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NM3507

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET

Complete Only Applicable Items

1. QA: QA

2. ☐ Analysis — Check all that apply

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

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

Describe use:

3. ☒ Model — Check all that apply

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

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

Describe use: This abstraction is planned to be used as input to the TSPA to calculate waste form degradation, radionuclide solubilities, waste package degradation, cladding degradation, and colloid generation.

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9. Checker	Pengchu Zhang (Technical)	Robert MacKinnon for	3/27/00
	William R. Hoey (Compliance)	William R. Hoey	3/27/00
10. Lead/Supervisor	James Nowak	Robert MacKinnon for	3/27/00
11. Responsible Manager	Robert MacKinnon	Robert MacKinnon	3/27/00

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Enclosure 17

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL REVISION RECORD

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LIST OF ACRONYMS

AMR	Analysis Model Report
CC	cladding coverage
CDSP	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	United States Department of Energy
EBS	Engineered Barrier System
FEP's	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
TSPA	Total-System Performance Assessment
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 Development Plan (CRWMS M&O 1999a), is to develop the in-package (waste package) chemistry abstraction model. This model will use the in-package chemistry process models (CRWMS M&O 2000a) as the data source for the abstraction. 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 cladding coverage (CC) or glass dissolution rate (GDR)), from which Eh and total carbonate are calculated. The parameters of ionic strength, chloride, and fluoride will be set to fixed ranges. 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, therefore the abstraction has a relatively high importance.

2. QUALITY ASSURANCE

The Quality Assurance (QA) program applies to the development of this model abstraction documentation. The Performance Assessment Operations responsible manager has evaluated the technical document development activity in accordance with QAP-2-0, *Conduct of Activities*. The QAP-2-0 activity evaluation, *Activity Evaluation for Conduct of Performance Assessment* (CRWMS M&O 1999b), has determined that the preparation and review of this technical document is subject to *Quality Assurance Requirements and Description* (QARD) DOE/RW-0333P (DOE 2000) requirements.

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. The regression analysis performed using SigmaPlot is an intrinsic function of SigmaPlot, and, therefore, does not constitute a single use routine. 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 following document: *Summary of 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 dependant aqueous concentration data, also from the in-package process models (CRWMS M&O 2000a, DTN: SN9911T0811199.005). The model output from CRWMS M&O 2000a, which is under DTN: SN9911T0811199.005 is unqualified, due to the use of unqualified inputs in CRWMS M&O, 2000a, and therefore labeled TBV. Both of these data types were documented in the *Summary of 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 *Summary of 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 – these two parameters were suited for both the Commercial Spent Nuclear Fuels (CSNF) packages as well as the DOE co-disposal packages (CDSP) simulations. In addition, for the CSNF packages the fraction of cladding present was also varied and for the CDSP 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 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: SN9911T0811199.005)

EQ6 File Name (*.6i)	Water Flux (m^3/yr)	WP Corrosion Rate[1]	Cladding Coverage (%)	Glass Dissolution Rate (GDR)[2]
CSNF_000	0.0015	Low	1%	N/A
CSNF_001	0.015	Low	1%	N/A
CSNF_002	0.15	Low	1%	N/A
CSNF_010	0.0015	High	99%	N/A
CSNF_011	0.015	High	99%	N/A

Table 1 continued

EQ6 File Name (*.6l)	Water Flux (m^3/yr)	WP Corrosion Rate[1]	Cladding Coverage (%)	Glass Dissolution Rate[2]
CSNF_012	0.15	High	99%	N/A
CSNF_100	0.0015	Low	1%	N/A
CSNF_101	0.015	Low	1%	N/A
CSNF_102	0.15	Low	1%	N/A
CSNF_110	0.0015	High	99%	N/A
CSNF_111	0.015	High	99%	N/A
CSNF_112	0.15	High	99%	N/A
CSNF_200	0.0015	Low	20%	N/A
CSNF_201	0.015	Low	20%	N/A
CSNF_202	0.15	Low	20%	N/A
CSNF_210	0.0015	High	20%	N/A
CSNF_211	0.015	High	20%	N/A
CSNF_212	0.15	High	20%	N/A
CDSP_000	0.0015	Low	N/A	Low
CDSP_001	0.015	Low	N/A	Low
CDSP_002	0.15	Low	N/A	Low
CDSP_010	0.0015	High	N/A	High
CDSP_011	0.015	High	N/A	High
CDSP_012	0.15	High	N/A	High
CDSP_100	0.0015	Low	N/A	Low
CDSP_101	0.015	Low	N/A	Low
CDSP_102	0.15	Low	N/A	Low
CDSP_110	0.0015	High	N/A	High
CDSP_111	0.015	High	N/A	High
CDSP_112	0.15	High	N/A	High

1 – low A526 = 8.706E-12, low 316SS = 2.528E-14, low 316SS/B = 1.169E-14 (mol/cm^{2}s), (Section 6.1.1)
2 – low GDR = 1.983E-19$(H^+)^{-0.4721}$ + 6.144E-12$(H^+)^{0.6381}$, (mol/cm^{2}s) (Section 6.1.2), NOTE: high = 10Xlow

4.1.2 In-Package Output Chemistry

The aqueous geochemistry of the in-package environment for both the CSNF and CDSP packages is documented in the *Summary of In-Package Chemistry for Waste Forms* (CRWMS M&O 2000a), all of the input data (DTN: SN9911T0811199.005) required for the abstraction process were taken from this report. The time dependant 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 Development Plan (CRWMS M&O 1999a). That Development Plan 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 7.2.

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 radionulcide 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 (FEP's)

This AMR being an abstraction is not subject to FEP's in the sense that the abstraction is a mathematical simplification of the process model results. A discussion of the FEP's that may impact the in-package chemistry is covered in the *Summary of 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 *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 It is assumed that the in-package geochemical environment as represented by the in-package process models (CRWMS M&O 2000a) conservatively describes the expected in-package chemistries for the conditions simulated for CSNF and CDSP packages. As a subset of the in-package process models (CRWMS M&O 2000a), the in-package abstraction is subject to the same assumptions as the process models. The basis for this assumption is that output from this abstraction is based solely on the output from *Summary of In-Package Chemistry for Waste Forms* (CRWMS M&O 2000a). Therefore, it is an implicit assumption of the abstraction that all of the assumptions made in the

Summary of In-Package Chemistry for Waste Forms (CRWMS M&O 2000a) also stand for the abstracted model results. This assumption is applied to all of Section 6, and does not require confirmation.

5.2 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 equibria, 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.

5.3 At some critical maximum value of water flux through the waste package, Q, the pH of the solution exiting the WP will be the same as the pH of the solution entering (J-13) the WP. This is true because the residence time of the water in the waste package will be too short to allow reactions between the water and the waste package materials to occur. Furthermore, this critical maximum Q value can be linearly extrapolated from the expressions developed herein to calculate by solving them in terms of Q and using the J-13 pH value. This assumption is used in Section 6, and does not require confirmation.

5.4 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.

5.5 The time frame used in this abstraction is with regard to 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.

5.6 For CSNF waste packages the dissolution rate of the CSNF increases proportionally to hydrogen ion activity (CRWMS M&O 2000A). The basis for this assumption is the mathematical formulation of the CSNF dissolution rate law (CRWMS M&O 2000a). This assumption is used in Section 6, and does not require confirmation.

5.7 For CDSP waste packages the dissolution rate of the CDSP increases above and below pH = 7 (CRWMS M&O 2000a). The basis for this assumption is the mathematical formulation of the CDSP dissolution rate law (CRWMS M&O 2000a). 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 dependant chemistry into blocks of time where 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.

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 CDSP.

6.1 ABSTRACTION OF pH

The chemical parameter pH constitutes the most important in-package 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. Based on its magnitude of change, pH will be used to define the time dependence of it and all of the other chemical parameters. In other words, the time discretization for all of the abstracted parameters will be based on changes in pH.

Figures 1 and 2 show the pH of the in-package fluids as a function of time for CSNF and CDSP waste packages, respectively. Inspection of these figures reveals that for times less than 1000 years the in-package pH, and hence the pH as a barometer of the chemistry, was changing rapidly relative to times greater then 1000 years. For times greater than 1000 years the pH curves had stabilized to "steady state" conditions. Therefore, based on the trends in the pH data two time periods will be used to describe the in-package chemistry, 1) chemistry from 0 to 1000 years post-breach, and 2) chemistry after 1000 years post-breach. For both the CSNF and the CDSP packages the minimum pH values are realized in the period prior to 1000 years, the reason being the dissolution of carbon steel and the coincident production of protons (CRWMS M&O 2000a) which reduces the pH.

The pH abstraction follows two lines of reasoning based on the waste package type (CSNF or CDSP), and the difference in kinetic rate laws between the two. The rate law for CSNF is proportional to the hydrogen ion activity, i.e, proportional to pH, such that at low pH the dissolution rate increases (CRWMS M&O 2000a). For CDSP the rate law is "U" shaped with the minimum at pH 7 and the rate increasing above and below pH 7 (CRWMS M&O 2000a). Therefore, conservative assumptions for one waste form may not be conservative for the other. In the case of the CSNF, for example, assuming the lowest pH for the <1000 year abstraction, and the averaged pH for >1000 year abstraction would be the most conservative, while still honoring the pH – time history. However, for the CDSP package using the lowest observed pH would be conservative for the <1000 year period, but not for the >1000 year period when use of the maximum pH is conservative. The difference in the rate laws between CDSP and CSNF and the difference in their pH – time profiles for the two waste forms predicates the use of different assumptions in the abstractions.

Validation of the CSNF and CDSP pH abstractions is implicit in method by which the pH response surfaces were developed. The response surfaces are mathematical constructs whose limits were set by the process models inputs (CRWMS M&O 2000a) and outputs (DTN: SN9911T0811199.005). 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.

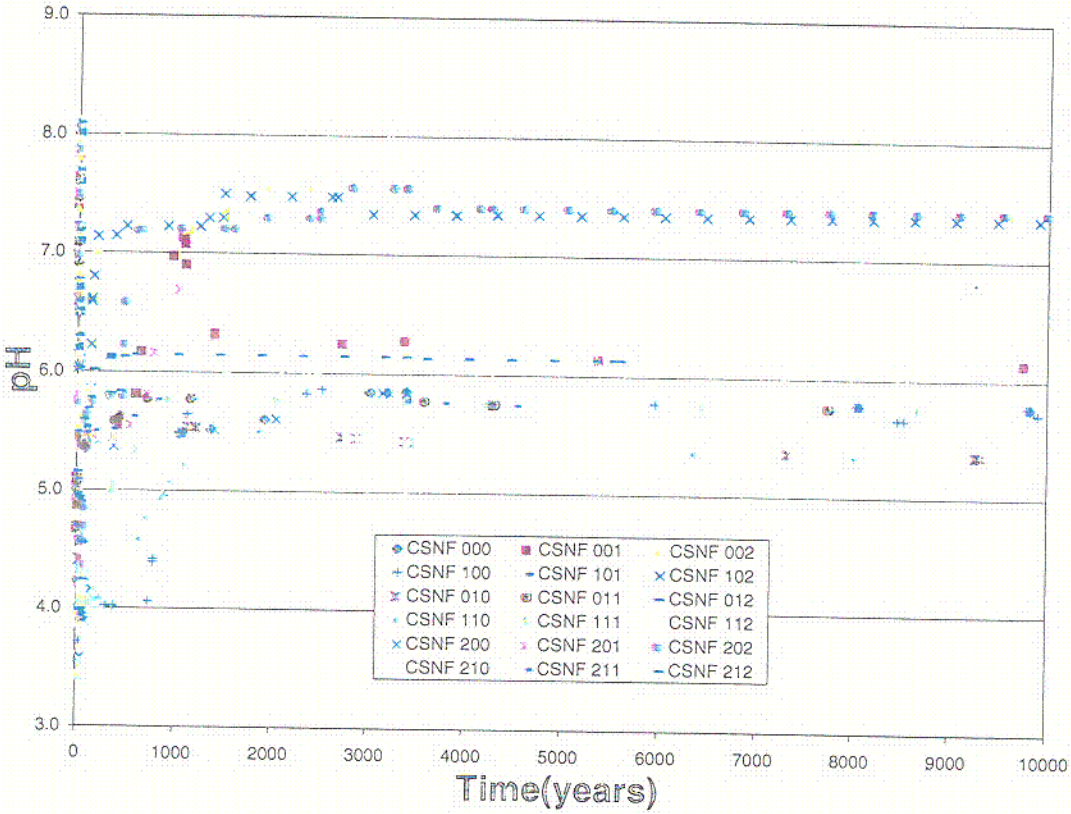

Figure 1 pH versus time for the CSNF packages (from CRWMS M&O 2000a, DTN: SN9911T0811199.005).

6.1.1 CSNF pH Abstraction

For the CSNF, at times less than 1000 years, the minimum pH value for each flux/cladding/corrosion scenario was extracted from the EQ6 output (CRWMS M&O 2000a). The minimum pH values for each scenario were compiled into a matrix along with the corresponding flux, cladding, and corrosion values such that response surfaces could be generated in SigmaPlot (Attachment I). It was necessary to generate two matrices (Tables 2 and 3) based on the corrosion rate of the metal components of the waste package, one for low corrosion rates, and a second for high corrosion rates. The waste package was modeled as being

composed of four component metal alloys where the dissolution rate of each alloy was simultaneously increased by an order of magnitude over a base case or "low" value 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 "high" and "low" groups, such that two response surfaces were created, one for low WP corrosion rates and the other for high WP corrosion rates. The axes of the three dimensional surfaces were x = cladding coverage, y = water flux, and z = pH.

This process was repeated for times greater than 1000 years where the average pH for the entire modeled duration (0 – 10, 0000 years post breach) was used to calculate the average pH. The average pH for the entire duration is conservative because it includes the low pH values at early times, which tends to lower the average value compared to averaging over the late time information (1000 – 10,000 years).

The results are four matrices of values (Tables 2 – 5), which in turn were used to generate four response surfaces, two surfaces for <1000 years (Figure 3), and two surfaces for time >1000 years (Figure 4). Thus, it is the parameter space between two surfaces that may be sampled in the TSPA where pH can be calculated as a function of time, water flux, WP corrosion rates, and cladding coverage or glass dissolution rate.

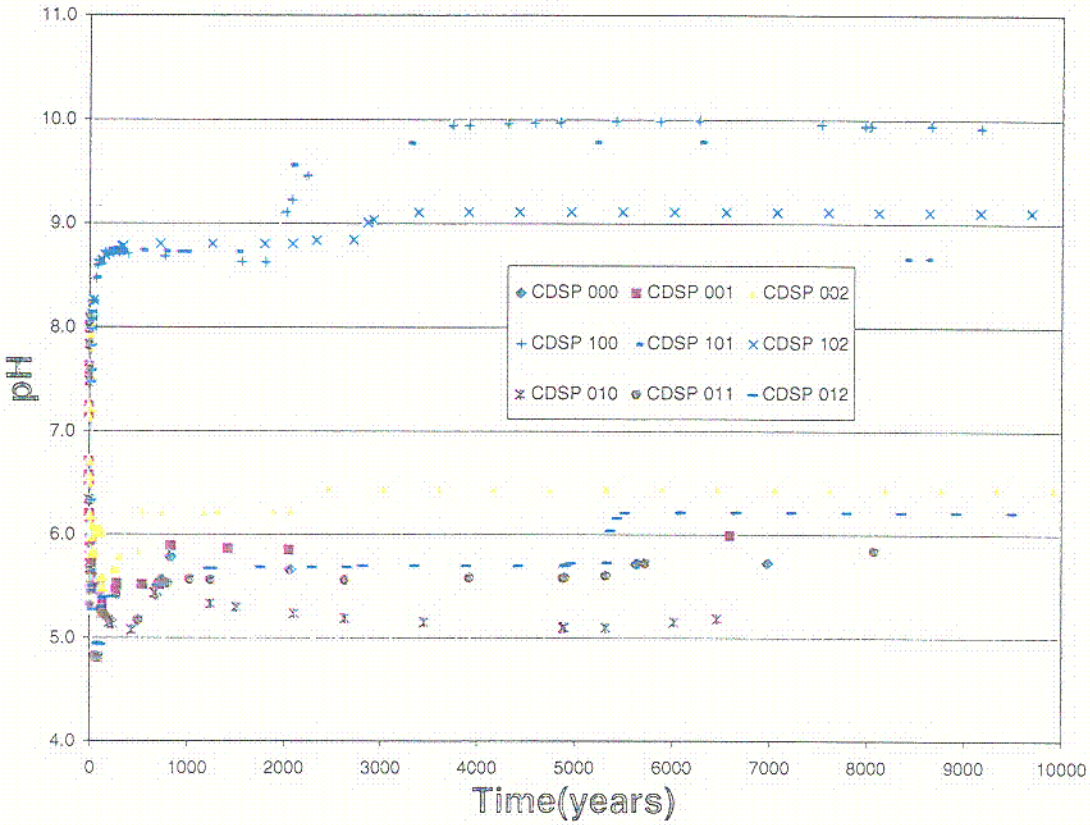

Figure 2 pH versus time for co-disposal waste packages (CDSP) (from CRWMS M&O 2000a, DTN: SN9911T0811199.005).

Table 2 CSNF matrix for low WP corrosion rates for the <1000 year time frame (from CRWMS M&O 1999a, DTN: SN9911T0811199.005).

EQ6 Input File (*.6i)	Q(m^3/yr)	Cladding Coverage	Minimum pH
CSNF_000	0.0015	0.01	5.3495
CSNF_001	0.015	0.01	5.3679
CSNF_002	0.15	0.01	5.4841
CSNF_100	0.0015	0.99	3.5606
CSNF_101	0.015	0.99	3.5425
CSNF_102	0.15	0.99	3.5855
CSNF_200	0.0015	0.2	4.1968
CSNF_201	0.015	0.2	4.2002
CSNF_202	0.15	0.2	4.2346

C2

Table 3 CSNF matrix for high WP corrosion rates for the <1000 year time frame (from CRWMS M&O 1999a, DTN: SN9911T0811199.005).

EQ6 Input File (*.6l)	Q(m^3/yr)	Cladding Coverage	Minimum pH
CSNF_010	0.0015	0.01	4.689
CSNF_011	0.015	0.01	4.6905
CSNF_012	0.15	0.01	4.7061
CSNF_210	0.0015	0.2	3.8815
CSNF_211	0.015	0.2	3.8907
CSNF_212	0.15	0.2	3.9776
CSNF_110	0.0015	0.99	3.4179
CSNF_111	0.015	0.99	3.4219
CSNF_112	0.15	0.99	3.4615

Table 4 CSNF matrix for low WP corrosion rates for the >1000 year time frame (from CRWMS M&O 1999a, DTN: SN9911T0811199.005).

EQ6 Input File (*.6l)	Q(m^3/yr)	Cladding Coverage	Average pH
CSNF_000	0.0015	0.01	6.9648
CSNF_001	0.015	0.01	7.0061
CSNF_002	0.15	0.01	7.3336
CSNF_100	0.0015	0.99	5.7469
CSNF_101	0.015	0.99	6.9407
CSNF_102	0.15	0.99	6.7581
CSNF_200	0.0015	0.2	6.7137
CSNF_201	0.015	0.2	6.7684
CSNF_202	0.15	0.2	7.1025

Table 5 CSNF matrix for high WP corrosion rates for the >1000 year time frame (from CRWMS M&O 1999a, DTN: SN9911T0811199.005).

EQ6 Input File (*.6l)	Q(m^3/yr)	Cladding Coverage	Average pH
CSNF_010	0.0015	0.01	6.6082
CSNF_011	0.015	0.01	6.6300
CSNF_012	0.15	0.01	6.6755
CSNF_210	0.0015	0.2	6.4892
CSNF_211	0.015	0.2	6.3922

Table 5 continued			
EQ6 Input File (*.6i)	Q(m^3/yr)	Cladding Coverage	Average pH
CSNF_212	0.15	0.2	6.5628
CSNF_110	0.0015	0.99	5.9180
CSNF_111	0.015	0.99	6.0356
CSNF_112	0.15	0.99	6.3527

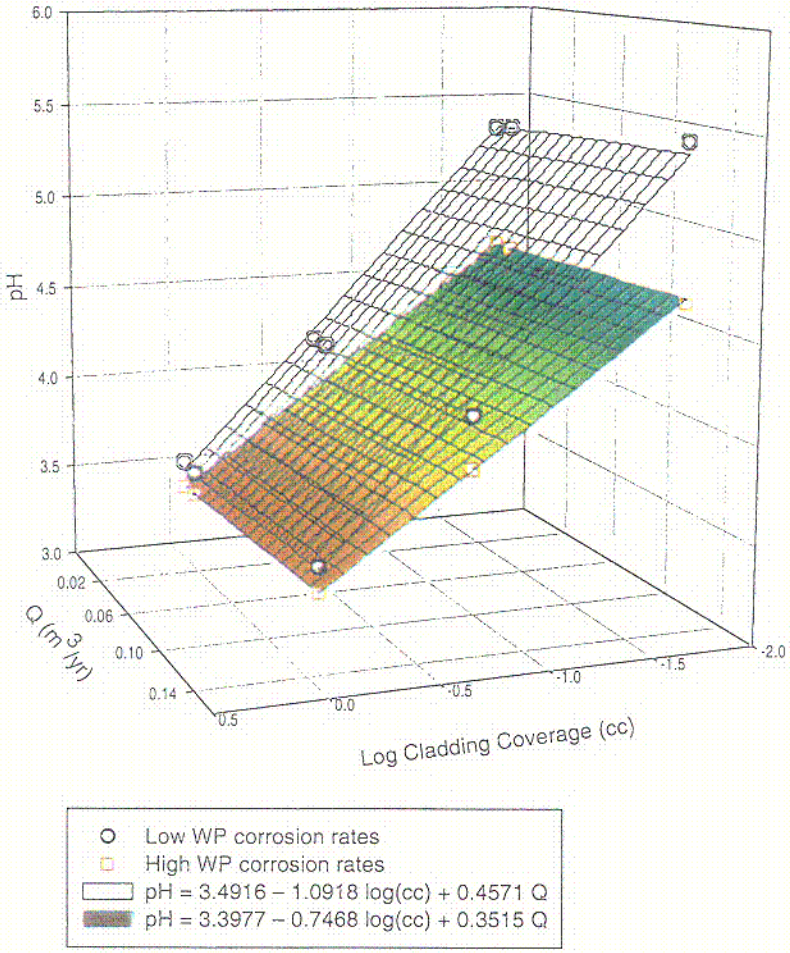

Figure 3 Response surface of pH for CSNF waste form for <1000 years (DTN: MO9911SPA CDP37.001).

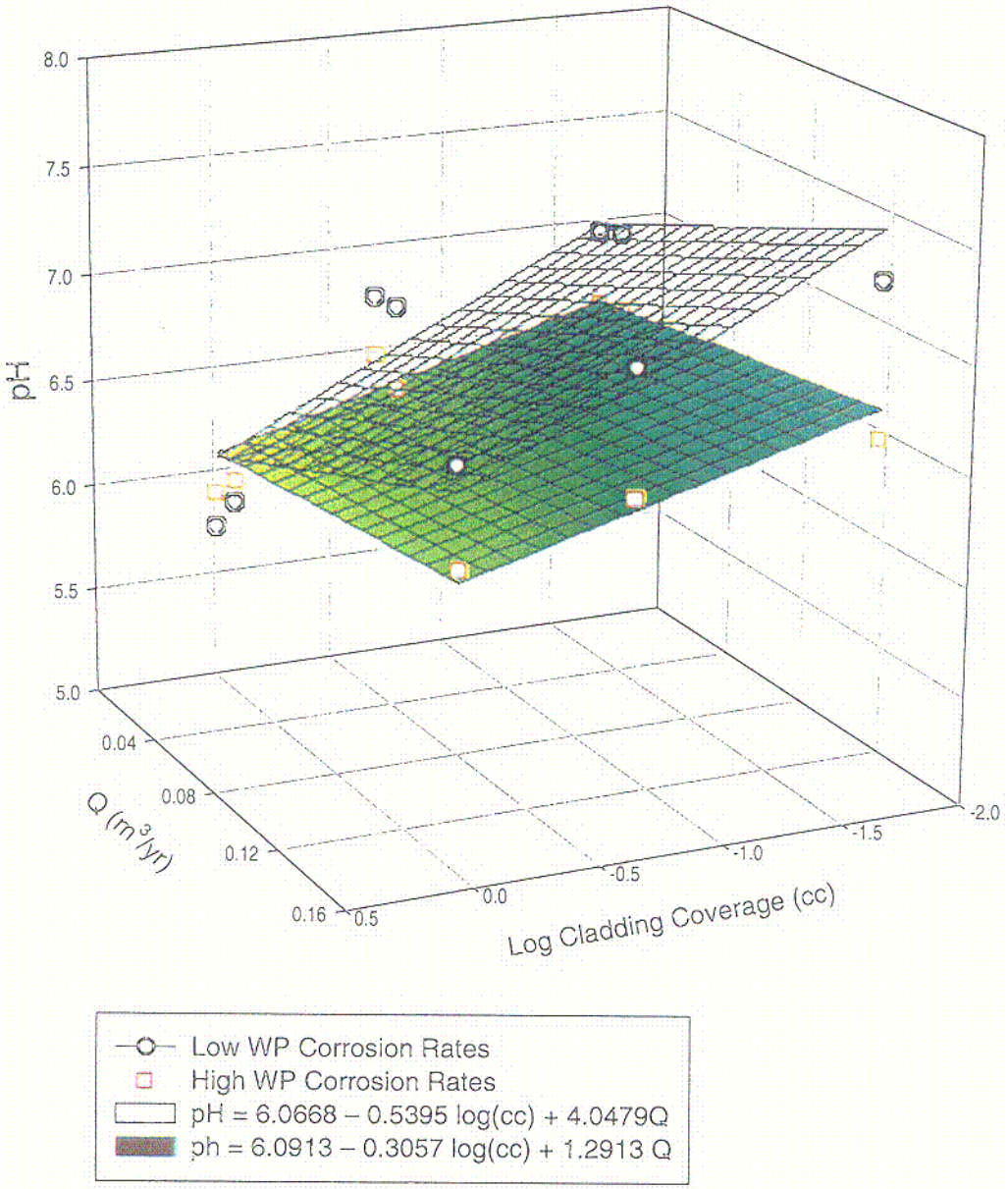

Figure 4 Response surface of pH for CSNF waste form for >1000 years (DTN: MO9911SPA CDP37.001).

Table 6 provides the equations of the planes that bound the pH parameter space for CSNF. Each plane represents either the low or high corrosion rate data for the waste package materials, 316 stainless steel, aluminum alloy, A-516 carbon steel, and borated stainless steel. In terms of which alloy is controlling the system pH it may be generalized that A-516 carbon steel dominates the early time (<1000 year), and aluminum alloy and stainless steel control the late time data (>1000 yr) (CRWMS M&O 2000a).

Table 6 Response surface parameters for CSNF.

$Z^1 = y_o + ax + by$			
Case	y_o	**a**	**b**
<1000 years, low corrosion rate	3.4916	-1.0918	0.4571
<1000 years, high corrosion rate	3.3977	-0.7468	0.3515
>1000 years, low corrosion rate	6.0668	-0.5395	4.0479
>1000 years, high corrosion rate	6.0913	-0.3057	1.2913
Z = pH, x = $\log_{10}$ (cladding coverage), y = water flux (m^3/yr)			

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

Due to the simplicity of the mathematical expressions used to calculate pH, it is possible, by increasing Q, to calculate unrealistic pH values. Therefore, it was necessary to set limits for the maximum allowable Q. Since the calculated pH from all of the expressions in Table 6 are directly proportional to water flux through the WP, and as the water flux increases the potential for reaction of the through flowing water with the WP/WF materials decreases, the pH of the water exiting the WP should approach that of J-13 water. Therefore, above some maximum Q-value the water exiting the WP should have the same pH as the water entering the WP. This critical value of Q was calculated by solving the expressions in Table 6 for Q and using the input, J-13, value for pH and assuming linear behavior.

Table 7 Maximum Q-values for CSNF.

$Y = (z - y_o - ax) / b$			
Period	*z*	*X*	*Y*
<1000 years, low corrosion rate	8.1	-2	5.3
>1000 years, low corrosion rate	8.1	-2	0.24
Z = pH, x = $\log_{10}$ (cladding coverage), y = maximum water flux (m^3/yr), y_o = coefficient from Table 6.			

The results (Table 7) indicate that for CSNF at time less then 1000 years the pH expressions (Table 6) are valid with the range of 0< Q < 5.3 (m^3/yr). Likewise when Q >= 5.3 m^3/yr, then the pH is constant at 8.1 (+/- 1). For time greater then 1000 years the pH expression (Table 6) is valid 0< Q < 0.24 (m^3/yr), and when Q >= 0.24 m^3/yr the pH is constant at 8.1 (+/- 1). Note that the maximum Q values are only calculated for the low WP corrosion rate and low cladding coverage value. The reason being that these conditions coupled with high water flux yield the highest pH values, and thus set the upper limit on water flux. Note that due to the conservative nature of the pH expressions they may be applied to times greater then 10,000 years.

6.1.2 CDSP pH Abstraction

For the CDSP waste form, at times <1000 years the minimum pH was extracted for each flux/glass dissolution rate/corrosion scenario from the EQ6 output (CRWMS M&O 2000a) and

compiled into matrices in Excel for generating response surfaces. Similarly, for the period 1000 to 10,000 years, the maximum pH was extracted and compiled in Excel. These matrices were copied into SigmaPlot for the regression analyses and generation of the response surfaces (Attachment I). Tables 8 - 11 summarize the data used in the regression analyses. Note that in Tables 8 – 11, as well as in the generation of the response surfaces, a "relative" glass dissolution rate was used. The reason being that the high-level waste glass (HLWG) kinetic rate law has two terms, each of which was simultaneously increased by an order of magnitude relative to the base case value (CRWMS M&O 2000a). Therefore, it was not possible to incorporate the change in the GDR directly into the abstraction, rather a "relative " GDR was used, where a value of "1" was assigned to the base case values and "10" was assigned to 10X GDR. This approach eliminates the need to use the absolute rate constants in the abstraction. Similar to the CSNF pH abstraction (Section 6.1.1) separate pH response surfaces (abstractions) were developed for high and low WP corrosion rates.

Table 8 CDSP matrix for low WP corrosion rates for the <1000 year time frame (from CRWMS M&O 2000a, DTN: SN9911T0811199.005).

EQ6 Input file (*.6l)	Q(m^3/yr)	Relative GDR	Minimum pH
CDSP_000	0.0015	1	5.2635
CDSP_001	0.015	1	5.2909
CDSP_002	0.15	1	5.4965
CDSP_100	0.0015	10	5.8006
CDSP_101	0.015	10	5.9212
CDSP_102	0.15	10	6.3929

Table 9 CDSP matrix for high WP corrosion rates for the <1000 year time frame (from CRWMS M&O 2000a, DTN: SN9911T0811199.005).

EQ6 Input file (*.6l)	Q(m^3/yr)	Relative GDR	Minimum pH
CDSP_010	0.0015	1	4.8111
CDSP_011	0.015	1	4.8219
CDSP_012	0.15	1	4.9441
CDSP_110	0.0015	10	5.5285
CDSP_111	0.015	10	5.6411
CDSP_112	0.15	10	5.6554

Table 10 CDSP matrix for low WP corrosion rates for the >1000 year time frame (from CRWMS M&O 2000a, DTN: SN9911T0811199.005).

EQ6 Input file (*.6I)	Q(m^3/yr)	Relative GDR	Maximum pH
CDSP_000	0.0015	1	8.0958
CDSP_001	0.015	1	8.8107
CDSP_002	0.15	1	8.2195
CDSP_100	0.0015	10	10.0010
CDSP_101	0.015	10	9.7936
CDSP_102	0.15	10	9.1194

Table 11 CDSP matrix for high WP corrosion rates for the >1000 year time frame (from CRWMS M&O 2000a, DTN: SN9911T0811199.005).

EQ6 Input file (*.6I)	Q(m^3/yr)	Relative GDR	Maximum pH
CDSP_010	0.0015	1	9.8231
CDSP_011	0.015	1	9.1973
CDSP_012	0.15	1	8.0958
CDSP_110	0.0015	10	8.0958
CDSP_111	0.015	10	8.8903
CDSP_112	0.15	10	8.9959

Table 12 provides the equations of the planes that bound the pH parameter space for CDSP. Each plane represents either the low or high corrosion rate data for the waste package materials. In terms of which alloy is controlling the system pH it may be generalized that A-516 carbon steel dominates the early time (<1000 year), and HLWG controls the late time data (>1000 year). Figures 5 and 6 show the response surfaces for the CDSP waste form.

Table 12 Response surface parameters for CDSP (DTN: MO9911SPA CDP37.001).

$Z^1 = y_o + ax + by$			
Case	y_o	a	b
<1000 years, low corrosion rate	5.1257	2.6692	0.0764
<1000 years, high corrosion rate	4.7324	0.7307	0.0837
>1000 years, low corrosion rate	8.4247	-3.4173	0.1403
>1000 years, high corrosion rate	9.2554	-3.1280	-0.0418
Z = pH, x = water flux (m^3/yr), y = relative glass dissolution rate			

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

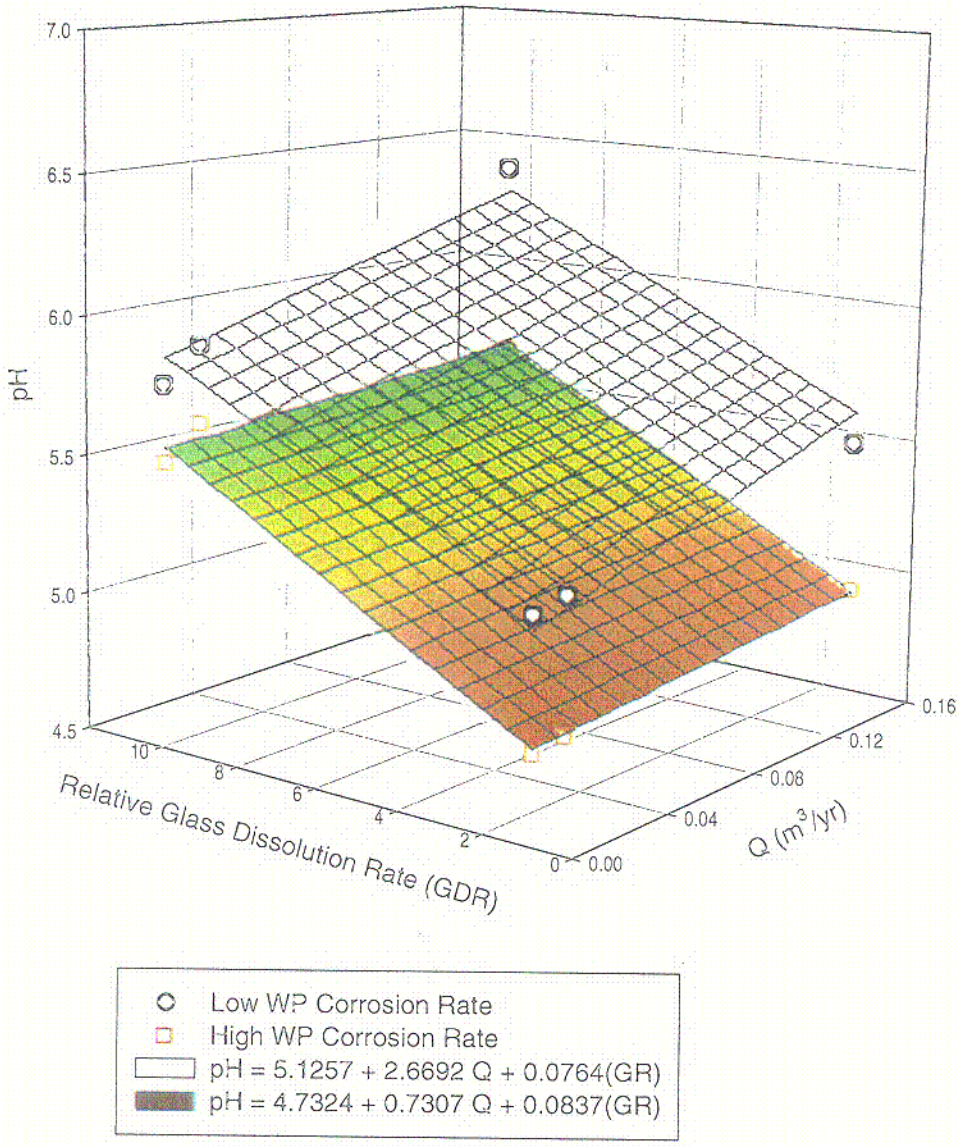

Figure 5 Response surface of pH for CDSP waste form for <1000 years (DTN: MO9911SPA CDP37.001).

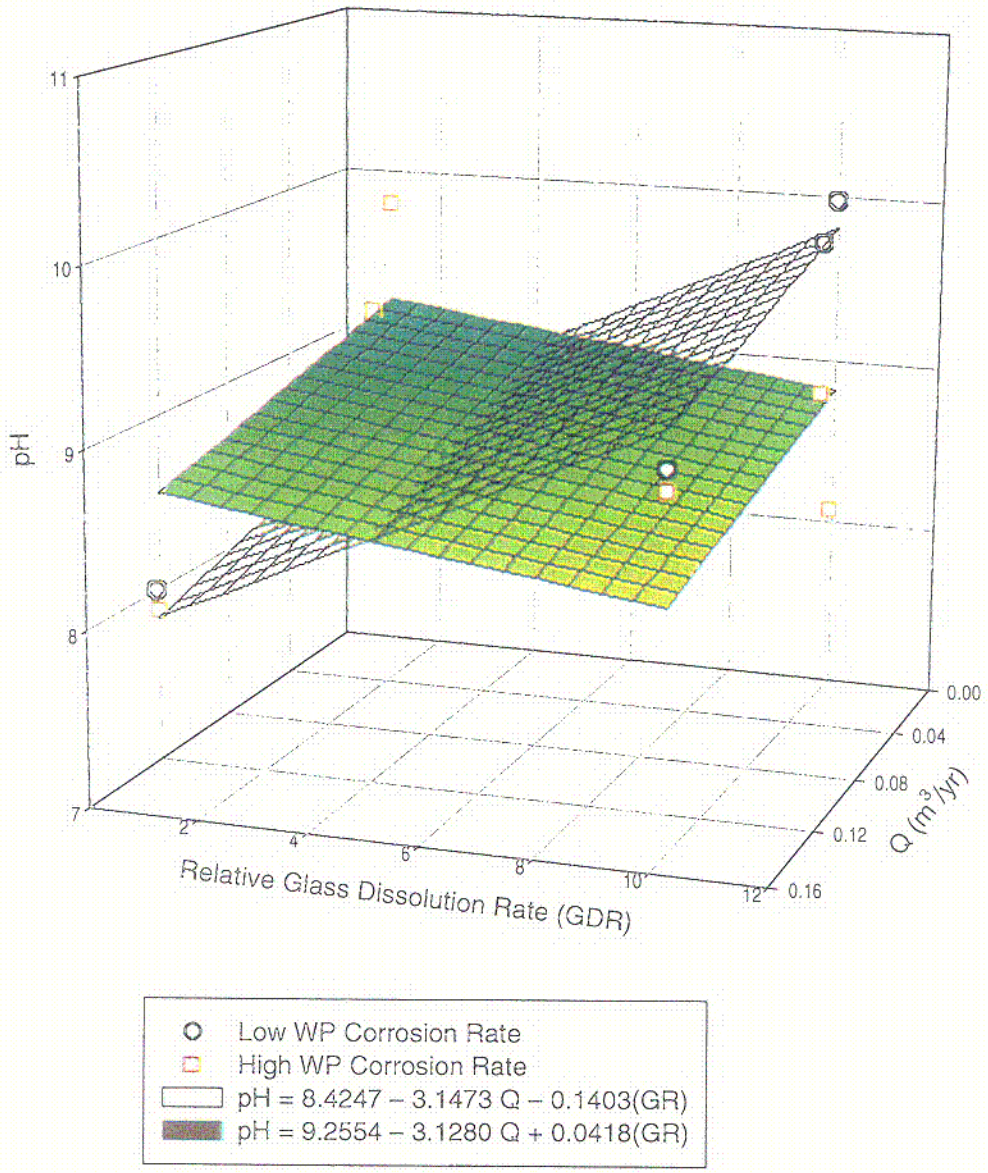

Figure 6 Response surface of pH for CDSP waste form for >1000 years (DTN: MO9911SPA CDP37.001).

As with the CSNF it was also necessary to calculate the upper limit of Q for the pH response surfaces for CDSP. This critical value of Q was calculated by solving the expressions in Table 12 for Q and using the input, J-13, value for pH and assuming linear behavior.

Table 13 Maximum Q-values for CDSP.

$X = (z - y_o - by) / a$			
Period	***z***	***Y***	***X***
<1000 years, high corrosion rate	8.1	1	1.1
>1000 years, low corrosion rate	8.1	1	0.36
Z = pH, x = maximum water flux (m^3/yr), y = relative dissolution glass rate			

The results (Table 13) indicate that for CDSP at time less then 1000 years the pH expressions (Table 12) are valid with the range of 0< Q < 1.1 (m^3/yr). Likewise when Q > = 1.1 m^3/yr, then the pH is constant at 8.1 (+/- 1). For time greater then 1000 years the pH expression (Table 12) is valid 0< Q < 0.36 (m^3/yr), and when Q > = 0.36 m^3/yr the pH is constant at 8.1 (+/- 1). Note that due to the conservative nature of the pH expressions they may be applied to times greater then 10,000 years.

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 results for the process model for CSNF are plotted in Figure 7. In a system where the partial pressure of carbon dioxide (CO_2) is fixed and the pH known, the total carbonate can be calculated using the equilibrium mass action expressions.

Where the total carbonate (0<pH<14) is equal to:

0) $\Sigma C = [CO_2\,(aq)] + [HCO_3^-] + [CO_3^{2-}]$

1) $CO_2(g) \Leftrightarrow CO_2\,(aq)$ $\log K = -1.47^*$

$[CO_2\,(aq)] = P_{CO2(g)}\, 10^{-1.47}$

2) $CO_2\,(aq) \Leftrightarrow H^+ + HCO_3^-$ $\log K = -6.35^*$

$[HCO_3^-] = (P_{CO2(g)}\, 10^{-1.47}\, 10^{-6.35})/10^{-pH}$

3) $HCO_3^- \Leftrightarrow H^+ + CO_3^{2-}$ $\log K = -10.33^*$

$[CO_3^{2-}] = [(P_{CO2(g)}\, 10^{-1.47}\, 10^{-6.35})/10^{-pH}]\, 10^{-10.33}/\, 10^{-pH}$

* - log K values have been rounded off to the nearest hundreth

Assuming that $\log(P_{CO2(g)}) = -3.0$ (CRMS M&O, 2000a), 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 (DTN: MO9911SPA CDP37.001).

$$\text{Total C} = 10^{-4.47} + (10^{-10.82})/10^{-pH} + (10^{-21.15})/10^{-2pH}$$

Solving this expression at a fixed partial pressure of carbon dioxide ($\log(P_{CO2(g)}) = -3.0$), and over a range of pH will yield a curve that closely approximates the output data from the in-package process model. Figures 7 and 8 depict the output from the CSNF and CDSP process models, respectively, and the calculated functional relationship between pH and total carbonate. 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.

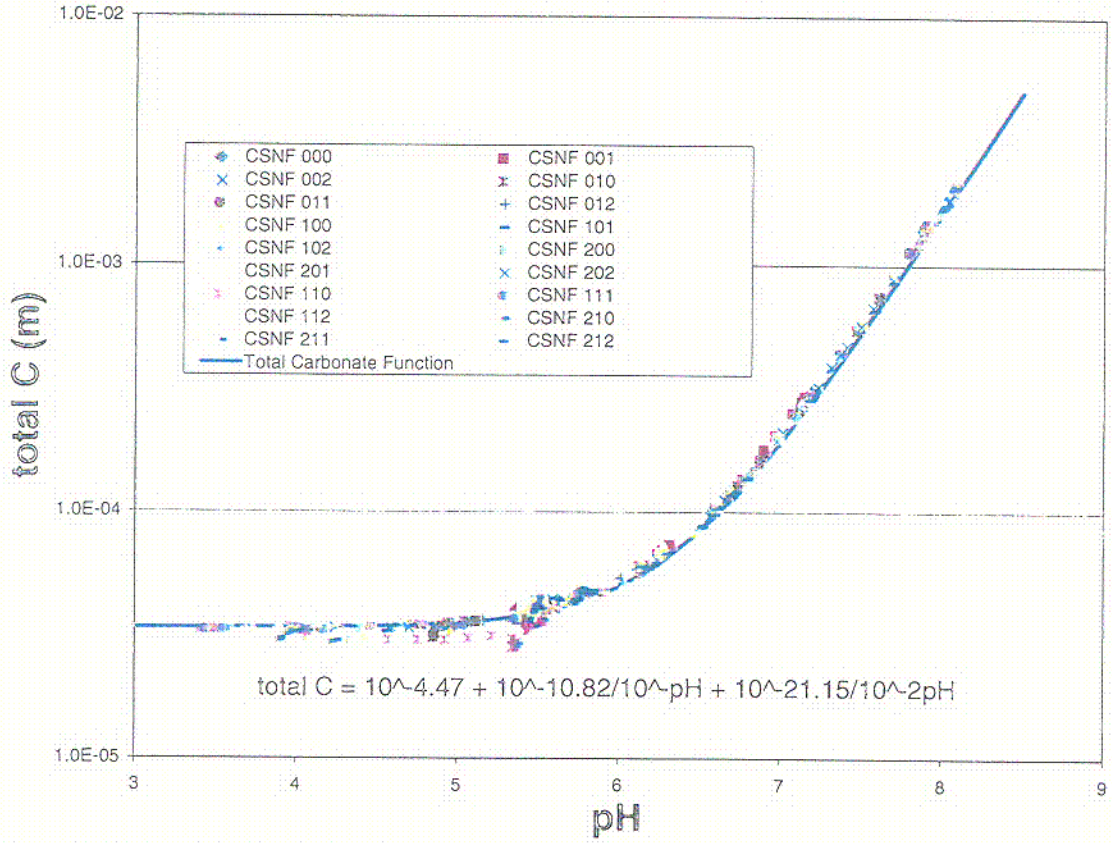

Figure 7 Plot of CSNF calculated total aqueous carbonate versus pH, and the functional relationship between the two (data from CRWMS M&O 2000a, DTN: SN9911T0811199.005, equation, DTN: MO9911SPA CDP37.001)

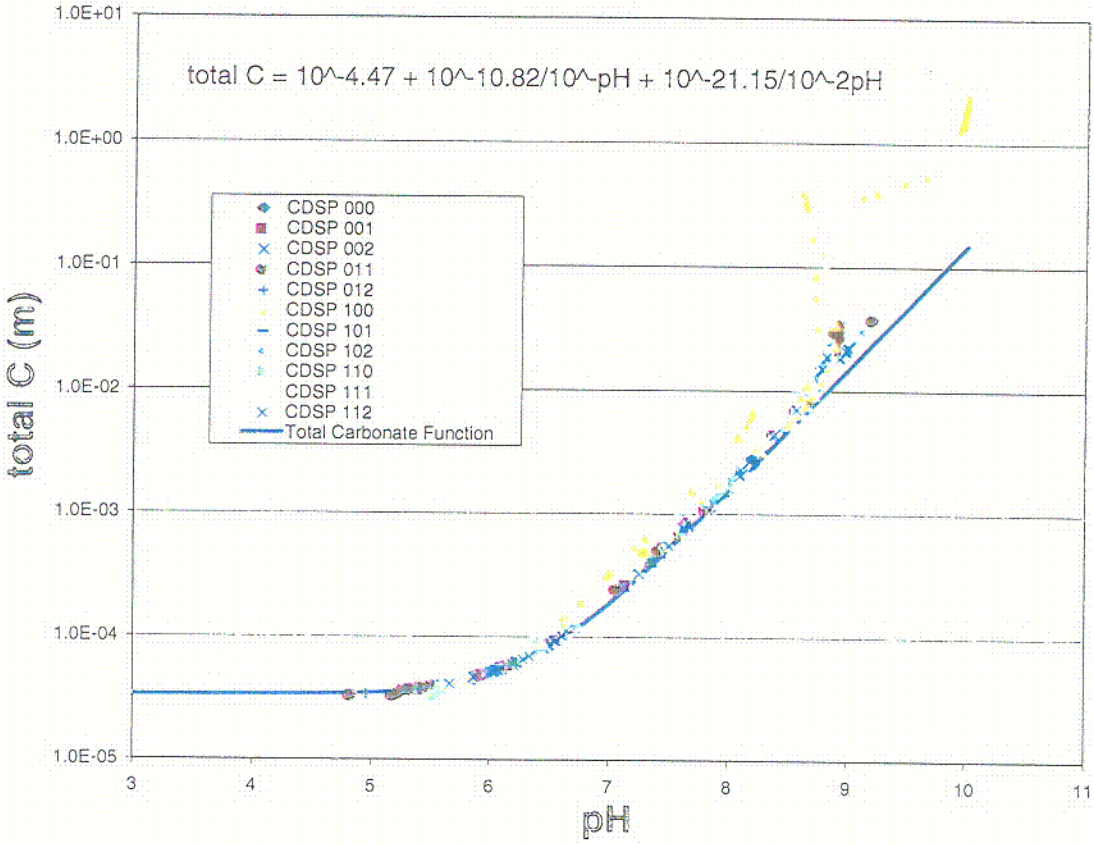

Figure 8 Plot of CDSP calculated total aqueous carbonate versus pH, and the functional relationship between the two (data from CRWMS M&O 2000a, DTN: SN9911T0811199.005, equation, DTN: MO9911SPA CDP37.001)

The total carbonate abstraction, for both the CSNF and CDSP, is reflective of the process model (Figure 7 and 8) output thus validating the abstraction. Uncertainty is built in to the carbonate abstraction by virtue of the input pH, which has associated uncertainty.

6.3 ABSTRACTION OF Eh

In aqueous systems in equilibrium with the atmosphere the Eh may be calculated directly from the pH. For the formation of water the pE^o may be calculated from the following expression, where ΔG^o is the Gibb's free energy of formation, F is the Faraday constant, Eh is the electron activity expressed in units of volts, and pE is the negative log base 10 of electron activity.

1) $1/2O_2 + 2H^+ + 2e^- = H_2O$ $\Delta G^o = -56.688$ kcal/mol (EQ6 database)

2) $\Delta G^o = -nFEh^o$ (Drever, 1988, page 285, eqn 13-6)

3) $pE = F/(2.303RT)Eh$ (Drever, 1988, page 284)

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

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

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^o results in:

$pE^o = 20.75$

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

$1/4O_2 + H^+ + e^- = 1/2H_2O$

$pE = pE^o + Log(P_{O2}^{1/4}[H^+])$

$pE = 20.75 - pH + 1/4\log(P_{O2})$

$\log(P_{O2}) = -0.7$

$pE = 20.575 - pH$

Converting to Eh we get the expression in Table 15. The expression for Eh as a function of pH (Table 15) is applicable for both CSNF and CDSP.

Table 15 Expression for Eh as a function of pH for use in the TSPA (DTN: MO9911SPA CDP37.001)

Eh = 1.217 – 0.059pH

The Eh abstraction, for both the CSNF and CDSP, is reflective of the process model output (Figure 9) thus validating the abstraction. Like the carbonate abstraction, uncertainty is built in to the Eh abstraction by virtue of the input pH, which has associated uncertainty.

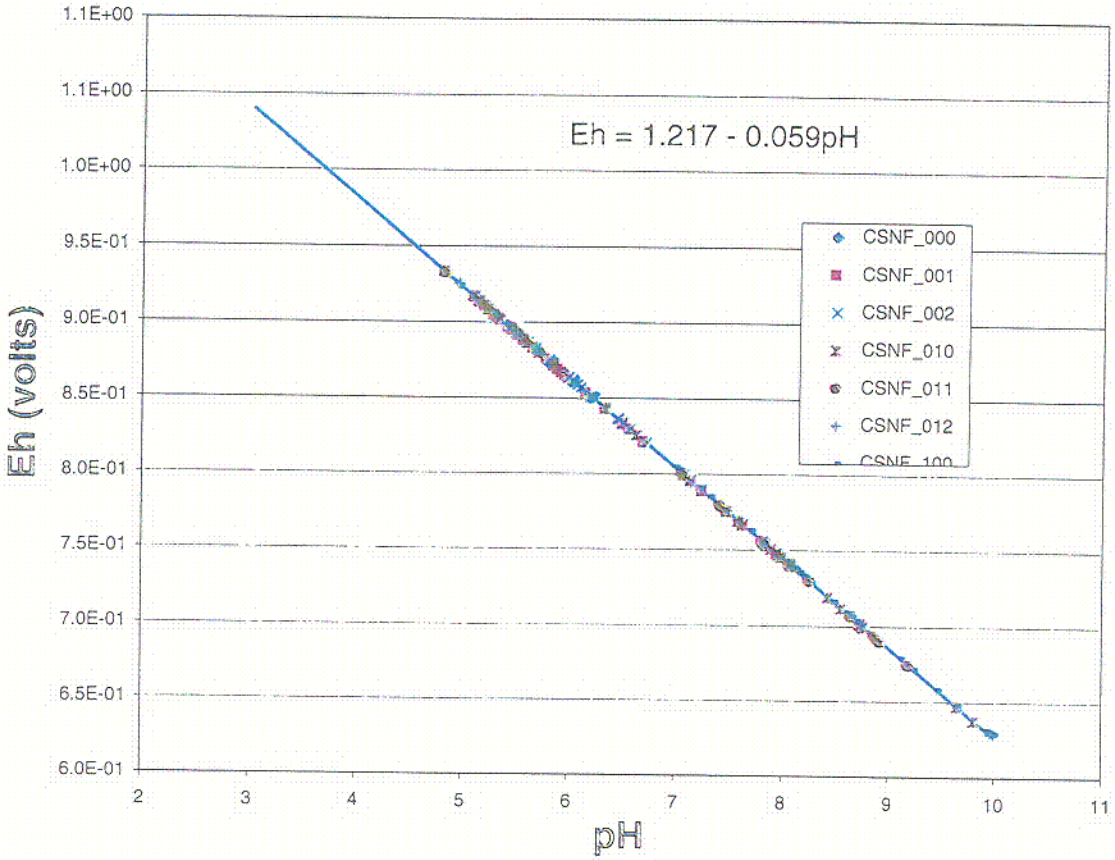

Figure 9 Eh as a function of pH, at $\log(pO_2) = -0.7$ (data values from CRWMS M&O 2000a, DTN: SN9911T0811199.005, equation, DTN: MO9911SPA CDP37.001)

6.4 IONIC STRENGTH, CHLORIDE, AND FLUORIDE ABSTRACTION

The ionic strength (I), chloride (Cl), and fluoride (F) abstractions apply the same constraints for both the CSNF and CDSP packages. In the following tables (16–19) it should be noted that the parameters listed at the bottom of each table (maximum, minimum, average, 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 values of ionic strength over the 10,000 years of each simulation for each scenario. While the maximum, minimum, average, and standard deviation listed at the bottom of Table 16 represent maximum of the minimums, the minimum of the minimums, 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.

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.

The DTN for the "raw" values in the following tables is SN991T08111.99.005. 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 MO9911SPACDP37.001, this is the abstracted "data" to be used in the TSPA.

6.4.1 Ionic Strength

The ionic strength is used in determining the colloid content of the water exiting the near-field environment. For the period before 1000 years the minimum ionic strength for each flux/cladding or glass dissolution rate/ corrosion rate scenario was calculated. These values are tabulated in Tables 16 and 18 for CSNF and CSDP, respectively, for <1000 year time period.

At times greater than 1000 years the average value of ionic strength will be used from each scenario to get the ionic strength range used in the abstraction. This is a conservative approach compared to using the maximum value because low ionic strength is conducive to colloid formation, and using the minimum value would also create the worst case which is not reflective of the actual in-package conditions.

6.4.2 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 2.014E-04 mol/kg.

6.4.3 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 CDSP package. The fluoride for the CSNF should be between 1.148E-04 - 9.114E-04 mol/ kg.

Table 16 CSNF <1000 years, ionic strength, chloride, and fluoride data (data from CRWMS M&O 2000a, DTN: SN9911T0811199.005, abstracted information, DTN: MO9911SPACDP37.001).

EQ6 Input file (*.6I)	Q(m^3/yr)	Cladding Coverage	Minimum Ionic Strength (m)	Maximum Chloride (m)	Maximum Fluoride (m)
CSNF_000	0.0015	0.02	2.757E-03	2.014E-04	1.150E-04
CSNF_001	0.015	0.02	2.757E-03	2.014E-04	1.945E-04
CSNF_002	0.15	0.02	2.757E-03	2.014E-04	1.982E-04
CSNF_100	0.0015	0.99	2.815E-03	2.014E-04	1.148E-04

Table 16 continued					
EQ6 Input file (*.6l)	Q(m^3/yr)	Cladding Coverage	Minimum Ionic Strength (m)	Maximum Chloride (m)	Maximum Fluoride (m)
CSNF_101	0.015	0.99	2.811E-03	2.014E-04	1.154E-04
CSNF_102	0.15	0.99	2.809E-03	2.014E-04	1.480E-04
CSNF_202	0.15	0.2	2.827E-03	2.014E-04	3.019E-04
CSNF_010	0.0015	0.01	2.792E-03	2.014E-04	1.312E-04
CSNF_011	0.015	0.01	2.792E-03	2.014E-04	5.559E-04
CSNF_012	0.15	0.01	2.792E-03	2.014E-04	1.271E-04
CSNF_210	0.0015	0.2	2.921E-03	2.014E-04	1.312E-04
CSNF_211	0.015	0.2	2.922E-03	2.014E-04	5.604E-04
CSNF_212	0.15	0.2	2.922E-03	2.014E-04	1.178E-04
CSNF_110	0.0015	0.99	2.819E-03	2.014E-04	1.309E-04
CSNF_111	0.015	0.99	2.819E-03	2.014E-04	9.114E-04
CSNF_112	0.15	0.99	2.818E-03	2.014E-04	1.168E-04
		Maximum	2.922E-03	2.014E-04	9.114E-04
		Minimum	2.757E-03	2.014E-04	1.148E-04
		Average	2.821E-03	2.014E-04	2.334E-04
		Standard Deviation	5.1716E-05	0.0	0.00022

Table 17 CSNF >1000 years, ionic strength, chloride, and fluoride data (data from CRWMS M&O 2000a, DTN: SN9911T0811199.005, abstracted information DTN: MO9911SPACDP37.001).

EQ6 Input file (*.6l)	Q(m^3/yr)	Cladding Coverage	Average Ionic Strength (m)	Maximum Chloride (m)	Maximum Fluoride (m)
CSNF_000	0.0015	0.01	9.763E-02	2.014E-04	1.150E-04
CSNF_001	0.015	0.01	3.842E-02	2.014E-04	1.945E-04
CSNF_002	0.15	0.01	1.228E-02	2.014E-04	1.982E-04
CSNF_100	0.0015	0.99	6.495E-02	2.014E-04	1.148E-04
CSNF_101	0.015	0.99	4.339E-03	2.014E-04	1.154E-04
CSNF_102	0.15	0.99	5.610E-03	2.014E-04	1.480E-04
CSNF_200	0.0015	0.2	8.387E-02	2.014E-04	1.148E-04
CSNF_201	0.015	0.2	2.827E-03	2.014E-04	1.156E-04
CSNF_202	0.15	0.2	8.109E-03	2.014E-04	3.019E-04
CSNF_010	0.0015	0.01	3.402E-01	2.014E-04	1.312E-04
CSNF_011	0.015	0.01	7.874E-02	2.014E-04	5.559E-04
CSNF_012	0.15	0.01	2.248E-02	2.014E-04	1.271E-04
CSNF_210	0.0015	0.2	3.713E-01	2.014E-04	1.312E-04
CSNF_211	0.015	0.2	8.026E-02	2.014E-04	5.604E-04
CSNF_212	0.15	0.2	1.705E-02	2.014E-04	1.178E-04
CSNF_110	0.0015	0.99	3.943E-01	2.014E-04	1.309E-04
CSNF_111	0.015	0.99	7.155E-02	2.014E-04	9.114E-04

Table 17 continued					
EQ6 Input file (*.6I)	Q(m^3/yr)	Cladding Coverage	Average Ionic Strength (m)	Maximum Chloride (m)	Maximum Fluoride (m)
CSNF_112	0.15	0.99	1.319E-02	2.014E-04	1.168E-04
		Maximum	3.943E-01	2.014E-04	9.114E-04
		Minimum	2.827E-03	2.014E-04	1.148E-04
		Average	9.484E-02	2.014E-04	2.334E-04
		Standard Deviation	0.13026125	0.0	0.00022

Table 18 CDSP <1000 years, ionic strength, chloride, and fluoride data (data from CRWMS M&O 2000a, DTN: SN9911T0811199.005, abstracted information DTN: MO9911SPACDP37.001).

EQ6 Input file (*.6I)	Q(m^3/yr)	Relative GDR	Minimum Ionic Strength (m)	Maximum Chloride (m)	Maximum Fluoride (m)
CDSP_000	0.0015	1	2.996E-03	2.014E-04	1.414E-04
CDSP_001	0.015	1	2.996E-03	2.014E-04	2.092E-04
CDSP_002	0.15	1	2.993E-03	2.014E-04	1.765E-04
CDSP_100	0.0015	10	3.269E-03	2.014E-04	2.287E-02
CDSP_101	0.015	10	3.269E-03	2.014E-04	3.082E-03
CDSP_102	0.15	10	3.268E-03	2.014E-04	2.544E-04
CDSP_010	0.0015	1	3.320E-03	2.014E-04	3.201E-03
CDSP_011	0.015	1	3.479E-03	2.014E-04	2.714E-04
CDSP_012	0.15	1	2.537E-03	2.014E-04	1.312E-04
CDSP_110	0.0015	10	3.479E-03	2.014E-04	1.351E-04
CDSP_111	0.015	10	3.067E-03	2.014E-04	1.096E-03
CDSP_112	0.15	10	3.479E-03	2.014E-04	2.320E-04
		Maximum	3.479E-03	2.014E-04	2.287E-02
		Minimum	2.537E-03	2.014E-04	1.312E-04
		Average	3.179E-03	2.014E-04	2.650E-03
		Standard Deviation	2.764E-04	0.000E+00	6.466E-03

Table 19 CDSP >1000 years, ionic strength, chloride, and fluoride data (data from CRWMS M&O 2000a, DTN: SN9911T0811199.005, abstracted information DTN: MO9911SPACDP37.001).

EQ6 Input file (*.6I)	Q(m^3/yr)	Relative GDR	Average Ionic Strength (m)	Maximum Chloride (m)	Maximum Fluoride (m)
CDSP_000	0.0015	1	1.280E-01	2.014E-04	1.414E-04
CDSP_001	0.015	1	4.216E-02	2.014E-04	2.092E-04
CDSP_002	0.15	1	7.860E-03	2.014E-04	1.765E-04
CDSP_100	0.0015	10	1.353E+00	2.014E-04	2.287E-02
CDSP_101	0.015	10	1.397E-01	2.014E-04	3.082E-03

Table 19 continued

EQ6 Input file (*.6l)	Q(m^3/yr)	Relative GDR	Average Ionic Strength (m)	Maximum Chloride (m)	Maximum Fluoride (m)
CDSP_102	0.15	10	2.361E-02	2.014E-04	2.544E-04
CDSP_010	0.0015	1	9.775E-01	2.014E-04	3.201E-03
CDSP_011	0.015	1	1.526E-01	2.014E-04	2.714E-04
CDSP_012	0.15	1	2.663E-02	2.014E-04	1.312E-04
CDSP_110	0.0015	10	9.965E-01	2.014E-04	1.351E-04
CDSP_111	0.015	10	1.633E-01	2.014E-04	1.096E-03
CDSP_112	0.15	10	4.984E-02	2.014E-04	2.320E-04
		Maximum	1.353E+00	2.014E-04	2.287E-02
		Minimum	7.860E-03	2.014E-04	1.312E-04
		Average	3.384E-01	2.014E-04	2.650E-03
		Standard Deviation	4.764E-01	0E+00	6.466E-03

6.5 OXYGEN AND CARBON DIOXIDE FUGACITY ABSTRACTION

Both oxygen (O_2) and carbon dioxide (CO_2) 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 20 summarizes the gas abstraction information. There is no uncertainty associated with the O_2 and CO_2 abstraction because they are a simple reflection of the process model (CRWMS M&O 2000a) input.

Table 20 Gas Abstraction Information (from CRWMS M&O 2000a, DTN: SN9911T0811199.005).

Gas	Log fugacity
Oxygen	-0.7
Carbon Dioxide	-3.0

7. CONCLUSIONS

7.1 ABSTRACTION MODEL SUMMARY

The purpose of this AMR, as directed by the Development Plan (CRWMS M&O 1999a) 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 either cladding coverage for CSNF packages, or glass dissolution rate for CDSP packages.

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.

It should be noted that as an abstraction this model uses mathematical relationships to fit the output of the process models. Therefore, the abstraction as such is adequate in its comparison to the output of the process models. It must be emphasized that this does not constitute validation of the process models output, but only that the abstraction can reproduce a subset of the process model output through the use of mathematical relationships.

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 covered under DTN: MO9911SPA CDP37.001.

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 RECOMMENDATIONS FOR FUTURE WORK

The statistical relevancy of the abstraction could be enhanced with a greater population of sensitivity runs. The generation of a response surface assumes that there exists a statistically relevant population of data points on which to perform a regression analysis. However, given the computational burden of generating these points it is not always feasible to produce the desired abundance of data.

7.4 TO BE VERIFIED (TBV) IMPACT

Since all of the input data used in the abstraction are TBV, it is possible that a future revision of the *Summary of In-Package Chemistry for Waste Forms* (CRWMS M&O 2000a) could produce results different from those cited herein. The affect of this would be to change the abstracted response surfaces provided in this report.

7.5 FEP'S EVALUATION

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

8. INPUTS AND REFERENCES

8.1 DOCUMENTS CITED

CRWMS M&O 1999a. *Develop the In-Package Chemistry Abstraction Model for TSPA-LA.* TDP-WIS-MD-000013 REV00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL. 19991028.0092.

CRWMS M&O 1999. *Conduct of Performance Assessment.* Activity Evaluation, September 30, 1999. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991028.0092.

CRWMS M&O 2000a. *Summary of In-Package Chemistry for Waste Forms.* ANL-EBS-MD-000050-REV00. Las Vegas, Nevada: CRWMS M&O.ACC: MOL. 20000127.0045.

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

8.2 DATA

SN9911T0811199.005. In-Package Chemical Evolution of Degradation of Waste Packages Containing Civilian and/or DOE Spent Fuel. Submittal date: 11/23/1999.

8.3 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

AP-3.10Q, Rev. 2, ICN 0. *Analyses and Models.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000217.0246.

ASTM C 1174-97. 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. Philadelphia , Pennsylvania: American Society for Testing and Materials. TIC: 246015

DOE (U.S. Department of Energy) 2000. *Quality Assurance Requirements and Description.* DOE/RW-0333P, Rev. 9. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19991028.0012.

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) to Dr. 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.

QAP-2-0, Rev. 5. *Conduct of Activities.* Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980826.0209.

64 FR 8640. Disposal of High-Level Radioactive Waste in a Proposed Geological Repository at Yucca Mountain. Readily Available.

8. ATTACHMENTS

Attachment	Title
I	SigmaPlot Regression Analyses Data Output

ATTACHMENT I

SigmaPlot, version 4.01. regression analyses output for the pH response surfaces.

CSNF, <1000 years, low WP corrosion rate
Nonlinear Regression

```
[Variables]
x = col(1)
y = col(2)
z = col(3)
'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 = 0.99750360 Rsqr = 0.99501343 Adj Rsqr = 0.99335124

Standard Error of Estimate = 0.0659

	Coefficient	Std. Error	t	P
y0	3.4916	0.0381	91.6142	<0.0001
a	-1.0918	0.0316	-34.5728	<0.0001
b	0.4571	0.3276	1.3953	0.2124

Analysis of Variance:

	DF	SS	MS	F	P
Regression	2	5.1988	2.5994	598.6156	<0.0001
Residual	6	0.0261	0.0043		
Total	8	5.2248	0.6531		

PRESS = 0.0627

Durbin-Watson Statistic = 1.6995

Normality Test: Passed (P = 0.4744)

Constant Variance Test: Passed (P = 0.9129)

Power of performed test with alpha = 0.0500: 1.0000

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
4	5.3473	0.0022	0.0337	0.0424	0.0388
5	5.3534	0.0145	0.2193	0.2693	0.2474
6	5.4152	0.0689	1.0462	1.5056	1.7423
7	4.2555	-0.0587	-0.8904	-0.9866	-0.9840
8	4.2616	-0.0614	-0.9324	-1.0138	-1.0166
9	4.3234	-0.0888	-1.3469	-1.6507	-2.0395
10	3.4971	0.0635	0.9636	1.1763	1.2242
11	3.5033	0.0392	0.5953	0.7102	0.6774
12	3.5650	0.0205	0.3114	0.4308	0.3995

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
4	0.0004	0.3685	0.0296
5	0.0123	0.3369	0.1763
6	0.8091	0.5171	1.8031
7	0.0739	0.1856	-0.4697
8	0.0624	0.1540	-0.4338
9	0.4559	0.3342	-1.4450
10	0.2260	0.3289	0.8569
11	0.0711	0.2973	0.4406
12	0.0565	0.4775	0.3819

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
4	5.3473	5.2494	5.4452	5.1587	5.5359
5	5.3534	5.2599	5.4470	5.1670	5.5399
6	5.4152	5.2992	5.5311	5.2166	5.6138
7	4.2555	4.1860	4.3249	4.0799	4.4310
8	4.2616	4.1984	4.3249	4.0884	4.4349
9	4.3234	4.2301	4.4166	4.1371	4.5096
10	3.4971	3.4046	3.5896	3.3112	3.6830
11	3.5033	3.4153	3.5912	3.3196	3.6869
12	3.5650	3.4536	3.6764	3.3690	3.7610

CSNF, <1000 years, high WP corrosion rate
Nonlinear Regression

```
[Variables]
x = col(1)
y = col(2)
z = col(4)
'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 = 0.99912123 Rsqr = 0.99824323 Adj Rsqr = 0.99765764

Standard Error of Estimate = 0.0267

	Coefficient	Std. Error	t	P
y0	3.3977	0.0155	219.8979	<0.0001
a	-0.7468	0.0128	-58.3296	<0.0001
b	0.3515	0.1328	2.6466	0.0382

Analysis of Variance:

	DF	SS	MS	F	P
Regression	2	2.4332	1.2166	1704.6789	<0.0001
Residual	6	0.0043	0.0007		
Total	8	2.4375	0.3047		

PRESS = 0.0080

Durbin-Watson Statistic = 0.8046

Normality Test: Passed (P = 0.0920)

Constant Variance Test: Passed (P = 0.9825)

Power of performed test with alpha = 0.0500: 1.0000

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
4	4.6670	0.0220	0.8247	1.0378	1.0459
5	4.6717	0.0188	0.7032	0.8636	0.8425
6	4.7192	-0.0131	-0.4891	-0.7039	-0.6708
7	3.9202	-0.0387	-1.4481	-1.6046	-1.9387
8	3.9249	-0.0342	-1.2814	-1.3932	-1.5462
9	3.9724	0.0052	0.1952	0.2392	0.2194
10	3.4015	0.0164	0.6151	0.7508	0.7200
11	3.4062	0.0157	0.5871	0.7004	0.6673
12	3.4537	0.0078	0.2932	0.4056	0.3754

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
4	0.2095	0.3685	0.7989
5	0.1263	0.3369	0.6006
6	0.1769	0.5171	-0.6942
7	0.1956	0.1856	-0.9254
8	0.1178	0.1540	-0.6598
9	0.0096	0.3342	0.1554
10	0.0921	0.3289	0.5040
11	0.0692	0.2973	0.4340
12	0.0501	0.4775	0.3589

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
4	4.6670	4.6273	4.7066	4.5905	4.7434
5	4.6717	4.6338	4.7097	4.5961	4.7473
6	4.7192	4.6722	4.7662	4.6387	4.7997
7	3.9202	3.8920	3.9483	3.8490	3.9914
8	3.9249	3.8993	3.9506	3.8547	3.9952
9	3.9724	3.9346	4.0102	3.8969	4.0479
10	3.4015	3.3640	3.4390	3.3261	3.4768
11	3.4062	3.3706	3.4419	3.3318	3.4807
12	3.4537	3.4085	3.4988	3.3742	3.5331

CSNF, >1000 years, low WP corrosion rate
Nonlinear Regression

```
[Variables]
x = col(1)
y = col(2)
z = col(3)
'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 = 0.91116623 Rsqr = 0.83022390 Adj Rsqr = 0.77363186

Standard Error of Estimate = 0.2565

	Coefficient	**Std. Error**	**t**	**P**
y0	6.0668	0.1483	40.8954	<0.0001
a	-0.5395	0.1229	-4.3889	0.0046
b	4.0479	1.2752	3.1744	0.0192

Analysis of Variance:

	DF	**SS**	**MS**	**F**	**P**
Regression	2	1.9303	0.9651	14.6703	0.0049
Residual	6	0.3947	0.0658		
Total	8	2.3250	0.2906		

PRESS = 0.8533

Durbin-Watson Statistic = 1.6314

Normality Test: Passed (P = 0.7258)

Constant Variance Test: Passed (P = 0.0769)

Power of performed test with alpha = 0.0500: 0.9639

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	6.9894	-0.0244	-0.0951	-0.1197	-0.1094
2	7.0440	-0.0379	-0.1477	-0.1814	-0.1661
3	7.5905	-0.2124	-0.8281	-1.1917	-1.2451
4	6.4499	0.3168	1.2352	1.3687	1.5066
5	6.5046	0.2759	1.0756	1.1694	1.2149
6	7.0510	0.0775	0.3021	0.3703	0.3419
7	6.0752	-0.3315	-1.2925	-1.5777	-1.8827
8	6.1298	-0.1950	-0.7604	-0.9071	-0.8914
9	6.6763	0.1310	0.5108	0.7066	0.6737

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.0028	0.3685	-0.0836
2	0.0056	0.3369	-0.1184
3	0.5069	0.5171	-1.2885
4	0.1423	0.1856	0.7191
5	0.0830	0.1540	0.5184
6	0.0229	0.3342	0.2423
7	0.4065	0.3289	-1.3179
8	0.1160	0.2973	-0.5798
9	0.1521	0.4775	0.6441

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	6.9894	6.6084	7.3704	6.2552	7.7236
2	7.0440	6.6797	7.4084	6.3184	7.7697
3	7.5905	7.1392	8.0418	6.8175	8.3636
4	6.4499	6.1796	6.7203	5.7665	7.1333
5	6.5046	6.2582	6.7509	5.8303	7.1788
6	7.0510	6.6882	7.4139	6.3261	7.7760
7	6.0752	5.7153	6.4351	5.3517	6.7987
8	6.1298	5.7876	6.4720	5.4150	6.8447
9	6.6763	6.2426	7.1100	5.9134	7.4392

CSNF, >1000 years, high WP corrosion rate
Nonlinear Regression

```
[Variables]
x = col(11)
y = col(12)
z = col(13)
'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 = 0.91134589 Rsqr = 0.83055132 Adj Rsqr = 0.77406843

Standard Error of Estimate = 0.1270

	Coefficient	**Std. Error**	**t**	**P**
y0	6.0913	0.0735	82.9250	<0.0001
a	-0.3057	0.0609	-5.0225	0.0024
b	1.2913	0.6314	2.0451	0.0868

Analysis of Variance:

	DF	**SS**	**MS**	**F**	**P**
Regression	2	0.4744	0.2372	14.7045	0.0049
Residual	6	0.0968	0.0161		
Total	8	0.5712	0.0714		

PRESS = 0.2244

Durbin-Watson Statistic = 2.1531

Normality Test: Passed (P = 0.6006)

Constant Variance Test: Passed (P = 0.1694)

Power of performed test with alpha = 0.0500: 0.9641

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	6.6126	-0.0026	-0.0207	-0.0260	-0.0238
2	6.6301	-0.0001	-0.0005	-0.0006	-0.0005
3	6.8044	-0.1244	-0.9793	-1.4093	-1.5730
4	6.3069	0.1831	1.4414	1.5972	1.9231
5	6.3244	0.0656	0.5168	0.5619	0.5270
6	6.4987	0.0613	0.4828	0.5917	0.5566
7	6.0946	-0.1746	-1.3747	-1.6780	-2.1027
8	6.1120	-0.0720	-0.5671	-0.6765	-0.6426
9	6.2863	0.0637	0.5012	0.6934	0.6600

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.0001	0.3685	-0.0182
2	0.0000	0.3369	-0.0004
3	0.7090	0.5171	-1.6278
4	0.1938	0.1856	0.9180
5	0.0192	0.1540	0.2249
6	0.0586	0.3342	0.3944
7	0.4599	0.3289	-1.4719
8	0.0646	0.2973	-0.4180
9	0.1465	0.4775	0.6309

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	6.6126	6.4240	6.8013	6.2491	6.9762
2	6.6301	6.4497	6.8105	6.2707	6.9894
3	6.8044	6.5809	7.0279	6.4216	7.1872
4	6.3069	6.1731	6.4408	5.9686	6.6453
5	6.3244	6.2024	6.4463	5.9905	6.6582
6	6.4987	6.3190	6.6783	6.1397	6.8576
7	6.0946	5.9164	6.2728	5.7364	6.4528
8	6.1120	5.9426	6.2815	5.7581	6.4660
9	6.2863	6.0716	6.5011	5.9086	6.6641

CDSP, <1000 years, low WP corrosion rate
Nonlinear Regression

```
[Variables]
x = col(1)
y = col(2)
z = col(3)
'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 = 0.98051046 Rsqr = 0.96140077 Adj Rsqr = 0.93566795

Standard Error of Estimate = 0.1099

	Coefficient	Std. Error	t	P
y0	5.1257	0.0800	64.0902	<0.0001
a	2.6692	0.6690	3.9898	0.0282
b	0.0764	0.0100	7.6683	0.0046

Analysis of Variance:

	DF	SS	MS	F	P
Regression	2	0.9021	0.4510	37.3609	0.0076
Residual	3	0.0362	0.0121		
Total	5	0.9383	0.1877		

PRESS = 0.2382

Durbin-Watson Statistic = 1.2074

Normality Test: Passed (P = 0.4494)

Constant Variance Test: Passed (P = 0.0600)

Power of performed test with alpha = 0.0500: 0.9794

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	5.2062	0.0573	0.5219	0.6983	0.6230
2	5.2422	0.0487	0.4433	0.5695	0.4924
3	5.6025	-0.1060	-0.9651	-1.6660	-4.9740
4	5.8941	-0.0935	-0.8509	-1.1386	-1.2336
5	5.9301	-0.0089	-0.0813	-0.1044	-0.0854
6	6.2905	0.1024	0.9322	1.6092	3.5523

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.1284	0.4414	0.5538
2	0.0703	0.3941	0.3971
3	1.8318	0.6644	-6.9989
4	0.3415	0.4414	-1.0967
5	0.0024	0.3941	-0.0689
6	1.7090	0.6644	4.9984

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	5.2062	4.9738	5.4385	4.7864	5.6260
2	5.2422	5.0227	5.4617	4.8293	5.6551
3	5.6025	5.3175	5.8876	5.1514	6.0537
4	5.8941	5.6618	6.1264	5.4743	6.3139
5	5.9301	5.7106	6.1497	5.5173	6.3430
6	6.2905	6.0055	6.5755	5.8394	6.7416

CDSP, <1000 years, high WP corrosion rate
Nonlinear Regression

```
[Variables]
x = col(12)
y = col(13)
z = col(14)
'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 = 0.99663016 Rsqr = 0.99327167 Adj Rsqr = 0.98878612

Standard Error of Estimate = 0.0442

	Coefficient	Std. Error	t	P
y0	4.7324	0.0322	147.0539	<0.0001
a	0.7307	0.2692	2.7145	0.0729
b	0.0837	0.0040	20.8688	0.0002

Analysis of Variance:

	DF	SS	MS	F	P
Regression	2	0.8657	0.4328	221.4379	0.0006
Residual	3	0.0059	0.0020		
Total	5	0.8715	0.1743		

PRESS = 0.0203

Durbin-Watson Statistic = 3.3550

Normality Test: Passed (P = 0.2783)

Constant Variance Test: Passed (P = 0.0600)

Power of performed test with alpha = 0.0500: 0.9998

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	4.8172	-0.0072	-0.1630	-0.2181	-0.1795
2	4.8271	-0.0071	-0.1600	-0.2055	-0.1690
3	4.9257	0.0143	0.3230	0.5575	0.4808
4	5.5705	-0.0405	-0.9170	-1.2269	-1.4193
5	5.5804	0.0596	1.3479	1.7318	76.9607
6	5.6791	-0.0191	-0.4310	-0.7440	-0.6726

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.0125	0.4414	-0.1596
2	0.0092	0.3941	-0.1363
3	0.2051	0.6644	0.6765
4	0.3966	0.4414	-1.2617
5	0.6503	0.3941	62.0743
6	0.3653	0.6644	-0.9465

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	4.8172	4.7237	4.9107	4.6483	4.9861
2	4.8271	4.7387	4.9154	4.6609	4.9932
3	4.9257	4.8110	5.0404	4.7442	5.1072
4	5.5705	5.4771	5.6640	5.4016	5.7395
5	5.5804	5.4921	5.6687	5.4143	5.7465
6	5.6791	5.5644	5.7937	5.4975	5.8606

CDSP, >1000 years, low WP corrosion rate
Nonlinear Regression

```
[Variables]
x = col(1)
y = col(2)
z = col(3)
'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 = 0.93311530 Rsqr = 0.87070416 Adj Rsqr = 0.78450694

Standard Error of Estimate = 0.3660

	Coefficient	Std. Error	t	P
y0	8.4247	0.2664	31.6217	<0.0001
a	-3.4173	2.2286	-1.5334	0.2227
b	0.1403	0.0332	4.2251	0.0242

Analysis of Variance:

	DF	SS	MS	F	P
Regression	2	2.7065	1.3532	10.1013	0.0465
Residual	3	0.4019	0.1340		
Total	5	3.1084	0.6217		

PRESS = 1.6213

Durbin-Watson Statistic = 1.6608

Normality Test: Passed (P = 0.4169)

Constant Variance Test: Passed (P = 0.0600)

Power of performed test with alpha = 0.0500: 0.8298

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	8.5599	-0.4641	-1.2679	-1.6965	-6.8702
2	8.5137	0.2970	0.8113	1.0424	1.0657
3	8.0524	0.1671	0.4565	0.7881	0.7226
4	9.8225	0.1785	0.4876	0.6524	0.5750
5	9.7764	0.0172	0.0470	0.0604	0.0493
6	9.3151	-0.1957	-0.5346	-0.9228	-0.8904

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.7582	0.4414	-6.1076
2	0.2356	0.3941	0.8595
3	0.4099	0.6644	1.0168
4	0.1121	0.4414	0.5112
5	0.0008	0.3941	0.0398
6	0.5620	0.6644	-1.2528

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	8.5599	7.7860	9.3338	7.1614	9.9584
2	8.5137	7.7825	9.2450	7.1384	9.8891
3	8.0524	7.1029	9.0019	6.5496	9.5552
4	9.8225	9.0486	10.5965	8.4241	11.2210
5	9.7764	9.0451	10.5077	8.4011	11.1517
6	9.3151	8.3656	10.2645	7.8123	10.8178

CDSP, >1000 years, high WP corrosion rate
Nonlinear Regression

```
[Variables]
x = col(11)
y = col(12)
z = col(13)
'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 = 0.46420143 Rsqr = 0.21548297 Adj Rsqr = -0.30752839

Standard Error of Estimate = 0.7606

	Coefficient	Std. Error	t	P
y0	9.2554	0.5537	16.7165	0.0005
a	-3.1280	4.6314	-0.6754	0.5478
b	-0.0418	0.0690	-0.6065	0.5870

Analysis of Variance:

	DF	SS	MS	F	P
Regression	2	0.4768	0.2384	0.4120	0.6949
Residual	3	1.7357	0.5786		
Total	5	2.2125	0.4425		

PRESS = 10.1826

Durbin-Watson Statistic = 1.0236

Normality Test: Passed (P = 0.5623)

Constant Variance Test: Passed (P = 0.0600)

Power of performed test with alpha = 0.0500: 0.1380

The power of the performed test (0.1380) 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.
1	9.2089	0.6111	0.8034	1.0750	1.1194
2	9.1667	0.0333	0.0438	0.0563	0.0460
3	8.7444	-0.6444	-0.8472	-1.4624	-2.2283
4	8.8323	-0.7323	-0.9627	-1.2881	-1.5732
5	8.7900	0.1000	0.1314	0.1689	0.1385
6	8.3677	0.6323	0.8312	1.4349	2.0917

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.3044	0.4414	0.9951
2	0.0007	0.3941	0.0371
3	1.4114	0.6644	-3.1354
4	0.4371	0.4414	-1.3985
5	0.0062	0.3941	0.1117
6	1.3588	0.6644	2.9432

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	9.2089	7.6006	10.8172	6.3026	12.1152
2	9.1667	7.6469	10.6864	6.3085	12.0249
3	8.7444	6.7712	10.7175	5.6214	11.8674
4	8.8323	7.2239	10.4406	5.9260	11.7385
5	8.7900	7.2703	10.3098	5.9318	11.6482
6	8.3677	6.3946	10.3409	5.2447	11.4