	3.5	8.5
10,000 - 300K years, base case corrosion rate	0.0	63	N/A	N/A	2.9	8.3
10,000 - 300K years, low corrosion rate	N/A	N/A	N/A	N/A	N/A	N/A
300K - 1E6 years, base case corrosion rate	N/A	N/A	N/A	N/A	N/A	N/A
300K - 1E6 years, low corrosion rate	N/A	N/A	N/A	N/A	N/A	N/A

6.1.2 Co-Disposal pH Abstraction

Figure 6 displays the pH as a function of time for the co-disposal waste packages (FFTF and Fermi). The pH time histories for the two WP types are nearly identical and show very little variation due to changes in the water flux (Table 1). Due to the lack of correlation between water flux and pH and the limited scenarios that were simulated no response surfaces or linear relationships were formulated for the co-disposal waste packages. Note that in the *In-Package Chemistry for Waste Forms* (CRMS M&O, 2000a) sensitivity runs were completed to test the effects of glass dissolution rate on resulting fluid chemistry.

It is recommended that a uniform distribution of pH be implemented in the TSPA for the co-disposal packages where the minimum and maximum value is set according to the values in Table 13.

Table 13. Descriptive statistics of pH for the co-disposal packages.

Statistical Parameters		EXCEL Intrinsic Function
Minimum	3.265	MIN
Maximum	10.011	MAX
Median	6.981	MEDIAN
Mean	6.644	AVERAGE
Standard Deviation	1.878	STDEV

The statistical output in Table 13 were generated in EXCEL using the intrinsic functions listed in Table 13 for the entire pH time history. Note that this information is available in the EXCEL spreadsheet “CO-DISPOSAL_ABSTRACTION.XLS” under DTN: MO0011SPAIPC37.002.

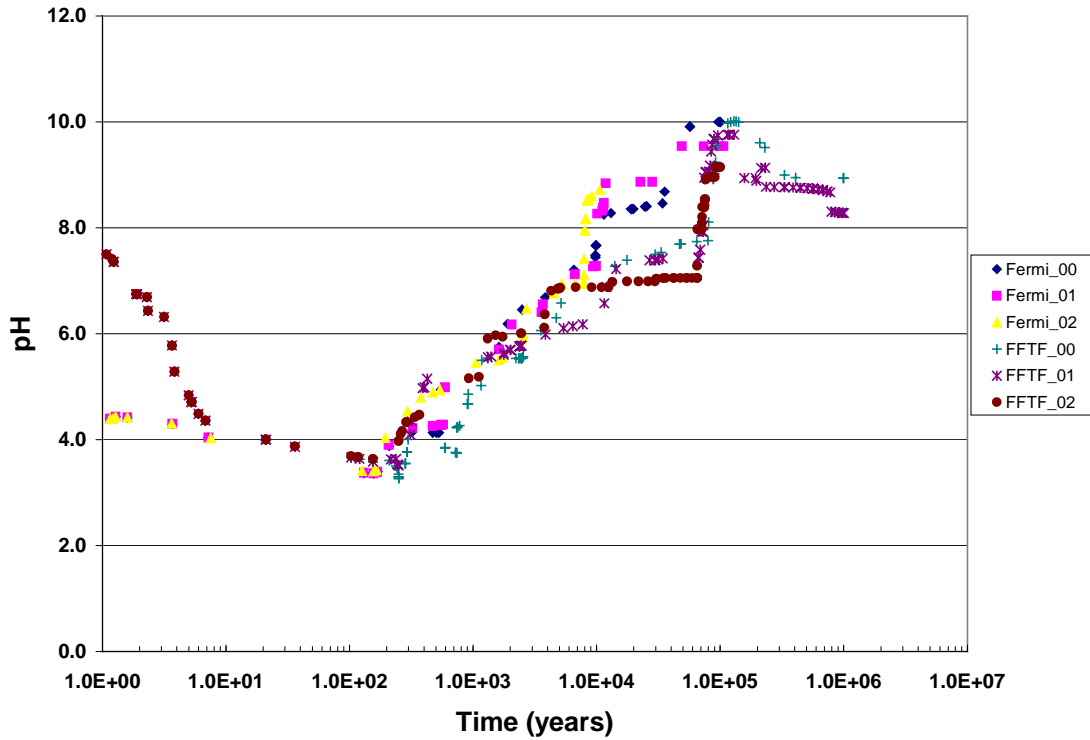


Figure 6. pH versus time for co-disposal waste packages (from CRWMS M&O 2000a, DTN: SN0009T0811199.008).

6.2 TOTAL CARBONATE ABSTRACTION

Total carbonate is used in the kinetic rate expression for the dissolution of CSNF, therefore, abstracted values are needed for the TSPA. The carbonate output data from the process model for CSNF and co-disposal are plotted in Figure 7 and 8, respectively. In a system where the fugacity of carbon dioxide (CO_2) is constant over the modeled period and the pH known, the total carbonate can be calculated using the equilibrium mass action expressions.

Where the total carbonate ($0 < \text{pH} < 14$) is equal to:

$$0) \Sigma C = [\text{CO}_2(\text{aq})] + [\text{HCO}_3^-] + [\text{CO}_3^{2-}]$$



$$[\text{CO}_2(\text{aq})] = F_{\text{CO}_2(\text{g})} 10^{-1.47}$$



$$[\text{HCO}_3^-] = (F_{\text{CO}_2(\text{g})} 10^{-1.47} 10^{-6.35}) / 10^{-\text{pH}}$$



$$[\text{CO}_3^{2-}] = [(F_{\text{CO}_2(\text{g})} 10^{-1.47} 10^{-6.35}) / 10^{-\text{pH}}] 10^{-10.33} / 10^{-\text{pH}}$$

* log K values have been rounded off to the nearest hundredth

Combining terms and substituting back into expression (0), the total carbonate for the system is equal to the expression in Table 14.

Table 14. Expression for total carbonate as a function of pH to be used in the TSPA.

$\text{Total C} = F_{\text{CO}_2(\text{g})} (10^{-1.47} + 10^{(\text{pH} - 7.82)} + 10^{(2\text{pH} - 18.15)})$

Solving the expression in Table 14 using EXCEL at a fixed fugacity of carbon dioxide ($\log(F_{\text{CO}_2(\text{g})}) = -3.0$), and over a range of pH (3 to 9) yields the curves displayed in Figures 7 and 8, which closely approximates the output data from the in-package process model. The expression for total carbonate is defined such that the fugacity of carbon dioxide is not a fixed value allowing total carbonate to be calculated over a range of carbon dioxide values.

Figures 7 and 8 depict the output from the CSNF and co-disposal process models, respectively, and the calculated functional relationship between pH and total carbonate. Both, Figures 7 and 8, as well as the input and output are contained in “CSNF_ABSTRACTION.XLS” and “CO-DISPOSAL_ABSTRACTION.XLS” under DTN: MO0011SPAIPC37.002, for CSNF and co-disposal, respectively. Implementation of the expression in Table 14 in the TSPA will provide a consistency in the solution chemistry by having carbonate values that correspond to the solution pH. Note that some of the process model data displayed in Figures 7 and 8 do not fall on the calculated curve. Some values fall below the calculated curve and the reason for this is an ionic strength effect, as the ionic strength exceeds a threshold value the solubility of carbon dioxide decreases and in turn the total carbonate decreases. Figure 7 shows some carbonate values that are above the calculated curve, these values occur at pH eight and above are likely due to additional carbon originating from the steel WP components. The observed uncertainty in the carbonate – pH relationship is inconsequential and is accounted for in the pH uncertainty.

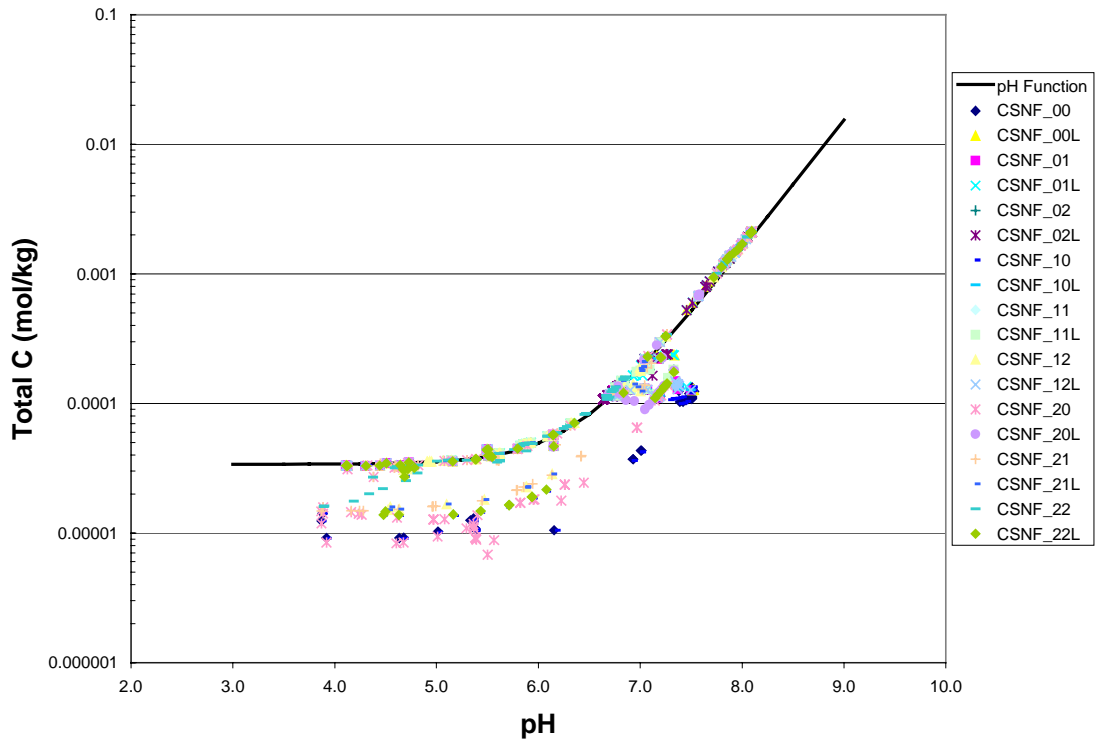


Figure 7. CSNF calculated total aqueous carbonate versus pH, and the process model output (data from CRWMS M&O 2000a, DTN: SN0009T0811199.008)

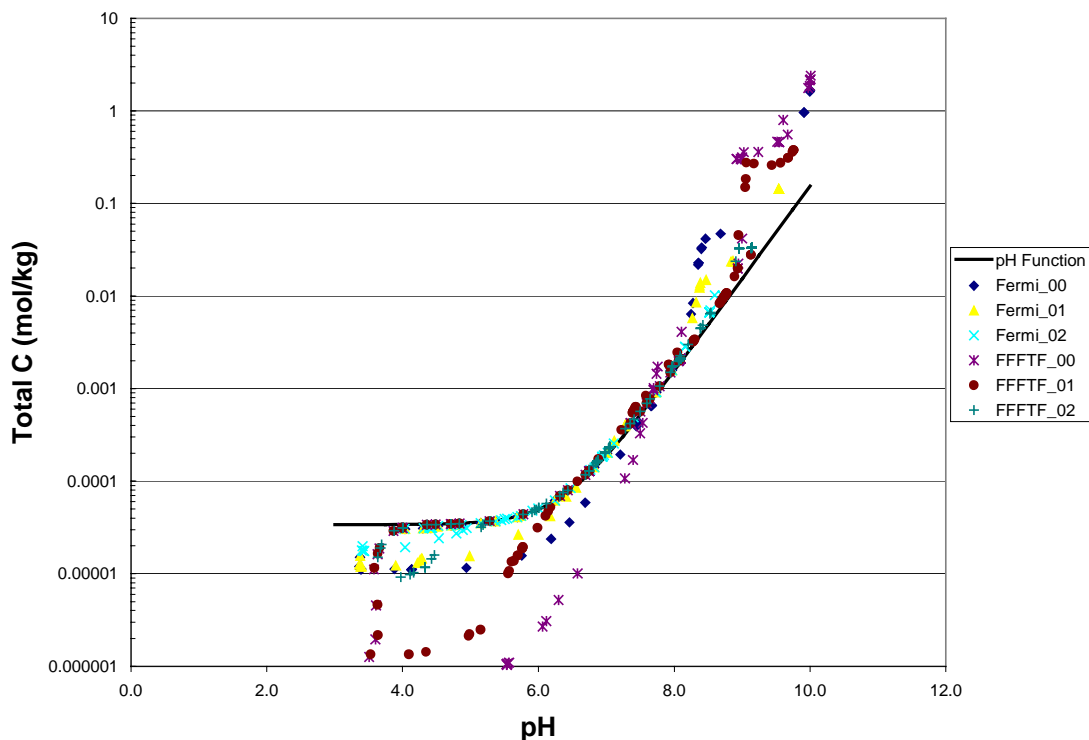


Figure 8. Co-Disposal calculated total aqueous carbonate versus pH, and the process model output (data from CRWMS M&O 2000a, DTN: SN0009T0811199.008)

Validation of the total carbonate abstraction, for both the CSNF and co-disposal, is displayed in Figures 7 and 8, where the process model output shows strong agreement with the abstracted relationship. Uncertainty is built in to the carbonate abstraction by virtue of the input pH, which has associated uncertainty of one pH unit.

6.3 ABSTRACTION OF Eh

In aqueous systems in equilibrium with oxygen at a constant fugacity the Eh may be calculated directly from the pH. For the formation of water the pE° may be calculated from the following expression, where ΔG° is the Gibb's free energy of formation, F is the Faraday constant (23.06 kcal/volt-gram equivalent), Eh is the electron activity expressed in units of volts, and pE is the negative log base 10 of electron activity.

$$1) \frac{1}{2}O_2 + 2H^+ + 2e^- = H_2O \quad \Delta G^{\circ} = -56.688 \text{ kcal/mol (EQ6 database)}$$

$$2) \Delta G^{\circ} = -nFEh^{\circ} \quad (\text{Drever, 1988, page 285, eqn 13-6})$$

$$3) pE = F/(2.303RT)Eh \quad (\text{Drever, 1988, page 284})$$

Solving (3) for Eh and substituting into (2) results in (4), establishing a relationship between ΔG° and pE°

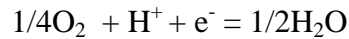
$$4) \Delta G^\circ = -2.303nRT(pE^\circ),$$

Where, n = number of electrons, (2), R = Gas Constant (1.987E-03 kcal/mol.K), and T = absolute temperature (25°C = 298.5K).

Solving for pE° results in:

$$pE^\circ = 20.75$$

Thus for the formation of water in terms of one electron mole we have:



$$pE = pE^\circ + \text{Log}(F_{O_2}^{1/4}[H^+])$$

$$pE = 20.75 - pH + 0.25\log(F_{O_2})$$

Converting to Eh we get the expression in Table 15. The expression for Eh as a function of pH and oxygen fugacity (Table 15) is applicable for both CSNF and co-disposal waste packages.

Table 15. Expression for Eh as a function of pH for use in the TSPA.

$Eh = 2.303RT/F(20.75 - pH + 0.25\log F_{O_2})$

The Eh function is displayed in Figures 9 and 10 and was calculated in EXCEL by solving the expression in Table 15 at a constant $\log F_{O_2} = -0.7$ and over a pH range 3 to 10. Both, Figures 9 and 10, as well as the input and output are contained in "CSNF_ABSTRACTION.XLS" and "CO-DISPOSAL_ABSTRACTION.XLS" under DTN: MO0011SPAIPC37.002, for CSNF and co-disposal, respectively.

Validation of the Eh abstraction, for both the CSNF and co-disposal, is shown in Figures 9 and 10, where the process model output strongly agrees with the Eh abstraction. Like the carbonate abstraction, uncertainty is built in to the Eh abstraction by virtue of the input pH, which has associated uncertainty of one pH unit.

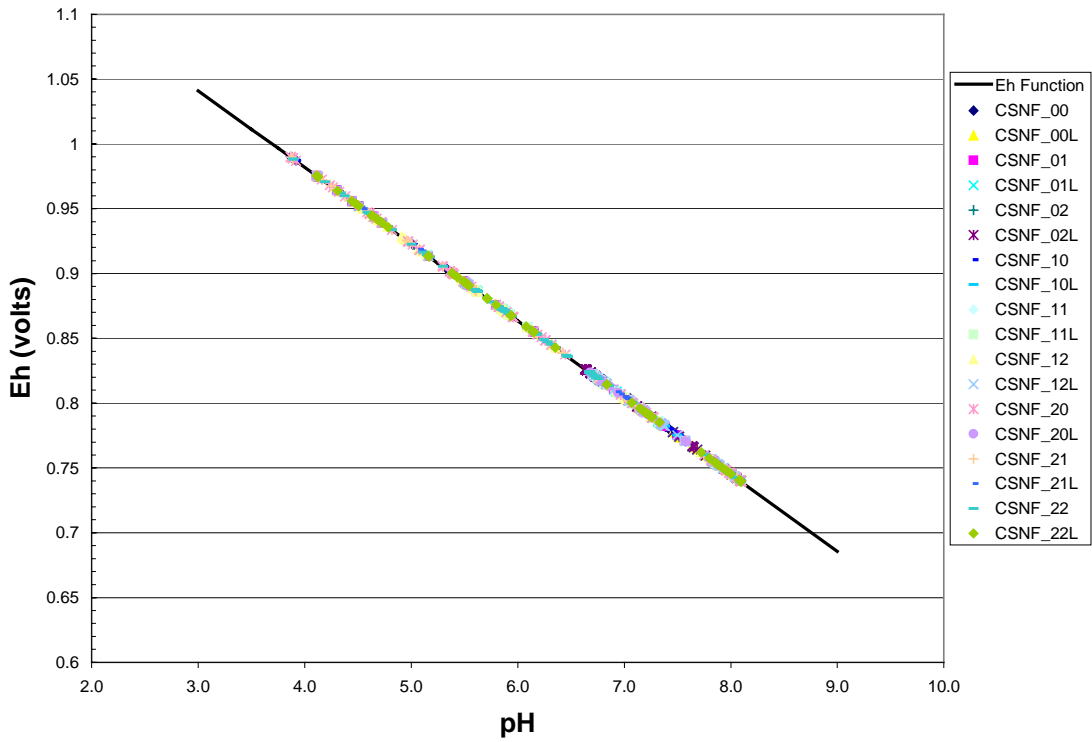


Figure 9. Eh as a function of pH for CSNF, at $\log(\text{FO}_2) = -0.7$ (data values from CRWMS M&O 2000a, DTN: SN0009T0811199.008)

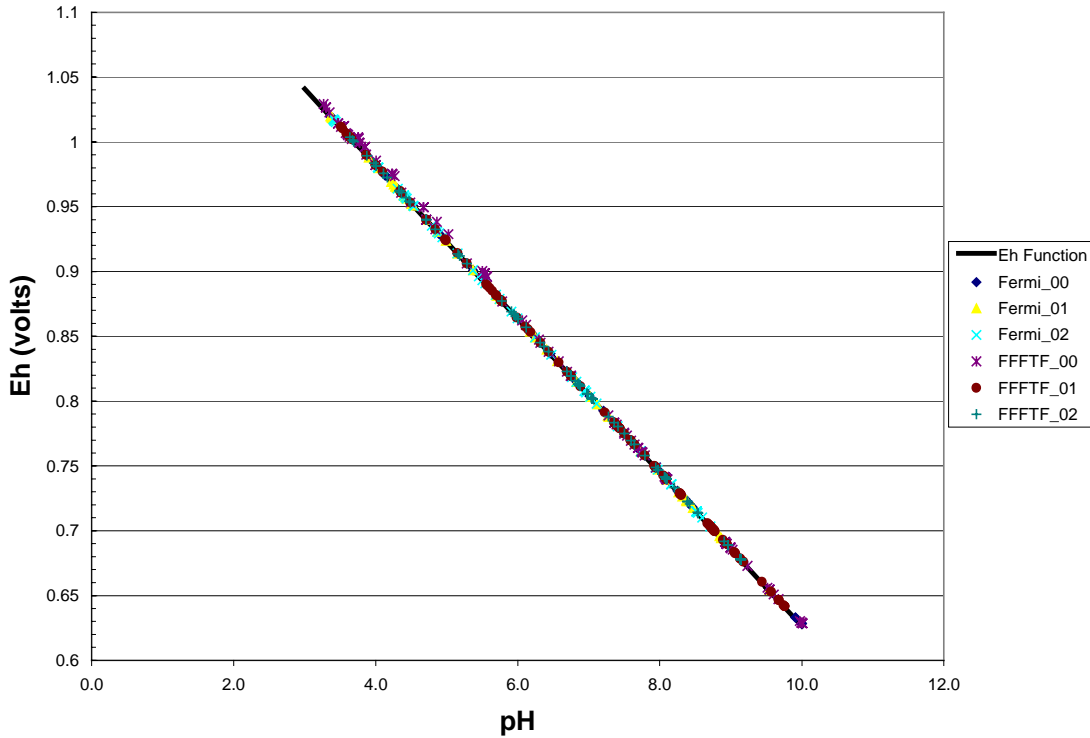


Figure 10. Eh as a function of pH for co-disposal, at $\log(\text{FO}_2) = -0.7$ (data values from CRWMS M&O 2000a, DTN: SN0009T0811199.008)

6.4 IONIC STRENGTH, CHLORIDE, AND FLUORIDE ABSTRACTION

The ionic strength (I), chloride (Cl), and fluoride (F) abstractions are discussed in the following subsections. In the following tables (Tables 16 – 20) it should be noted that the parameters listed at the bottom of each table (maximum, minimum, median, and standard deviation) refer to the relationship that value has with respect to the stated property at the top of the table. For example, in Table 16, the ionic strength values in the body of the table represent the minimum and maximum values of ionic strength over the stated period of each simulation for each scenario. While the maximum, minimum, median, and standard deviation listed at the bottom of Table 16 represents the minimum of the minimums, the maximum of the maximums, and so on. Therefore, for the TSPA the maximum and minimum values, as listed in the tables, should be used as bounds for each of these parameters, and sampling should occur within these bounds. Unless otherwise stated uniform distributions should be implemented for each sampled parameter.

Note that the minimum, maximum, median, and standard deviation values reported in Tables 16 - 20 were calculated in EXCEL using the “MIN”, “MAX”, “MEDIAN”, and “STDEV” intrinsic functions, respectively, for each time period. Tables 16 – 20 are contained in “CSNF_ABSTRACTION.XLS” and “CO-DISPOSAL_ABSTRACTION.XLS” under DTN: MO0011SPAIPC37.002, for CSNF and co-disposal, respectively.

The DTN for the “raw” values in the following tables is SN0009T0811199.008. These are the data which are output from the process model(s) (CRWMS M&O 2000a). Note also the DTN for the maximum, minimum, average and standard deviation listed at the bottom of each of the following tables is MO0011SPAIPC37.002, this is the abstracted “data” to be used in the TSPA.

Validation of the abstraction models for I, Cl, and F is implicit because simple ranges are used, or in the case of Cl a constant value, which directly reflects the process model output.

6.4.1 CSNF Ionic Strength Abstraction

The ionic strength is used in determining the colloid content of the water exiting the waste package. Figure 11 shows the ionic strength histories for the CSNF runs, which differ from the pH histories (Figure 1) in the timing of the trends. Therefore, a different time discretization was used for ionic strength as compared to the pH time discretization. The ionic strength abstraction is broken into three time periods where first and third period implements the same distribution and the second period implements a separate distribution. Figure 11 confirms that each of the modeled scenarios achieves a maximum between 200 and 100,000 years, therefore the ionic strength abstraction is divided into three periods, 0 –200 years, 200 – 100,000 years, and 100,000 to 1E6 years. Tables 16 and 17 summarize the values that should be used in the generation of distributions for the CSNF ionic strength abstraction.

Table 16. CSNF ionic strength distribution information for 0 – 200 years, and 100,000 to 1E6 years. (data from CRWMS M&O 2000a, DTN: SN0009T0811199.008, abstracted information, DTN: MO0011SPAIPC37.002).

EQ6 input file (*.6i)	Water Flux(l/yr)	Fuel Exposure	Corrosion Case	Minimum	Maximum
CSNF_10	0.15	0.1	Base Case	1.22E-03	4.05E-02
CSNF_11	1.5	0.1	Base Case	1.22E-03	3.54E-02
CSNF_12	15	0.1	Base Case	2.59E-03	2.62E-02
CSNF_20	0.15	0.01	Base Case	1.22E-03	3.70E-02
CSNF_21	1.5	0.01	Base Case	1.22E-03	3.65E-02
CSNF_22	15	0.01	Base Case	2.57E-03	3.19E-02
CSNF_10L	0.15	0.1	Low	1.22E-03	4.56E-02
CSNF_11L	1.5	0.1	Low	2.42E-03	8.63E-03
CSNF_12L	15	0.1	Low	1.22E-03	4.56E-02
CSNF_20L	0.15	0.01	Low	1.22E-03	4.55E-02
CSNF_21L	1.5	0.01	Low	2.51E-03	8.45E-03

In-Package Chemistry Abstraction

Table 16 continued

EQ6 input file (*.6i)	Water Flux(l/yr)	Fuel Exposure	Corrosion Case	Minimum	Maximum
CSNF_22L	15	0.01	Low	1.22E-03	4.55E-02
			Minimum	1.22E-03	N/A
			Maximum	N/A	4.56E-02
			Median		5.52E-03
			Standard Deviation		1.89E-02

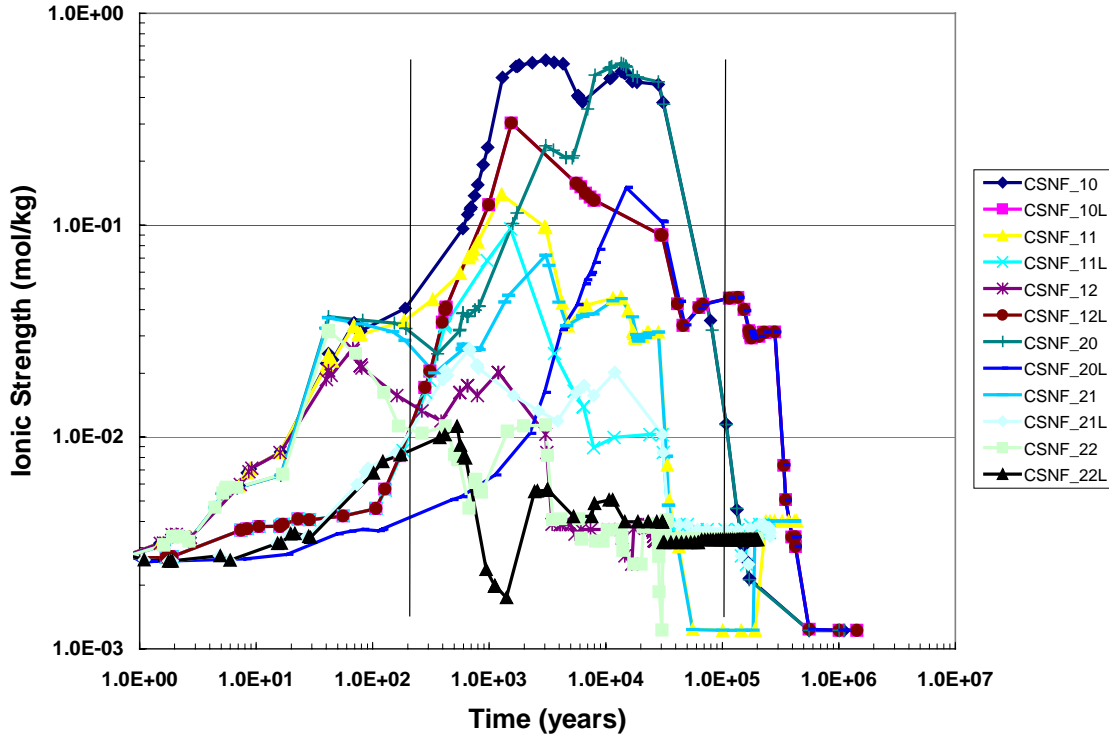


Figure 11. Ionic strength histories for CSNF waste packages (data values from CRWMS M&O 2000a, DTN: SN0009T0811199.008)

Table 17. CSNF ionic strength distribution information for 200 to 100,000. (data from CRWMS M&O 2000a, DTN: SN0009T0811199.008, abstracted information DTN: MO0011SPAIPC37.002).

EQ6 input file(*.6i)	Water Flux(l/yr)	Fuel Exposure	Corrosion Case	Minimum	Maximum
CSNF_10	0.15	0.1	base case	3.55E-02	6.00E-01
CSNF_11	1.5	0.1	base case	1.24E-03	1.40E-01
CSNF_12	15	0.1	base case	2.51E-03	2.02E-02
CSNF_20	0.15	0.01	base case	2.47E-02	5.82E-01
CSNF_21	1.5	0.01	base case	1.23E-03	7.21E-02
CSNF_22	15	0.01	base case	1.23E-03	1.14E-02
CSNF_10L	0.15	0.1	low	1.71E-02	3.03E-01

Table 17 continued					
EQ6 input file(*.6i)	Water Flux(l/yr)	Fuel Exposure	Corrosion Case	Minimum	Maximum
CSNF_11L	1.5	0.1	low	3.48E-03	9.60E-02
CSNF_12L	15	0.1	low	1.71E-02	3.03E-01
CSNF_20L	0.15	0.01	low	5.06E-03	1.50E-01
CSNF_21L	1.5	0.01	low	3.48E-03	2.62E-02
CSNF_22L	15	0.01	low	2.19E-02	1.40E-01
			Minimum	1.23E-03	NA
			Maximum	NA	6.00E-01
			Median	2.33E-02	
			Standard Deviation	1.73E-01	

6.4.2 Co-Disposal Ionic Strength Abstraction

The ionic strength histories for co-disposal packages are displayed in Figure 12. Like the CSNF ionic strength abstraction the co-disposal abstraction for ionic strength may be discretized using the same time divisions, 0 –200 years, 200 – 100,000 years, and 100,000 to 1E6 years.

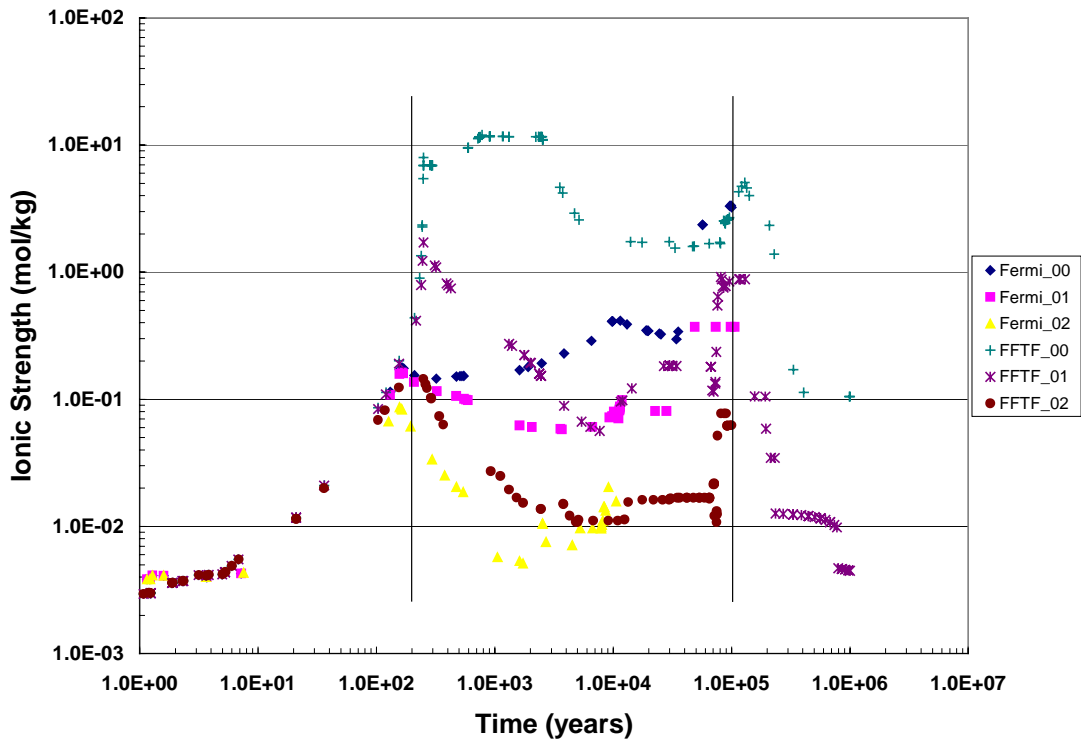


Figure 12. Ionic strength histories for co-disposal packages (data values from CRWMS M&O 2000a, DTN: SN0009T0811199.008)

Table 18 and 19 provide the distribution information for the ionic strength abstraction. It is suggested that a triangular distribution be used to describe the ionic strength behavior for co-disposal packages. The corners of the triangle should be defined by the minimum, maximum and median values. The rationale for using a triangular distribution is that the maximum value of ionic strength is very high and assigning the maximum probability to the median would tend to remove some of the bias for the high values, and would be conservative with respect to colloid generation.

Table 18. Co-Disposal ionic strength distribution information for 0 - 200 and 100,000 to 1E6 years. (data from CRWMS M&O 2000a, DTN: SN0009T0811199.008, abstracted information DTN: MO0011SPAIPC37.002).

EQ6 File (*.6i)	Q(I/yr)	Minimum	Maximum
FFTF_00	0.15	2.64E-03	5.07E+00
FFTF_01	1.5	2.64E-03	8.80E-01
FFTF_02	15	2.64E-03	1.23E-01
Fermi_00	0.15	2.55E-03	1.78E-01
Fermi_01	1.5	2.55E-03	1.63E-01
Fermi_02	15	2.55E-03	8.68E-02
	Minimum	2.55E-03	NA
	Maximum	NA	5.07E+00
	Median	4.47E-02	
	Standard Deviation	1.446085	

Table 19. Co-Disposal ionic strength distribution information for 200 to 100,000 years. (data from CRWMS M&O 2000a, DTN: SN0009T0811199.008, abstracted information DTN: MO0011SPAIPC37.002).

EQ6 File (*.6i)	Q(I/yr)	Minimum	Maximum
FFTF_00	0.15	4.38E-01	1.20E+01
FFTF_01	1.5	5.64E-02	1.71E+00
FFTF_02	15	1.08E-02	1.45E-01
Fermi_00	0.15	1.46E-01	3.34E+00
Fermi_01	1.5	5.80E-02	3.71E-01
Fermi_02	15	5.12E-03	3.37E-02
	Minimum	5.12E-03	NA
	Maximum	NA	1.20E+01
	Median	1.45E-01	
	Standard Deviation	3.439424	

6.4.3 Chloride

Chloride is used for the waste package corrosion model. Since chloride is geochemically conservative under the modeled conditions, the value used in the abstraction is equal to J-13 input value of 2.023E-04 mol/kg. It should be noted that because of its conservative nature the concentration of chloride contacting a waste package will vary in accordance to the composition of the seepage dripping on to a package. However, in the absence of further data it is not possible in this abstraction model to pose other chloride values.

6.4.4 Fluoride

Fluoride is used in the cladding model. A simple range of values should be applied to the entire duration consisting of the maximum values. Fluoride is only pertinent for the CSNF because there is no cladding in the co-disposal package. Table 20 provides the distribution information for fluoride, it is suggested that a uniform distribution be applied to the fluoride data.

Table 20. CSNF fluoride distribution information for 0 to 1E6 years (data from CRWMS M&O 2000a, DTN: SN0009T0811199.008, abstracted information DTN: MO0011SPAIPC37.002).

EQ6 input file(*.6i)	Q(l/yr)	Fuel Exposure	Corrosion Case	Minimum F	Maximum F
CSNF_10	0.15	0.1	base case	9.48E-06	1.38E-04
CSNF_11	1.5	0.1	base case	1.21E-05	2.06E-04
CSNF_12	15	0.1	base case	1.57E-05	7.71E-04
CSNF_20	0.15	0.01	base case	1.11E-05	1.37E-04
CSNF_21	1.5	0.01	base case	1.41E-05	2.74E-04
CSNF_22	15	0.01	base case	2.51E-05	7.71E-04
CSNF_10L	0.15	0.1	low	1.22E-03	3.03E-01
CSNF_11L	1.5	0.1	low	2.42E-03	9.60E-02
CSNF_12L	15	0.1	low	2.82E-05	2.03E-04
CSNF_20L	0.15	0.01	low	2.74E-05	2.07E-04
CSNF_21L	1.5	0.01	low	1.57E-05	7.71E-04
CSNF_22L	15	0.01	low	1.21E-05	2.06E-04
			Minimum	9.48E-06	NA
			Maximum	NA	3.03E-01
			Median	1.71E-04	
			Standard Deviation	6.40E-02	

6.5 OXYGEN AND CARBON DIOXIDE FUGACITY ABSTRACTION

Both oxygen (O₂) and carbon dioxide (CO₂) fugacities were set to constant values for all times in the process models (CRWMS M&O 2000a). Therefore, the abstracted gas fugacities are also set to constants for the modeled duration. Table 21 summarizes the gas abstraction information.

There is no uncertainty associated with the O₂ and CO₂ abstraction because they are a simple reflection of the process model (CRWMS M&O 2000a) input.

Note that alternate fugacities for O₂ were run as a sensitivity case in CRWMS M&O 2000a and the pH ranges obtained for these alternate gas compositions was not out of the range of those used in the CSNF pH abstraction (Section 6.1.1). Given that the total carbonate and Eh abstractions (Sections 6.2 and 6.3) were derived as functions of CO₂ and O₂ fugacity, the range of applicable gas fugacities may be expanded to include the range used in CRWMS M&O 2000a.

Table 21. Gas Abstraction Information (from CRWMS M&O 2000a, DTN: SN0009T0811199.008).

Gas	Log fugacity
Oxygen	-3.5 to -0.7
Carbon Dioxide	-3.0 to -2.0

6.6 ABSTRACTION VALIDATION

This abstraction model uses mathematical relationships and statistical distributions to fit TPO, i.e., TPO is used as input for the abstraction. Thus, TPO was used to generate the abstraction model, i.e., to generate the mathematical relationships and statistical distributions. Therefore, the acceptance criteria, for the abstraction relationships, is that they reflect the TPO used in their generation. In other words, validation of the abstraction model requires comparison of abstracted parameter values to their corollary TPO parameter values. It must be emphasized that this does not constitute validation of the TPO, but only that the abstraction can reproduce a subset of the process model output through the use of mathematical relationships.

Validation of the CSNF and co-disposal pH abstractions is implicit in method by which the pH response surfaces, lines and distributions were developed. The validation process used for the CSNF pH abstraction was comparison of the abstracted pH for each time period to the TPO value from CRWMS M&O 2000a for a given set of input parameters within the ranges defined in Table 12. The response surfaces are mathematical constructs whose limits were set by the process models inputs (CRWMS M&O 2000a) and outputs (DTN: SN0009T0811199.008). The pH abstractions represent a best fit to the process model data, and are therefore able to reproduce the process model output for given set of input conditions within a range of uncertainty, thus rendering them self validating.

The total carbonate and Eh relationships use process model input data and an abstracted pH value to calculate a total carbonate concentration and Eh values in solution at a given time. The ability for these relationships to reproduce process model output was demonstrated in Sections 6.2 and 6.3, respectively. In other words the total carbonate and ionic strength abstractions were validated by comparison to TPO.

The remaining parameters, ionic strength, fluoride, and chloride concentrations were set to distributions where the values were taken directly from the TPO for both CSNF and co-disposal and are thus self validated.

7. CONCLUSIONS

7.1 ABSTRACTION MODEL SUMMARY

The purpose of this AMR, as directed by the TWP (CRWMS M&O 2000b) was to develop the in-package chemistry abstraction model. This was accomplished by using the input for and the output from the in-package process models (CRWMS M&O 2000a) and then reducing it to a form usable by the TSPA.

The chemical parameter pH was used as a “key” parameter where response surfaces were generated with pH as a function of the independent parameters, water flux, WP corrosion rate, and fuel exposure for CSNF packages, for co-disposal packages a distribution of pH was generated. Relationships were formulated between pH and total carbonate and pH and Eh such that for any set of independent parameters the pH, total carbonate, and Eh could be directly calculated.

The additional parameters of ionic strength, chloride, and fluoride also included in the abstraction model showed only small variability in concentration over the time domain of the models. Therefore, sampling ranges for their concentrations were set. No systematic variation of these parameters was observed with respect to pH, therefore, it was not possible to derive a formulation to explicitly calculate their concentration as a function of pH.

The data developed under this abstraction model include mathematical formulations and parameter ranges for specific aqueous chemical properties and/or constituents. All of the developed data are contained in DTN: MO0011SPAIPC37.002.

7.2 EVALUATION OF NRC ISSUE RESOLUTION STATUS REPORT CRITERIA

As this documentation contains only the abstraction of the in-package chemistry for waste forms, not all of the criteria in Section 4.2 can be evaluated nor do they all apply at this time.

From Section 4.2.1.1 (Data and Model Justification Acceptance Criteria), as an abstraction this AMR does not address the criteria in this section.

From Section 4.2.1.2 (Data Uncertainty and Verification Acceptance Criteria), as an abstraction this AMR does not address the criteria in this section.

For Section 4.2.1.3 (Model Uncertainty Acceptance Criteria), as an abstraction this AMR does not address the criteria in this section.

For Section 4.2.1.4 (Model Verification Acceptance Criteria), as an abstraction this AMR does not address the criteria in this section.

7.3 TO BE VERIFIED (TBV) IMPACT

There are no TBV's in this AMR, all of the data used for this abstraction are TPO. Note: this document may be affected by technical product input information that requires confirmation. Any changes to the document or its conclusions that may occur, as a result of completing the confirmation activities will be reflected in subsequent revisions. The status of the technical product input information quality may be confirmed by review of the DIRS database.

7.4 FEPs EVALUATION

This AMR being an abstraction is not subject to FEPs in the sense that as an abstraction it is a mathematical simplification of the process model results. A discussion of the FEPs that may impact the in-package chemistry is covered in the *In-Package Chemistry for Waste Forms* (CRWMS M&O 2000a).

8. INPUTS AND REFERENCES

8.1 DOCUMENTS CITED

CRWMS M&O 2000a. *Summary of In-Package Chemistry for Waste Forms*. ANL-EBS-MD-000050 REV 01. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0735

CRWMS M&O 2000b. *Technical Work Plan for Waste Form Degradation Process Model Report for SR*. TWP-EBS-MD-000006 Rev. 00. Las Vegas, Nevada: CRWMS M&O.ACC: MOL.20001204.0036.

Drever, J.I. 1988. *The Geochemistry of Natural Waters*. 2nd Edition. Englewood Cliffs, New Jersey: Prentice Hall. TIC: 242836.

8.2 DATA

SN0009T0811199.008. Revised Range of Waste Package Effluent Compositions. Submittal date: 09/28/2000.

8.3 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

Procedures listed below are retrievable from the OCRWM Program Documents database contained in Lotus Notes 4.6 and the BSC INTRANET.

AP-3.10Q, Rev. 2, ICN 3, BSCN 1. *Analyses and Models*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management.

AP-SV.1Q, Rev. 0, ICN 2. *Control of the Electronic Management of Information*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management.

AP-2.21Q, Rev. 0, ICN 0, BSCN 1. *Quality Determinations and Planning for Scientific, Engineering, and Regulatory Compliance Activities*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management.

ASTM C 1174-97. 1998. *Standard Practice for Prediction of the Long-Term Behavior of Materials, Including Waste Forms, Used in Engineered Barrier Systems (EBS) for Geological Disposal of High-Level Radioactive Waste*. West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 246015

Dyer, J.R. 1999. "Revised Interim Guidance Pending Issuance of New U.S. Nuclear Regulatory Commission (NRC) Regulations (Revision 01, July 22, 1999), for Yucca Mountain, Nevada." Letter from J.R. Dyer (DOE/YMSCO) to D.R. Wilkins (CRWMS M&O), September 3, 1999, OL&RC:SB-1714, with enclosure, "Interim Guidance Pending Issuance of New NRC Regulations for Yucca Mountain (Revision 01)." ACC: MOL.19990910.0079.

NRC (U.S. Nuclear Regulatory Commission) 1999. *Issue Resolution Status Report Key Technical Issue: Evolution of the Near-Field Environment*. Rev. 2. Washington, D.C.: U.S. Nuclear Regulatory Commission. ACC: MOL.19990810.0640.

64 FR 8640. Disposal of High-Level Radioactive Wastes in a Proposed Geologic Repository at Yucca Mountain, Nevada. Proposed rule 10 CFR Part 63. Readily Available.

QAP-2-3, Rev. 10, BSCN 2. Classification of Permanent Items. Las Vegas, Nevada: CRWMS M&O.

YMP (Yucca Mountain Site Characterization Project) 2000. Q-List. YMP/90-55Q, Rev. 6. Las Vegas, Nevada: Yucca Mountain Site Characterization Office. ACC: MOL.20000510.0177.

8. ATTACHMENTS

Attachment	Title
I	SigmaPlot Regression Analyses Data Output

ATTACHMENT I
SigmaPlot Regression Analyses Data Output

<200 years Base Case Corrosion Rates
Nonlinear Regression

[Variables]
x = col(2)
y = col(3)
z = col(5)
'Automatic Initial Parameter Estimates
F(q,r)=ape(q,r,1,0,1)
[Parameters]
y0=F(x,z)[1] "Auto
a=F(x,z)[2] "Auto
b=F(y,z)[2] "Auto
[Equations]
f=y0+a*x+b*y
fit f to z
[Constraints]
[Options]
tolerance=0.000100
stepsize=100
iterations=100

R = 0.99989944 Rsqr = 0.99979889 Adj Rsqr = 0.99966481

Standard Error of Estimate = 0.0062

	Coefficient	Std. Error	t	P
y0	3.7950	0.0045	844.5058	<0.0001
a	0.0025	0.0004	6.7105	0.0068
b	6.8296	0.0560	121.9389	<0.0001

Analysis of Variance:

	DF	SS	MS	F	P
Regression	2	0.5684	0.2842	7457.0668	<0.0001
Residual	3	0.0001	0.0000		
Total	5	0.5686	0.1137		

PRESS = 0.0008

Durbin-Watson Statistic = 1.4936

Normality Test: Passed (P = 0.3919)

Constant Variance Test: Passed (P = 0.0600)

In-Package Chemistry Abstraction for TSPA-LA

Power of performed test with alpha = 0.0500: 1.0000

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
2	4.4784	-0.0034	-0.5472	-0.7322	-0.6597
3	4.4818	-0.0028	-0.4509	-0.5793	-0.5019
4	4.5158	0.0062	0.9981	1.7230	13.8047
5	3.8637	0.0033	0.5326	0.7127	0.6384
6	3.8671	0.0029	0.4669	0.5999	0.5221
7	3.9012	-0.0062	-0.9996	-1.7255	-16.2666

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
2	0.1412	0.4414	-0.5865
3	0.0728	0.3941	-0.4048
4	1.9593	0.6644	19.4243
5	0.1338	0.4414	0.5676
6	0.0780	0.3941	0.4211
7	1.9650	0.6644	-22.8884

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
2	4.4784	4.4653	4.4914	4.4548	4.5020
3	4.4818	4.4694	4.4941	4.4586	4.5050
4	4.5158	4.4998	4.5319	4.4905	4.5412
5	3.8637	3.8507	3.8768	3.8401	3.8873
6	3.8671	3.8548	3.8795	3.8439	3.8903
7	3.9012	3.8852	3.9172	3.8758	3.9265

<200 years, Low Corrosion Rates
Nonlinear Regression

[Variables]

x = col(8)

y = col(9)

z = col(11)

'Automatic Initial Parameter Estimates

F(q,r)=ape(q,r,1,0,1)

[Parameters]

y0=F(x,z)[1] "Auto

a=F(x,z)[2] "Auto

b=F(y,z)[2] "Auto

[Equations]

f=y0+a*x+b*y

fit f to z

[Constraints]

[Options]

tolerance=0.000100

stepsize=100

In-Package Chemistry Abstraction for TSPA-LA

iterations=100

R = 0.76519908 Rsqr = 0.58552963 Adj Rsqr = 0.30921605

Standard Error of Estimate = 0.8637

	Coefficient	Std. Error	t	P
y0	5.4198	0.6287	8.6209	0.0033
a	-0.0394	0.0526	-0.7501	0.5077
b	15.0214	7.8356	1.9171	0.1511

Analysis of Variance:

	DF	SS	MS	F	P
Regression	2	3.1615	1.5808	2.1191	0.2668
Residual	3	2.2379	0.7460		
Total	5	5.3994	1.0799		

PRESS = 8.0655

Durbin-Watson Statistic = 2.2187

Normality Test: Passed (P = 0.2214)

Constant Variance Test: Passed (P = 0.0600)

Power of performed test with alpha = 0.0500: 0.4157

The power of the performed test (0.4157) is below the desired power of 0.8000.
You should interpret the negative findings cautiously.

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
2	6.9160	-0.2130	-0.2466	-0.3300	-0.2744
3	6.8627	-0.1597	-0.1850	-0.2376	-0.1959
4	6.3302	0.3728	0.4316	0.7451	0.6739
5	5.5641	1.1179	1.2944	1.7319	104.9039
6	5.5108	-0.8358	-0.9677	-1.2433	-1.4580
7	4.9783	-0.2823	-0.3268	-0.5642	-0.4872

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
2	0.0287	0.4414	-0.2440
3	0.0122	0.3941	-0.1580
4	0.3664	0.6644	0.9482
5	0.7902	0.4414	93.2597
6	0.3352	0.3941	-1.1760
7	0.2101	0.6644	-0.6855

95% Confidence:

In-Package Chemistry Abstraction for TSPA-LA

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
2	6.9160	5.0898	8.7422	3.6160	10.2160
3	6.8627	5.1371	8.5884	3.6173	10.1082
4	6.3302	4.0897	8.5707	2.7841	9.8763
5	5.5641	3.7378	7.3903	2.2640	8.8641
6	5.5108	3.7852	7.2364	2.2654	8.7562
7	4.9783	2.7378	7.2187	1.4322	8.5244

200 - 10K years, Base Case Corrosion Rates
Nonlinear Regression

[Variables]

x = col(2)

y = col(3)

z = col(5)

'Automatic Initial Parameter Estimates

F(q,r)=ape(q,r,1,0,1)

[Parameters]

y0=F(x,z)[1] "Auto

a=F(x,z)[2] "Auto

b=F(y,z)[2] "Auto

[Equations]

f=y0+a*x+b*y

fit f to z

[Constraints]

[Options]

tolerance=0.000100

stepsize=100

iterations=100

R = 0.90134342 Rsqr = 0.81241995 Adj Rsqr = 0.68736659

Standard Error of Estimate = 0.2838

	Coefficient	Std. Error	t	P
y0	6.0496	0.2066	29.2841	<0.0001
a	-0.0084	0.0173	-0.4860	0.6603
b	9.1963	2.5748	3.5717	0.0375

Analysis of Variance:

	DF	SS	MS	F	P
Regression	2	1.0466	0.5233	6.4966	0.0812
Residual	3	0.2416	0.0805		
Total	5	1.2882	0.2576		

PRESS = 1.3888

Durbin-Watson Statistic = 1.5796

In-Package Chemistry Abstraction for TSPA-LA

Normality Test: Passed (P = 0.1386)

Constant Variance Test: Passed (P = 0.0600)

Power of performed test with alpha = 0.0500: 0.7265

The power of the performed test (0.7265) is below the desired power of 0.8000.
You should interpret the negative findings cautiously.

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
2	6.9680	0.2960	1.0429	1.3954	1.9233
3	6.9567	-0.0717	-0.2526	-0.3245	-0.2697
4	6.8433	-0.2243	-0.7903	-1.3643	-1.8080
5	6.1404	-0.0654	-0.2303	-0.3081	-0.2556
6	6.1290	-0.1820	-0.6413	-0.8239	-0.7648
7	6.0156	0.2474	0.8716	1.5046	2.4797

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITs
2	0.5130	0.4414	1.7098
3	0.0228	0.3941	-0.2175
4	1.2283	0.6644	-2.5440
5	0.0250	0.4414	-0.2273
6	0.1472	0.3941	-0.6169
7	1.4939	0.6644	3.4891

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
2	6.9680	6.3679	7.5681	5.8836	8.0524
3	6.9567	6.3896	7.5237	5.8902	8.0231
4	6.8433	6.1071	7.5795	5.6781	8.0085
5	6.1404	5.5403	6.7405	5.0560	7.2247
6	6.1290	5.5620	6.6961	5.0626	7.1955
7	6.0156	5.2794	6.7519	4.8504	7.1809

200 - 10K years, Low Corrosion Rates
Nonlinear Regression

[Variables]

x = col(8)

y = col(9)

z = col(11)

'Automatic Initial Parameter Estimates

F(q,r)=ape(q,r,1,0,1)

[Parameters]

y0=F(x,z)[1] "Auto

In-Package Chemistry Abstraction for TSPA-LA

a=F(x,z)[2] "Auto
 b=F(y,z)[2] "Auto
 [Equations]
 f=y0+a*x+b*y
 fit f to z
 [Constraints]
 [Options]
 tolerance=0.000100
 stepsize=100
 iterations=100

R = 0.81242016 Rsqr = 0.66002652 Adj Rsqr = 0.43337753

Standard Error of Estimate = 0.4267

	Coefficient	Std. Error	t	P
y0	6.4146	0.3106	20.6524	0.0002
a	-0.0180	0.0260	-0.6938	0.5377
b	8.9477	3.8711	2.3114	0.1039

Analysis of Variance:

	DF	SS	MS	F	P
Regression	2	1.0605	0.5302	2.9121	0.1982
Residual	3	0.5462	0.1821		
Total	5	1.6067	0.3213		

PRESS = 2.1538

Durbin-Watson Statistic = 2.0956

Normality Test: Passed (P = 0.4745)

Constant Variance Test: Passed (P = 0.0600)

Power of performed test with alpha = 0.0500: 0.5017

The power of the performed test (0.5017) is below the desired power of 0.8000.
 You should interpret the negative findings cautiously.

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
2	7.3067	-0.0377	-0.0882	-0.1181	-0.0966
3	7.2823	-0.1923	-0.4507	-0.5791	-0.5017
4	7.0390	0.2300	0.5390	0.9305	0.9008
5	6.5014	0.5406	1.2670	1.6953	6.7535
6	6.4770	-0.3610	-0.8461	-1.0870	-1.1400
7	6.2337	-0.1797	-0.4211	-0.7270	-0.6539

Influence Diagnostics:

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Row	Cook'sDist	Leverage	DFFITS
2	0.0037	0.4414	-0.0859
3	0.0727	0.3941	-0.4046
4	0.5714	0.6644	1.2675
5	0.7571	0.4414	6.0039
6	0.2562	0.3941	-0.9195
7	0.3488	0.6644	-0.9201

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
2	7.3067	6.4044	8.2089	5.6763	8.9370
3	7.2823	6.4298	8.1349	5.6789	8.8857
4	7.0390	5.9321	8.1459	5.2871	8.7909
5	6.5014	5.5991	7.4036	4.8710	8.1317
6	6.4770	5.6245	7.3296	4.8736	8.0804
7	6.2337	5.1268	7.3406	4.4818	7.9856

10K to 300K years, Base Case Corrosion Rates
Nonlinear Regression

[Variables]

x = col(2)

y = col(5)

'Automatic Initial Parameter Estimate Functions

F(q)=ape(x,y,1,0,1)

[Parameters]

y0=F(0)[1] "Auto

a=F(0)[2] "Auto

[Equations]

f=y0+a*x

fit f to y

[Constraints]

[Options]

tolerance=0.000100

stepsize=100

iterations=100

R = 0.98967427 Rsqr = 0.97945516 Adj Rsqr = 0.97431895

Standard Error of Estimate = 0.0819

	Coefficient	Std. Error	t	P
y0	3.9306	0.0434	90.5192	<0.0001
a	0.0689	0.0050	13.8093	0.0002

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	1.2802	1.2802	190.6961	0.0002
Residual	4	0.0269	0.0067		

In-Package Chemistry Abstraction for TSPA-LA

Total 5 1.3071 0.2614

PRESS = 0.0585

Durbin-Watson Statistic = 2.3462

Normality Test: Passed (P = 0.1573)

Constant Variance Test: Passed (P = 0.0600)

Power of performed test with alpha = 0.0500: 0.9953

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
2	3.9410	-0.0710	-0.8662	-1.0171	-1.0231
3	4.0340	0.0770	0.9400	1.0695	1.0961
4	4.9640	-0.0560	-0.6840	-0.9652	-0.9544
5	3.9410	-0.0700	-0.8540	-1.0028	-1.0038
6	4.0340	0.0780	0.9522	1.0834	1.1162
7	4.9640	0.0420	0.5120	0.7225	0.6710

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
2	0.1960	0.2748	-0.6297
3	0.1684	0.2275	0.5948
4	0.4616	0.4977	-0.9501
5	0.1905	0.2748	-0.6178
6	0.1728	0.2275	0.6057
7	0.2586	0.4977	0.6680

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
2	3.9410	3.8217	4.0602	3.6841	4.1978
3	4.0340	3.9255	4.1425	3.7819	4.2860
4	4.9640	4.8035	5.1245	4.6856	5.2425
5	3.9410	3.8217	4.0602	3.6841	4.1978
6	4.0340	3.9255	4.1425	3.7819	4.2860
7	4.9640	4.8035	5.1245	4.6856	5.2425

10K - 300K years, Low Corrosion Rate

Nonlinear Regression

[Variables]

x = col(8)

y = col(11)

'Automatic Initial Parameter Estimate Functions

F(q)=ape(x,y,1,0,1)

[Parameters]

y0=F(0)[1] "Auto

In-Package Chemistry Abstraction for TSPA-LA

a=F(0)[2] "Auto
[Equations]
f=y0+a*x
fit f to y
[Constraints]
[Options]
tolerance=0.000100
stepsize=100
iterations=100

The regression produces a perfect fit

R = >1e20 Rsqr = >1e20 Adj Rsqr = >1e20

Standard Error of Estimate = 0.0000

	Coefficient
y0	4.1110
a	0.0000

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	0.0000	0.0000	>1e20	1.0000
Residual	2	0.0000	0.0000		
Total	3	0.0000	0.0000		

PRESS = 0.0000

Durbin-Watson Statistic = >1e20

Normality Test: Failed (P = <0.0001)

Constant Variance Test: Failed (P = <0.0001)

Power of performed test with alpha = 0.0500: 1.0000