OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
CALCULATION COVER SHEET

1. QA: QA
Page: 1 Of: 37

2. Calculation Title
Microbial Communities Model Parameter Calculations for TSPA/SR

MOL.20010828.0002

3. Document Identifier (including Revision Number)
CAL-EBS-PA-000001 REV 00

4. Total Attachments	5. Attachment Numbers - Number of pages in each
0	N/A

	Print Name	Signature	Date
6. Originator	Darren Jolley		7/16/01
7. Checker	Amy Loch		16 July 2001
8. Lead	Jim Nowak For	J. Blink EBS PMR Mgr	16 Jul 01

9. Remarks
The following TBVs can be closed out with the use of this calculation:

TBV-0370
TBV-3763
TBV-4227

The results of this calculation (Table 6.2-1) supercededs the following DTN: MO9909SPAMING1.003

This calculation also documents the impacts of TBV-4659 on the In-Drift Microbial Communities AMR (ANL-EBS-MD-000038 Rev 00 ICN 01).

The results of this calculation also replace the majority of Attachment II (excepting II-5.3) in the In-Drift Microbial Communities AMR (ANL-EBS-MD-000038 Rev 00 ICN 01) and replaces and adds some parameters to Table 32 of that document.

Revision History

10. Revision No.	11. Description of Revision
00	Initial Issue

CONTENTS

Page

LIST OF TABLES

Page

LIST OF FIGURES

Page

1. PURPOSE

This calculation has several purposes. First the calculation reduces the information contained in *Committed Materials in Repository Drifts* (BSC 2001a) to useable parameters required as input to MING V1.0 (CRWMS M&O 1998, CSCI 30018 V1.0) for calculation of the effects of potential in-drift microbial communities as part of the microbial communities model. The calculation is intended to replace the parameters found in Attachment II of the current In-Drift Microbial Communities Model revision (CRWMS M&O 2000c) with the exception of Section II-5.3.

Second, this calculation provides the information necessary to supercede the following DTN: MO9909SPAMING1.003 and replace it with a new qualified dataset (see Table 6.2-1). The purpose of this calculation is to create the revised qualified parameter input for MING that will allow ΔG (Gibbs Free Energy) to be corrected for long-term changes to the temperature of the near-field environment. Calculated herein are the quadratic or second order regression relationships that are used in the energy limiting calculations to potential growth of microbial communities in the in-drift geochemical environment.

Third, the calculation performs an impact review of a new DTN: MO0012MAJIONIS.000 that is intended to replace the currently cited DTN: GS980908312322.008 for water chemistry data used in the current *In-Drift Microbial Communities Model* revision (CRWMS M&O 2000c).

Finally, the calculation updates the material lifetimes reported on Table 32 in section 6.5.2.3 of the *In-Drift Microbial Communities* AMR (CRWMS M&O 2000c) based on the inputs reported in BSC (2001a). Changes include adding new specified materials and updating old materials information that has changed.

This work activity has been evaluated in accordance with the AP-2.21 procedure, *Quality Determinations and Planning for Scientific, Engineering, and Regulatory Compliance Activities* Revision 1, BSCN 1, and is subject to QA controls (BSC 2001c). The calculation is developed in accordance with the AP-3.12 procedure, *Calculations*, Revision 0, ICN 4, and prepared in accordance with the *Technical Work Plan For EBS Department Modeling FY 01 Work Activities* (BSC 2001c) which includes controls for the management of electronic data.

2. METHOD

2.1 REPOSITORY SUBSURFACE DESIGN INPUT PARAMETERS

Data or information that has been delivered to EBS may be complete and necessary for other EBS calculations but for use in MING may be overly detailed or in a format that cannot be directly used. This calculation extracts the necessary information from BSC (2001a) and places it into a format that can be used. This calculation also reduces the extemporaneous data from the sources and tabulates the results.

MING requires all chemical compositions of the repository design materials to be reported in two ways.

1- The material compositions (wt %) are required as a minimum for the following elements: C, N, P, S, Mn, and Fe.
2- The mass of each material in the design should be in terms of kilograms per linear meter of either waste package or repository.

All input information is converted into this format as necessary from the information in BSC (2001a).

2.2 TEMPERATURE DEPENDENT GIBBS FREE ENERGY PARAMETERS

In this calculation, temperature dependent ΔG_r° data for each selected redox half reaction were obtained using the same sources of data used to prepare the qualified dataset in DTN MO0008THRMODYN.000. This data was taken from either an accepted electronic handbook or from references cited by those handbooks and formatted for use in SUPCRT92 (STN: 10058-1.0-00). This software is used to define the temperature ΔG_r° dependent parameters that could be incorporated into the energy calculations performed in MING.

Each half reaction that is of interest is entered into SUPCRT92 and the output is saved to a file. This file produces ΔG_r° in calories per mol, thus need to be converted to kilojoules per mol for use in MING. The conversion is made using the following conversion factor (Morel and Hering, 1993, inside back cover).

$$1 \text{ Calorie} = 4.184 \text{ Joules} = 4.184e^{-3} \text{ Kilojoules}$$

The ΔG_r° and temperature data from SUPCRT92 for each half reaction were entered into the SigmaPlot program and are plotted in a simple XY format to which the second order regression tool is applied. This routine then plotted the regressed curve through the plotted data and calculated the second order regression coefficients (B_0, B_1 and B_2) . Temperature dependent regression variables are used in MING the following way (Eq. 1)

$$\Delta G_{r\,(temp)}^\circ = B_0 + B_1 T + B_2 T^2 \qquad \text{(Eq. 1)}$$

2.3 DTN IMPACT REVIEW

Comparison of the two DTN's for any deviation in values will be conducted and recommendations will be made to use the new or existing input.

2.4 MATERIAL LIFETIMES

Another input that may be varied in the calculations below is the material lifetimes used to calculate the availability of materials in both the nutrient and energy calculations. Material lifetime inputs for the calculations below are given in Table 32 of CRWMS M&O (2000c). The reference case values (median lifetimes) are thought to be a reasonable lifetime of the given material based on the calculations below.

3. ASSUMPTIONS

3.1 REPOSITORY SUBSURFACE DESIGN INPUT PARAMETERS

1. Even though information was reported about the specific composition of all Swellex rock bolt sets components, all compositional data reported are based on the composition of the bolts only [used in Section 6.1.1].

2. Due to the lack of information on the composition of the steel fittings that are part of the rail fittings and conductor bar, the fittings were assumed to be A572 steel [used in Section 6.1.1].

3 Due to lack of information about the composition of ceramic insulators, this material is not included in the information to be evaluated for the rail fittings [used in Section 6.1.1].

The general rationale and/or basis for all of the assumptions above are encompassed in one or the other of the following two reasons. First, the composition of materials assumed will be a good approximation for the replaced materials as the masses and compositions are not going to be dramatically different from those assumed. For example, comparing the compositions of the various steel alloys reported in Section 6.1.1 below, the steels are similar in composition. Second, the masses of these materials are generally small in comparison to the masses of some of the major alloys that are used in the system. For example, the mass of the commo cable is two orders of magnitude less than that of the steel invert (See Table 6.1.2-1 below).

4. Because silica fume can vary in composition (CRWMS M&O 1997 Table 7.2 and DTN MO9912DTMKCCOF.000) and is used to lower the pH of concrete emplaced in the repository environment by the presence of elevated SiO_2, the values selected for use are found on Table 5.1.2-1 [used in Section 5.1.2].

The rationale for this assumption is that the values reported in CRWMS M&O (1997) and in DTN MO9912DTMKCCOF.000 show Table 5.1.2-1 to have the highest SiO_2 content. This composition is more likely to be used by design than the values with lower SiO_2 content based on the desire to lower the pH of the cement because of the uncertainty in using cement in the repository (CRWMS M&O 1997, Section 7.4.3), even though the higher iron and sulfur contents for silica fume are found on Table 7.2. and would provide more nutrients and energy for microbial catalysis. Additionally, the values on Table 5.1.2-1 have been reported as representative of the silica fume produced in North America (Bhattacharyya 2000, Attachment II, page 1).

5. Due to the absence of an exact compositional information for WWF, the use of ASTM A 36 carbon steel will be used (Table 6.1.1-1) for the unspecified general carbon steel composition.

The rationale for this assumption is that the compositions will be similar as BSC (2001a Section 3.2.2.2 and 6.2.1) indicates that the wire is fabricated from carbon steel. They assumed that it would be similar to ASTM A 36 steel [used in section 6.1.1].

3.2 TEMPERATURE DEPENDENT GIBBS FREE ENERGY PARAMETERS

Extending the temperatures to which MO0008THRMODYN.000 was qualified is an acceptable use of the data and does not violate its qualification status. According to the Data Qualification report which produced MO0008THRMODYN.000, the data is valid for temperatures up to 100°C. However, for microbial calculations in MING the temperature range for this data needs to be expanded to at least 120°C in order for the range of potential microbial growth to be utilized.

The rationale for this assumption is based on the following argument. SUPCRT92 is a qualified code that is designed to make the appropriate temperature extrapolations to thermodynamic data over the following ranges in temperature (0 to 1000°C) and pressure (1 to 5000 bar), therefore should produce accurate results at 120°C and above. For our purposes, extending the temperature range by 50°C beyond its range of qualification status should be valid in this case.

3.3 DTN IMPACT REVIEW

No assumptions were made.

3.4 MATERIAL LIFETIMES

No assumptions were made.

4. USE OF COMPUTER SOFTWARE AND MODELS

4.1 REPOSITORY SUBSURFACE DESIGN INPUT PARAMETERS

No software was developed in the preparation of the calculation.

4.2 TEMPERATURE DEPENDENT GIBBS FREE ENERGY PARAMETERS

4.2.1 SUPCRT92

SUPCRT92, Version 1.0, STN: 10058-1.0-00 is a qualified acquired software product obtained from Software Configuration Management (SCM) and was used only within the range of validation in accordance with AP-SI.1Q. SUPCRT92 was used on a a Dell PowerEdge 2200 PC (CPU 112370) with dual Pentium II - 266 MHz chips, 128 MB of RAM, in a Windows NT 4.0 operating system. SUPCRT92 calculates the variation of thermodynamic properties with temperature using the modified Helgeson/Kirkham/Flowers equation of state (Tanger and Helgeson 1988) for aqueous species and the Maier-Kelly expression (Helgeson et al. 1978) for solids and gases. This program is appropriate to make the temperature dependent extrapolations for ΔG of half reactions from 0 to at least 120°C as these algorithms can produce extrapolations of thermodynamic properties to temperatures exceeding 1000°C and 500 bars of pressure.

4.2.2 Sigma Plot

SigmaPlot 4.0 is an appropriate commercial off the shelf software application in that it is able to perform linear regression calculations given two input variables. The second order linear regression routine found in the SigmaPlot 4.0 software package was used to provide the temperature dependent parameters for ΔG. Sigma Plot Version 4.0 is an exempt software product in accordance with AP-SI.1Q, Revision 3, ICN, Section 2.1.1.

4.3 DTN IMPACT REVIEW

No software was used.

4.4 MATERIAL LIFETIMES

No software was used.

5. CALCULATION

5.1 REPOSITORY SUBSURFACE DESIGN INPUT PARAMETERS

The source of most information found herein is BSC (2001a) and is based on preliminary design information. Of the information provided in BSC (2001a) and used in this attachment, the sources from ASTM standards (see Section 7.2) are considered to be accepted data. Two other sources of accepted data used in this calculation are the periodic table of elements (Sargent–Welch Scientific Company 1979) and the chemical formulas for various organic materials found in a widely used organic chemistry text book (Morrison and Boyd 1992).

5.1.1 Type K Cement Composition

Type K cement is part of the grout formulation used to anchor rock bolts in the repository drift ground support (BSC 2001a) and its characteristics are found in the following DTN: MO9912SEPMKTDC.000. Compositions of Type K cement are given in oxide weight percentage. These have to be converted to elemental weight percentage, as explained below, in order to be fed into MING as input. The oxide composition is shown in Table 5.1.1-1.

Step 1: Calculate formula weights for each oxide. This is done by multiplying each element formula weight (Sargent-Welch 1979) by the number of atoms of that element and summing all of the values (e.g., for SiO_2 do the following 1[Si]*28+2[O]*16 = 60). Applicable formula weights are found in Table 5.1.1-2.

Step 2: Determine the fraction of the oxide weight % for each element then sum the resulting elemental weight percents. This is done by taking the elemental weight % and multiplying by the number of atoms of each element then dividing by the oxide formula weight and then multiplying by the oxide weight % (e.g. for P in P_2O_5: 31*2/142*0.1=0.044). This gives the fraction of the element in the oxide in terms of the oxide weight %. These values are then summed for each element to give the elemental weight %. Results are found on Table 6.1.1-5 below.

Table 5.1.1-1. Oxide Composition of Type K Expansive Cement Manufactured to ASTM C 845-96.

Oxide Component	Wt %
SiO_2	19.4
Al_2O_3	5.2
Fe_2O_3	2.8
CaO	61.9
MgO	1.4
SO_3	6.9
Na_2O	0.1
K_2O	0.59
SrO	0.05
ZnO	0.02
TiO_2	0.28
P_2O_5	0.1
MnO_3	0.04
LOI	1.1
Total	99.88

DTN: MO9912SEPMKTDC.000

Table 5.1.1-2. Formula Weights for Elements and Minerals in Type K Cement.

Element	Formula Wt	Oxide	Formula Wt
Ca	40	SiO_2	60
Si	28	Al_2O_3	102
O	16	Fe_2O_3	160
Al	27	CaO	56
Fe	56	MgO	40
S	32	SO_3	80
K	39	Na_2O	62
Na	23	K_2O	94
Mg	24	SrO	104
Sr	88	ZnO	81
Zn	65	TiO_2	80
Ti	48	P_2O_5	142

Mn	55	MnO_3	103
P	31		

5.1.2 Silica Fume Composition

Silica fume is part of the cement admixtures used in the grout formulation to anchor rock bolts in the repository drift ground support (BSC 2001a). The source of the oxide composition of silica fume (5.1.2-1) is discussed in assumption 4 above. These values need to be converted to elemental weight percentages so that they can be used directly in MING V1.0. This is done following the same steps used to calculate the elemental formula weight percents in the Type K cement (see Section 5.1.1). Data for the formula weights were taken from Sargent-Welch (1979). Results are found on Table 6.1.1-6 below.

Table 5.1.2-1. Oxide Composition of Silica Fume.

Oxide	Wt %
SiO_2	95.0
Al_2O_3	0.7
Fe_2O_3	0.3
CaO	0.3
MgO	0.2
Na_2O	0.3
K_2O	0.3
SO_3	0.8
C	1.3

Table 5.1.2-2. Formula Weights for Elements and Oxides Found in this Section.

Element	Formula Wt	Oxide	Formula Wt
Ca	40	SiO_2	60
Si	28	Al_2O_3	102
O	16	Fe_2O_3	160
Al	27	CaO	56
Fe	56	MgO	40
S	32	Na_2O	62
K	39	K_2O	94
Na	23	SO_3	80
Mg	24		

5.1.3 Communications Cable Composition

Communications cables are part of the repository drift ground support design reported in BSC (2001a) . This section represents the calculations to determine the appropriate elemental Wt % of materials for the communications cable to enter into MING. Composition of the functional groups for polyethylene polymer was taken from Morrison and Boyd (1992). Formula weights for each element were taken from Sargent-Welch Scientific Company (1979).

The appropriate Wt fraction of polyethylene found in the communications cable was determined by taking the composition reported in Morrison and Boyd (1992, CH_2CH_2, Page 350) and formula weights (FW) found in Sargent-Welch Scientific Company (1979), and dividing the elemental FW by the total FW. The values are then normalized to 50% based on design input that the cable is 50% (by weight) polyethylene (BSC 2001a).

Table 5.1.3-1. Normalized Wt Fraction of Polyethylene

CH_2CH_2	2*C	4*H	Total
FW (from periodic table)	24.022	4.0316	28.0536
Wt fraction (FW/ total FW)	0.8563	0.1437	1.00000
Normalized Wt fraction (50%)	0.4282	0.0718	0.50000

Table 6.1.1-9 below was developed from the values Table 5.1.3-1 above and the communications cable composition assumptions from BSC (2001a).

- 50% Cu
- 50% Polyethylene

5.1.4 Rail Fittings Composition

This section calculates the appropriate composition for rail fittings given an unknown steel composition from BSC (2001a) and a 75% to 25% steel copper mix. Because the steel composition is unspecified, we have chosen to use an A572 composition (See assumption 2 in Section 3.1).

Step 1: Convert steel values found in Table 6.1.1-1 below to values at 75% using the following formula (Formula = Wt % (from Table 6.1.1-1 below) * 0.75).

Table 5.1.4-1. Results of Step 1.

Element	Wt %
C	0.1725
P	0.03
S	0.0375
Si	0.3
Mn	1.2375
V	0.1125
Fe	73.11

Step 2: Create Table 6.1.1-8 below with the values above and 25% Cu.

5.1.5 ASTM Standard Materials

ASTM standard materials are specified by BSC (2001a) for many of the ground support items and as such the standard material specifications for composition are to be used as noted in Section 6.1 below.

5.2 TEMPERATURE DEPENDENT GIBBS FREE ENERGY PARAMETERS

As discussed in CRWMS M&O 2000c, Section 6.3.1.1, Table 5.2-1 below lists the possible redox half reactions that are associated with microbial catalysis. This table however does not include the half reactions for reducing U(VI) to U(IV). Microbes that are involved in iron reduction can also reduce uranium. CRWMS M&O 2000c (Section 7.7) also recommends that these reactions be included in the energy calculations as there is a potential for increased microbial growth due to these reactions.

5.2.1 Half Reactions and Reactant Compositions

Table 5.2-2 below lists the half reactions that will be added as a result of uranium reduction. All of these half reactions will be entered into SUPCRIT92 to develop the appropriate temperature dependent ΔG values. Table 5.2-2 also lists the necessary reactant compositions to be able to associate the material composition with the associated half reaction. Based on the methodology described in Attachment V of CRWMS M&O 2000c, the reactant composition is based on the general redox state. Because the redox state of uranium in spent fuels tends to be in the U(VI) state (BSC 2001b Section 4.1.1) the associated ion would be the UO_2^{2+} ion.

Table 5.2-1. Redox Half Reactions Associated with Microbial Catalysis Used in Previous MING Calculations (CRWMS M&O 2000c, Table 9).

Redox half reaction	Redox half reaction
Carbon	**Iron**
$CO_2 + H^+ + 2e^- = HCOO^-$	$Fe_2O_3 + 6H^+ + 6e^- = 2Fe + 3H_2O$
$CO_2 + 4H^+ + 4e^- = CH_2O + H_2O$	$Fe^{2+} + 2e^- = Fe$
$CO_2 + 6H^+ + 6e^- = CH_3OH + H_2O$	$Fe^{3+} + e^- = Fe^{2+}$
$HCOO^- + 3H^+ + 2e^- = CH_2O + H_2O$	$Fe_3O_4 + 8H^+ + 8e^- = 3Fe + 4H_2O$
$CO_2 + 8H^+ + 8e^- = CH_4 + 2H_2O$	$FeOOH + 3H^+ + e^- = Fe^{2+} + 2H_2O$
$CH_2O + 2H^+ + 2e^- = CH_3OH$	**Manganese**
$HCOO^- + 7H^+ + 6e^- = CH_4 + 2H_2O$	$MnO_2 + 4H^+ + 2e^- = Mn^{2+} + 2H_2O$
$CH_2O + 4H^+ + 4e^- = CH_4 + H_2O$	$Mn_3O_4 + 8H^+ + 2e^- = 3Mn^{2+} + 4H_2O$
$CH_3OH + 2H^+ + 2e^- = CH_4 + H_2O$	**Sulfur**
$CO_3^{2-} + 10H^+ + 8e^- = CH_4 + 3H_2O$	$S + H^+ + 2e^- = HS^-$
$CO_3^{2-} + 6H^+ + 4e^- = CH_2O + 2H_2O$	$S + 2H^+ + 2e^- = H_2S$

Redox half reaction	Redox half reaction
$CO_3^{2-} + 8H^+ + 6e^- = CH_3OH + 2H_2O$	$SO_4^{-2} + 9H^+ + 8e^- = HS^- + 4H_2O$
$CO_3^{2-} + 3H^+ + 2e^- = HCOO^- + H_2O$	$SO_4^{-2} + 10H^+ + 8e^- = H_2S + 4H_2O$
Nitrogen	$HSO_4^- + 7H^+ + 6e^- = S + 4H_2O$
$N_2 + 6H^+ + 6e^- = 2NH_3$	$SO_4^{-2} + 8H^+ + 6e^- = S + 4H_2O$
$N_2 + 8H^+ + 6e^- = 2NH_4^+$	$SO_2 + 4e^- + 4H^+ = S + 2H_2O$
$NO_2^- + 7H^+ + 6e^- = NH_3 + 2H_2O$	$SO_3^{2-} + 7H^+ + 6e^- = HS^- + 3H_2O$
$NO_3^- + 2H^+ + 2e^- = NO_2^- + H_2O$	$2SO_4^{-2} + 10H^+ + 8e^- = S_2O_3^{-2} + 5H_2O$
$NO_3^- + 10H^+ + 8e^- = NH_4^+ + 3H_2O$	**Hydrogen**
$NO_2^- + 8H^+ + 6e^- = NH_4^+ + 2H_2O$	$H^+ + e^- = 0.5H_2$
$NO_3^- + 6H^+ + 5e^- = 0.5N_2 + 3H_2O$	**Oxygen**
$2NO_2^- + 8H^+ + 6e^- = N_2 + 4H_2O$	$O_2 + 4H^+ + 4e^- = 2H_2O$
$NO_3^- + 9H^+ + 8e^- = NH_3 + 3H_2O$	

Table 5.2-2. Redox Half Reaction Associated with Microbial Reduction of Uranium (IV) to Uranium (VI) and the associated reactant compositions to augment the parameter table for each of the spent fuel compositions (Table V-2) found in attachment V of CRWMS M&O (2000c)

Uranium	Reactant Compositions		
$UO_2^{2+} + 4H^+ + 2e^- = U^{4+} + 2H_2O$	CSNF PWR	CSNF BWR	DHLW
	UO_2^{2+}	UO_2^{2+}	UO_2^{2+}

5.2.2 SUPCRT92 INPUT (smicrobe.dat)

A database (schkfil5.dat; CRWMS M&O 2000a, Appendix J) for use in the SUPCRT92 software code was generated during the derivation of the Data0.ymp data file (MO0008THRMODYN.000) for use in other geochemical modeling work. The data used in the generation of the qualified data set was taken from several online databases and electronic handbooks that have been designated as acceptable for use on the project. These files are documented in the data qualification report (CRWMS M&O 2000a). The starting point for the development of the data required to build the input table for MING is taken from this report and is documented below.

Using the schkfil5.dat database file as a starting place, a new database file was generated titled smicrobe.dat. Because smicrobe.dat will support modeling of microbial activity in the Engineered Barrier System, several organic species, several minerals, and several inorganic aqueous species had to be added to the existing schkfil5.dat database. Most of the species were taken directly from 2 electronic handbooks that are documented in the *Data Qualification Report for Thermodynamic Data File, Data0.ymp.R0 for Geochemical Code, EQ3/6* (CRWMS M&O 2000a, Appendix J): slop98.dat and sprons96.dat. Species extracted from the handbooks were copied and pasted into the ASCII file using Microsoft Wordpad. These species and the source are listed in Table 5.2.2-1.

Table 5.2.2-1. Species added to schkfil5.dat from electronic handbooks to create smicrobe.dat

Species	Classification	Datasource
CO3-2	Aqueous species	slop98.dat
NH4+	Aqueous species	slop98.dat
NO2-	Aqueous species	slop98.dat
Fe2O3	Mineral species that undergoes 2 phase transitions	slop98.dat
Fe	Mineral species that undergoes 3 phase transitions	sprons96.dat
Fe3O4	Mineral species that undergoes 1 phase transition	slop98.dat
Fe+3	Aqueous species	slop98.dat
Mn+2	Aqueous species	slop98.dat
H2S	Aqueous species	slop98.dat
S	Mineral species that undergoes 2 phase transitions	slop98.dat
SO3-2	Aqueous species	slop98.dat
H2	Aqueous species	slop98.dat

Three minearls, MnO_2 (pyrolusite), Mn_3O_4 (hausmanite), and α–FeOOH (goethite) required derivation from other available data. Species in the database require values for the free energy of formation, entropy, enthalpy, and molar volume for the species at 298.15 K. In addition, the coefficients for the Maier-Kelly expansion must be determined from constant pressure molar heat capacity (C_p) for the species (Eq. 2)

$$C_p = a + bT + \frac{c}{T^2} \qquad \text{(Eq. 2)}$$

The coefficients a, b, and c are specific to each species and, in this document, have the units of cal/mol·K, cal/mol·K^2, and cal·K/mol, respectively. For the manganese minerals, the thermodynamic and heat capacity data came from Robie and Hemingway (1995). For goethite, the data was taken from Robie et al. (1979). This second reference does not contain all of the heat capacity data, but refers the reader to the original publication. Therefore, the heat capacity data for goethite was taken from King and Weller (1970). All of the thermodynamic and molar volume data is listed in Table 5.2.2-2. Note: these three data sources are part of the references for the accepted electronic handbooks. Therefore, they are considered accepted data sources themselves.

Table 5.2.2-2. Thermodynamic and molar volume data for pyrolusite, hausmanite, and goethite.

Parameter	Goethite	Hausmannite	Pyrolusite
$\Delta G°_f$ (cal/mol @ 298.15 K)	-116766	-306524	-111138
$\Delta H°_f$ (cal/mol @ 298.15 K)	-133683	-330903	-124283
$S°_{T,P}$ (cal/mol·K @ 298.15 K)	14.43	39.22	12.607
$V°_{T,P}$ (cm^3/mol)	20.82	46.95	16.61

The regression wizard function of SigmaPlot 4.0, a built-in fuction of the software, was used to fit the available heat capacity data to the Maier-Kelly expansion equation. This fit determined the coefficients a, b, and c for each species. The resulting equations are:

Goethite: $$C_{p,Goethite} = -0.15 + 0.0628T - \frac{6823.5}{T^2} \quad \text{(Eq. 3)}$$

Hausmannite: $$C_{p,Hausmannite} = 34.36 + 0.01T - \frac{310943}{T^2} \quad \text{(Eq. 4)}$$

Pyrolusite: $$C_{p,Pyrolusite} = 17.5 + 9.66E^{-3}T - \frac{421146}{T^2} \quad \text{(Eq. 5)}$$

The C_p data and the regression fit are plotted in Figures 5.2.2-1, 5.2.2-2 and 5.2.2-3.

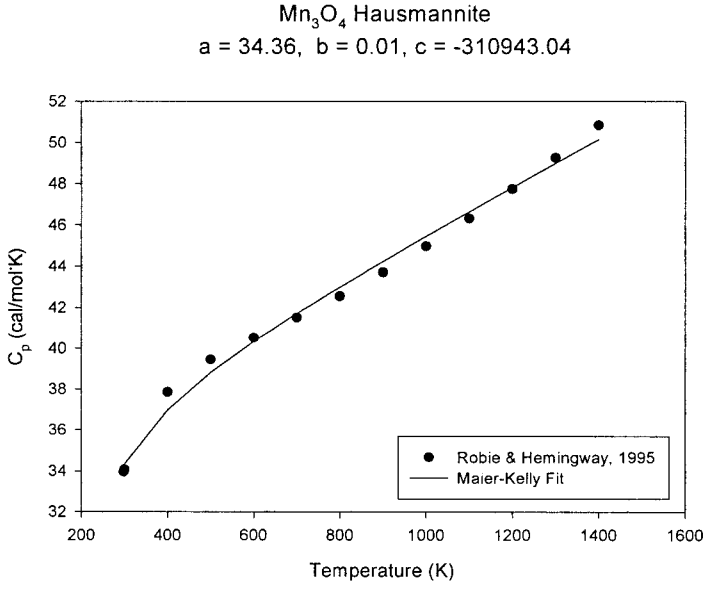

Figure 5.2.2-1 Determination of Maier-Kelly Expansion Coefficients for Hausmannite.

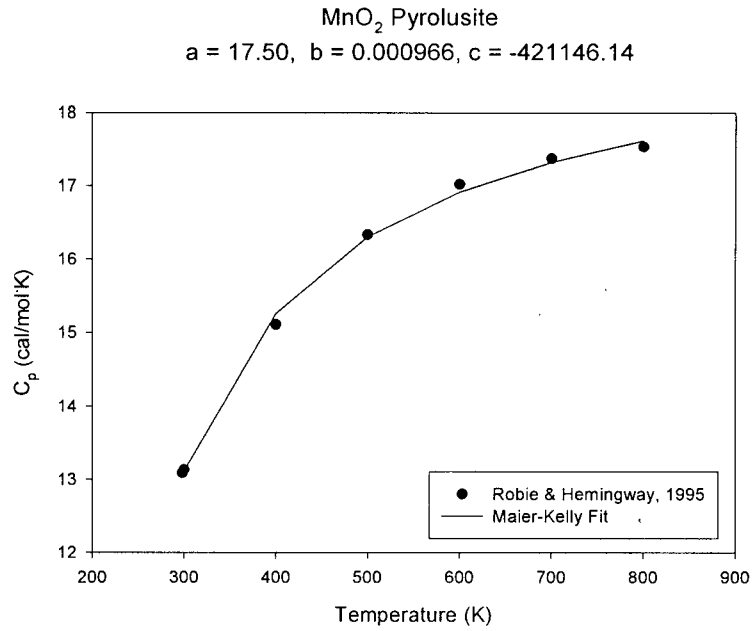

Figure 5.2.2-2 Determination of Maier-Kelly Expansion Coefficients for Pyrolusite

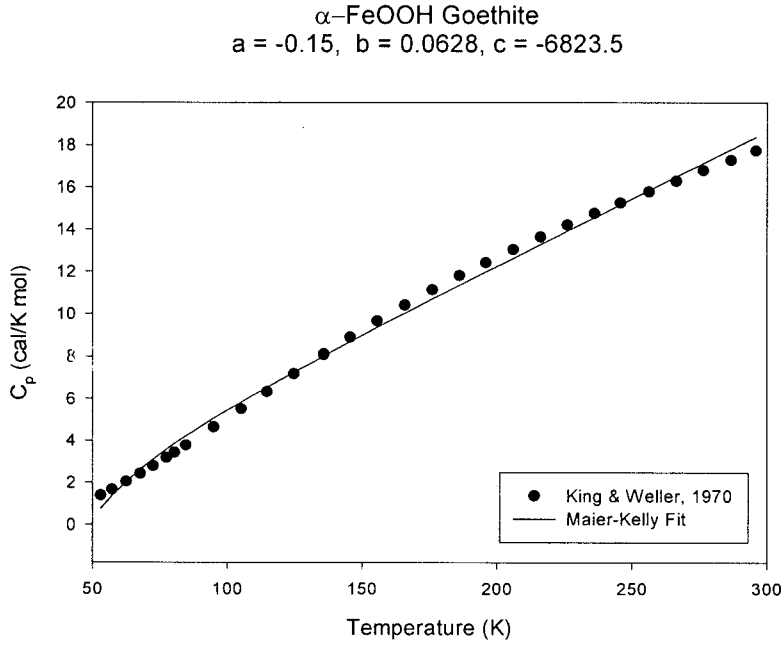

Figure 5.2.2-2 Determination of Maier-Kelly Expansion Coefficients for Goethite.

5.2.3 SUPCRT92 Calculations

The smicrobe.dat file was converted to the dmicrobe.dat file using the conversion routine CPRONS92 which is part of the SUPCRT92 software package. The instructions are given in Appendix 3 of Johnson et al (1992). This file (dmicrobe.dat) was used in the calculations below as direct input.

Each half reaction listed in Table 5.2-1 above was entered into SUPCRT92 following the instructions given in Appendix 4 of Johnson et al. (1992). The use of the dmicrobe.dat was specified instead of the default database in Step 1.0. For Step 2, the EQ3/6 one-phase/sat curve was selected as one of the three default reaction-independent parameters as this produced results for the following required points on each of our reaction curves (0, 25, 60, 100, and 150°C). For Step 3, new reaction files (*_rxn; see Table 6.2-2) were specified for each half reaction and given the reaction number as listed on Table 6.2-1. Each half reaction listed on Tables 5.2-1 and 5.2-2 were entered following the instructions given in Step 3.4. Names for tabulated output files were also specified in the same manner (RXN #.out; see Table 6.2-2) in Step 4.0. X-Y plot files were also produced and the files associated with Gibbs free energy (*.gxy; see Table 6.2-2) were saved in Step 4.1.

The results for each of the half reactions were converted from calories to kilojoules and entered into Sigma Plot 4.0 where the second order regression wizard was applied and the results plotted. These results were then entered onto Table 6.2-1 below.

5.3 DTN IMPACT REVIEW

This section reports the average values for manganese, phosphate and nitrogen oxide abundances found in a new DTN MO0002MAJIONIS.000 (qualified in *Data Qualification Report: Water and Mineral Chemistry Data for Use on the Yucca Mountain Project*, CRWMS M&O 2000b which replaced DTN GS980908312322.008) and compares those to the values used in section 6.5.1.3 of the *In Drift Microbial Communities* AMR (CRWMS M&O, 2000c). Data from the above DTN was averaged and the averages for each are shown in Table 5.3-1 below

Table 5.3-1 Comparison of Mean Values for Manganese, Phosphate and Nitrogen Oxide from a New Qualified DTN vs Old Unqualified DTN Used in Previous Calculations.

Species	Values Reported in CRWMS M&O (2000c) section 6.5.1.3	Values Averaged from DTNMO0002MAJIONIS.000
Manganese	5.697 ug/l	5.697 ug/l
Phosphate	0.016975 mg/l	0.016975 mg/l
Nitrogen Oxides	0.790875 mg/l	0.790875 mg/l

5.4 MATERIAL LIFETIMES

In order to calculate a material lifetime, material thicknesses need to be specified that correspond to the general masses of materials in the drift. Material thickness is determined by taking the thickest of the minimal dimensions (for beams, the selected component would be the flange thickness instead of the web thickness) for the given material. Information for these inputs was taken from BSC (2001, Table 1 and Figure 1) and AISC (1995). The results of this section will only replace the equivalent values found on Table 32 in CRWMS M&O (2000c) and report those design components that were not on that table (i.e. the waste package design materials remain unchanged).

Table 5.4-1. Material Thickness of Repository Design Materials Taken from BSC (2001a, Table 1)

Material	Component	Thickness (mm)
ASTM F432-95	Rock Bolts	13.0
ASTM A 32	Welded wire fabric	5.72
ASTM A572 Steel	Steel Sets	9.27
ASTM A759-85 Steel	Gantry Rail	47.62
Unspecified	Rail Fittings (Joint Bar)	30.17
ASTM A242	Gantry Runway (Cap Plate)	43.70
ASTM A709	Transverse Support Beam	14.61
ASTM A53	Pipe Spacers	3.56
ASTM A307	Tie Rods	15.88

For carbon steel corrosion rates, data supplied by the following DTN LL980704605924.035 was used where 6-month corrosion tests for aqueous general corrosion of A387, A516 and cast carbon steel values were averaged. The minimum and maximum rates represent one standard deviation of the average of these 12 values. The rates are given on Table 5.4-2. These rates are applied to the materials found in Table 5.4-1 above. These rates will be divided by the average thickness of the material as shown on Table 5.4-1 and the results will be provided on Table 6.4-1.

Table 5.4-2. Selected Aqueous General Corrosion Rates for Mild Carbon Steel.

Minimum Rate (-1STD) (μm/yr)	Maximum Rate (+1STD) (μm/yr)	Median Rate (AVG) (μm/yr)
23.5	95.34	59.42

LL980704605924.035

6. RESULTS

6.1 REPOSITORY SUBSURFACE DESIGN INPUT PARAMETERS

The results of each calculation are presented in the individual attachment. The tables presented here are the necessary input tables that need to be entered into MING software code. The results in the tables are either the value generated from the above calculations and/or a simple recompilation of the data provided in BSC (2001a).

6.1.1 Material Compositions

The values found on Tables 6.1.1-1 to 6.1.1-4 and 6.1.1-10 to 6.1.1-13 are considered accepted data having been taken from the ASTM standards listed in Section 7.2. Note that assumptions 2 and 3 apply to the use of Table 6.1.1-1.

Table 6.1.1-1. Composition of ASTM A572 Steel
Used in Rail Fittings, Conductor Bar Fittings, Gantry Rail, and Steel Set
Ground Support.

Element	Wt %
C	0.23
P	0.04
S	0.05
Si	0.4
Mn	1.65
V	0.15
Fe	97.48

Table 6.1.1-2. Composition of ASTM-F432-95 Steel
used in Rock Bolts. Note: Bolt Component
Values used for All Components of the Set (see assumption 1)

Element	Wt %
C	0.79
P	0.058
S	0.13
Fe	99.022

Table 6.1.1-3. Composition of A759-85 Steel used in Gantry Rails

Element	Wt %
C	0.82
Mn	1
P	0.04
Si	0.05
S	0.5
Fe	97.59

Values found on Table 6.1.1-4 were taken from ASTM A36 based on Assumption 5 above.

Table 6.1.1-4. Composition of Steel used in WWF

Element	Wt %
C	0.26
P	0.04
S	0.05
Si	0.4
Fe	99.25

The values found on Table 6.1.1-5 below show the elemental composition of Type K Cement.

Table 6.1.1-5. Composition of Type K Cement as Calculated in Section 5.1.1

Element	Wt %
Ca	44.21
Si	9.05
O	36.34
Al	2.75
Fe	1.96
S	2.76
K	0.49
Na	0.07
Mg	0.84
Sr	0.04
Zn	0.02
Ti	0.17
Mn	0.02
P	0.04

The values found on Table 6.1.1-6 below show the composition of silica fume.

Table 6.1.1-6. Elemental Composition of Silica Fume as Calculated in Section 5.1.2

Element	Wt %
Ca	0.214
Si	44.333
O	51.860
Al	0.371
Fe	0.21
S	0.32
K	0.249
Na	0.223
Mg	0.12
C	1.30

Table 6.1.1-7. Composition of Superplasticizer as Calculated in BSC (2001a)

Element	Wt %
C	51.15
H	3.9
S	12.41
O	24.78
Ca	7.76

The results found on Table 6.1.1-8 below are based on assumption 2 reported in Section 3 above.

Table 6.1.1-8. Composition of Rail Fittings
as Calculated in Section 5.1.6.

Element	Wt %
C	0.1725
P	0.03
S	0.0375
Si	0.30
Mn	1.2375
V	0.1125
Fe	73.11
Cu	25.00

Table 6.1.1-9. Composition of Commo Cable
as Calculated in Section 5.1.5.

Element	WT %
Cu	50.000
C	42.82
H	7.18

Table 6.1.1-10. Composition of ASTM A 242 Steel Used in the Longitudinal Support Beams, and Guide Beams (ASTM A 242) .

Element	WT %
C	0.15
Mn	1.0
P	0.45
S	0.05
Cu	0.2
Fe	98.15

Table 6.1.1-11. Composition of ASTM A 709 Steel Used in the Transfer Support Beam and Appurtenances (ASTM A 709, Table 2).

Element	WT %
C	0.27
Mn	0.9
P	0.04
S	0.05
Si	0.4
Cu	0.2
Fe	98.14

Table 6.1.1-12. Composition of ASTM A 53 Steel Used in Pipe Spacers (ASTM A 53, Table 1).

Element	WT %
C	0.3
Mn	1.2
P	0.5
S	0.45
Cu	0.4
Ni	0.4
Cr	0.4
Mo	0.15
V	0.08
Fe	96.975

Table 6.1.1-13. Composition of ASTM A 307 Steel Used in the Tie Rods (ASTM A 307, Table 1).

Element	WT %
C	0.33
Mn	0.93
P	0.041
S	0.051
Fe	98.648

6.1.2 Material Quantities

The masses reported below are taken and summarized from in BSC (2001a).

Table 6.1.2-1. Quantities of Materials in a One Linear Meter Segment of Repository Drift for Lithophysal Areas (~70% of Emplacement Drift Length)

Item	Elemental Composition	Quantity kg/m
Steel Sets	Table II-12	333
WWF Steel	Table II-15	45.9
Gantry Rail	Table II-14	133.9
Pipe Spacers	Table II-23	37.2
Tie Rods	Table II-24	17.1
Rail Fittings*	Table II-19	13.7
Transverse Support Beam	Table II-22	185.4
Gantry Runway	Table II-21	313.3
Longitudinal Support Beam	Table II-21	89.2
Guide Beams	Table II-21	59.5
Commo cable	Table II-20	2.0

*Includes the conductor bar fittings

Note: conductor bar not included as it is made of copper and is not part of the modeled microbial redox.

Table 6.1.2-2. Quantities of Materials in a One Lineal Meter Segment of Repository Drift Nonlithophysal Areas (~30% of Emplacement Drift Length)

Item	Elemental Composition	Quantity kg/m
Steel Sets	Table II-12	333
WWF Steel	Table II-15	45.9
Gantry Rail	Table II-14	133.9
Pipe Spacers	Table II-23	37.2
Tie Rods	Table II-24	17.1
Rail Fittings*	Table II-19	13.7
Transverse Support Beam	Table II-22	185.4
Gantry Runway	Table II-21	313.3
Longitudinal Support Beam	Table II-21	89.2
Guide Beams	Table II-21	59.5
Commo cable	Table II-20	2.0
Rock Bolts	Table II-13	74.4
Type K Cement	Table II-16	112.0
Silica Fume	Table II-17	12.4
Superplasticizer	Table II-18	2.5

*Includes the conductor bar fittings

Note: conductor bar not included as it is made of copper and is not part of the modeled microbial redox.

6.2 TEMPERATURE DEPENDENT GIBBS FREE ENERGY PARAMETERS

The filenames for each independent half reaction from SUPCRT92 and the associated Sigmaplot files are summarized in Table 6.2-2. The symbol * will often represent the RXN # found on Table 6.2-1 (the exception being the *.dat files that represent inputs to SUPCRT92). These files along with the files used to generate smicrobe.dat have been submitted to the TDMS under the following model warehouse DTN: MO0106MWDTDG01.035. The information used to generate Table 6.2-1 below is found in the associated Sigma plot files. For illustration purposes, Figure 6.2-1 below is an example of the regression analysis results. Note: the signs for each of the coefficients (B0, B1, and B2) reported in Table 6.2.1 are appropriate for use in MING. They are however, reversed in the output from SUPCRT92. Additionally, Table 6.2.1 is written with an apparent pH dependence on the free energy reactions. This is intentional, as it is required for use as MING input.

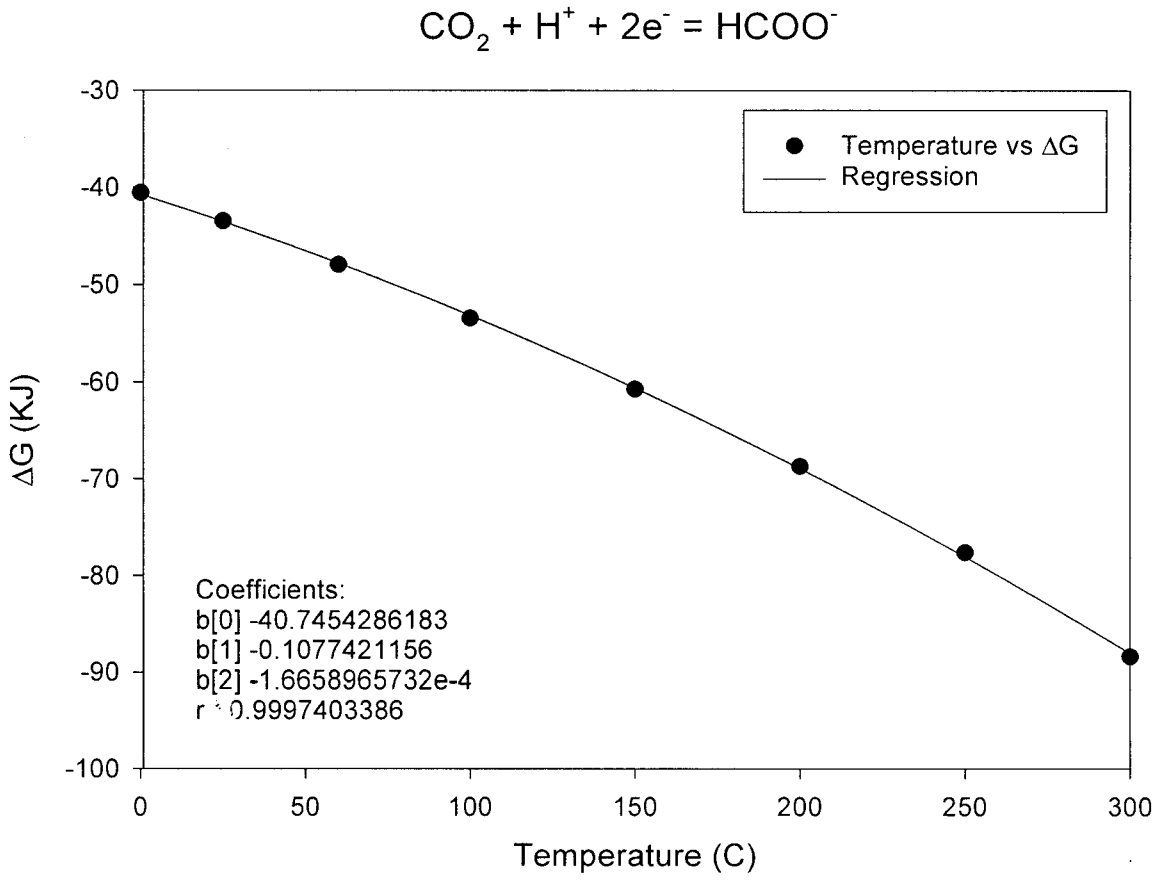

Figure 6.2-1 An Example of a Regression Analysis for Determination of Gibbs Free Energy Temperature Dependence Coefficients.

Table 6.2-1 Temperature Dependent ΔG Relationships for the Selected Redox Half Reactions found on Tables 5.2-1 and 5.2-2. These Data Supercede DTN: MO9909SPAMING1.003.

Redox Half Reaction		Δ°Gr (kJ/mol) vs. T(°C)		
	RXN #	B0	B1	B2
Carbon				
$CO_2 + H^+ + 2e^- = HCOO^-$	C1	40.7454	0.1077	1.6658e-4
$CO_2 + 4H^+ + 4e^- = CH_2O + H_2O$	C2	-35.1181	0.0353	4.8168e-4
$CO_2 + 6H^+ + 6e^- = CH_3OH + H_2O$	C3	-19.0661	0.0166	-2.5150e-4
$HCOO^- + 3H^+ + 2e^- = CH_2O + H_2O$	C4	6.3612	-0.0736	-3.4507e-4
$CO_2 + 8H^+ + 8e^- = CH_4 + 2H_2O$	C5	-114.3373	-5.6395e-3	-4.0214e-4

Redox Half Reaction		Δ°Gr (kJ/mol) vs. T(°C)		
	RXN #	B0	B1	B2
$CH_2O + 2H^+ + 2e^- = CH_3OH$	C6	-66.1411	-0.0175	-7.3149e-5
$HCOO^- + 7H^+ + 6e^- = CH_4 + 2H_2O$	C7	-154.9582	-0.1142	-5.6428e-4
$CH_2O + 4H^+ + 4e^- = CH_4 + H_2O$	C8	-161.3965	-0.0339	-2.4447e-4
$CH_3OH + 2H^+ + 2e^- = CH_4 + H_2O$	C9	-95.1077	-0.0244	-1.4081e-4
$CO_3^{2-} + 10H^+ + 8e^- = CH_4 + 3H_2O$	C10	-210.2704	-0.2960	-1.0161e-3
$CO_3^{2-} + 6H^+ + 4e^- = CH_2O + 2H_2O$	C11	-48.9273	-0.2572	-7.9106e-4
$CO_3^{2-} + 8H^+ + 6e^- = CH_3OH + 2H_2O$	C12	-115.0967	-0.2746	-8.6484e-4
$CO_3^{2-} + 3H^+ + 2e^- = HCOO^- + H_2O$	C13	-55.2133	-0.1845	-4.4713e-4
Nitrogen				
$N_2 + 6H^+ + 6e^- = 2NH_3$	N1	-52.8196	-0.0194	-1.6830e-4
$N_2 + 8H^+ + 6e^- = 2NH_4^+$	N2	-157.8665	-0.0357	-8.4085e-5
$NO_2^- + 7H^+ + 6e^- = NH_3 + 2H_2O$	N3	-466.1398	-0.1037	-4.3778e-4
$NO_3^- + 2H^+ + 2e^- = NO_2^- + H_2O$	N4	-156.8907	-0.0470	-5.5727e-5
$NO_3^- + 10H^+ + 8e^- = NH_4^+ + 3H_2O$	N5	-675.9929	-0.1544	-4.6004e-4
$NO_2^- + 8H^+ + 6e^- = NH_4^+ + 2H_2O$	N6	-754.0787	-0.1760	-4.9901e-4
$NO_3^- + 6H^+ + 5e^- = 0.5N_2 + 3H_2O$	N7	-597.2461	-0.1342	-4.2457e-4
$2NO_2^- + 8H^+ + 6e^- = N_2 + 4H_2O$	N8	-878.9891	-0.1898	-7.0731e-4
$NO_3^- + 9H^+ + 8e^- = NH_3 + 3H_2O$	N9	-623.0305	-0.1508	-4.9350e-4
Iron				
$Fe_2O_3 + 6H^+ + 6e^- = 2Fe + 3H_2O$	F1	38.2658	-0.1731	-1.9358e-4
$Fe^{2+} + 2e^- = Fe$	F2	94.6318	-0.1220	-1.1699e-4
$Fe^{3+} + e^- = Fe^{2+}$	F3	-70.1995	-0.1605	-1.0569e-4
$Fe_3O_4 + 8H^+ + 8e^- = 3Fe + 4H_2O$	F4	71.5929	-0.2109	-2.5541e-4
$FeOOH + 3H^+ + e^- = Fe^{2+} + 2H_2O$	F5	-77.7134	0.0139	3.2389e-5
Manganese				
$MnO_2 + 4H^+ + 2e^- = Mn^{2+} + 2H_2O$	M1	-239.0315	-0.0302	-2.5681e-5
$Mn_3O_4 + 8H^+ + 2e^- = 3Mn^{2+} + 4H_2O$	M2	-359.3919	0.0602	2.9471e-5
Sulfur				
$S + H^+ + 2e^- = HS^-$	S1	13.2571	-0.0571	2.3278e-4
$S + 2H^+ + 2e^- = H_2S$	S2	-25.6245	-0.0922	1.3593e-4
$SO_4^{-2} + 9H^+ + 8e^- = HS^- + 4H_2O$	S3	-182.7211	-0.2997	-5.9307e-4
$SO_4^{-2} + 10H^+ + 8e^- = H_2S + 4H_2O$	S4	-223.0548	-0.3393	-9.7424e-4
$HSO_4^- + 7H^+ + 6e^- = S + 4H_2O$	S5	-188.9704	-0.1559	-4.8888e-4
$SO_4^{-2} + 8H^+ + 6e^- = S + 4H_2O$	S6	-197.8705	-0.2466	-8.3085e-4
$SO_2 + 4e^- + 4H^+ = S + 2H_2O$	S7	-172.9306	-0.0109	-2.0250e-4
$SO_3^{2-} + 7H^+ + 6e^- = HS^- + 3H_2O$	S8	-206.0158	-0.2744	-5.7195e-4
$2SO_4^{-2} + 10H^+ + 8e^- = S_2O_3^{-2} + 5H_2O$	S9	-211.1992	-0.3248	-9.2009e-4
Hydrogen				
$H^+ + e^- = 0.5H_2$	H1	9.5513	-0.0265	-8.8270e-5
Oxygen				
$O_2 + 4H^+ + 4e^- = 2H_2O$	O1	-490.0311	-0.0378	8.0135e-5
Uranium				
$UO_2^{2+} + 4H^+ + 2e^- = U^{4+} + 2H_2O$	U1	-55.8741	0.1679	-5.1626e-5

DTN: MO0106SPAIDM01.034

Table 6.2-2 File types and descriptions for electronic output found in DTN:MO0106MWDTDG01.035.

File Type	Description
*.jnb	Sigma Plot 4.0 regression files
*.out	SUPCRIT combined output file
*_rxn	SUPCRIT reaction output file
*.gxy	SUPCRIT Gibbs free energy xy plot file
*_gxy.xls	Microsoft Excel file to convert *.gxy data to kilojoules
*.dat	Data files used as inputs to SUPCRT92

6.3 DTN IMPACT REVIEW

The new DTN MO0002MAJIONIS.000 reports the exact same data that is found in the current revision of the *In-Drift Microbial Communities* AMR (CRWMS M&O 2000c). There are no differences as shown on Table 5.3.1. Therefore, there is no impact to the existing parameters that were developed from DTN GS980908312322.008.

6.4 MATERIAL LIFETIMES

Table 6.4-1 reports the material lifetimes required by MING to evaluate the changes to the subsurface design reported by BSC (2001a). This table replaces the equivalent out of date parameters and augments the parameter set found in CRWMS M&O (2000c Table 32) to add the new information from previously undefined design components.

Table 6.4-1. Minimum, Median and Maximum Material Lifetimes (years) used in the MING Calculations.

Component	Material Name	Minimum Lifetime	Median Lifetime	Maximum Lifetime
Rock Bolts	ASTM F432-95*	136	219	553
Welded wire fabric	ASTM A 36	60	96	243
Steel Sets	ASTM A572 Steel*	97	156	394
Gantry Rail	ASTM A759-85 Steel*	499	801	2026
Rail Fittings (Joint Bar)	Rail Fittings Steel*	316	508	1284
Gantry Runway (Cap Plate)	ASTM A242	458	735	1860
Transverse Support Beam	ASTM A709	153	246	622
Pipe Spacers	ASTM A53	37	60	151
Tie Rods	ASTM A307	167	267	676

*Replaces previous parameter reported on Table 32 in CRWMS M&O (2000c)

7. REFERENCES

7.1 DOCUMENTS CITED

AISC (American Institute of Steel Construction) 1997. *Manual of Steel Construction, Allowable Stress Design.* 9th Edition, 2nd Revision, 2nd Impression. Chicago, Illinois: American Institute of Steel Construction. TIC: 240772.

Bhattacharyya, K.K. 2000. "Request for Approval of Analysis and Modeling Report Input as 'Accepted Data' - Composition of Silica Fume." Letter from K.K. Bhattacharyya (CRWMS M&O) to S.P. Mellington (DOE/YMSCO), February 15, 2000, LV.SSFD.KKB.02/00-001, with attachments. ACC: MOL.20000504.0594.

BSC (Bechtel SAIC Company) 2001a. *Committed Materials in Repository Drifts.* CAL-GCS-GE-000002 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010412.0157.

BSC (Bechtel SAIC Company) 2001b. *In-Package Chemistry for Waste Forms.* ANL-EBS-MD-000056 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010322.0490.

BSC (Bechtel SAIC Company) 2001c. *Technical Work Plan For EBS Department Modeling FY 01 Work Activities.* TWP-MGR-MD-000015 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. URN-0872.

CRWMS M&O 1997. *Materials for Emplacement Drift Ground Support.* BCAA00000-01717-0200-00003 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19971029.0493.

CRWMS M&O 2000a. *Data Qualification Report for Thermodynamic Data File, Data0.ympR0 for Geochemical Code, EQ3/6.* TDR-EBS-MD-000012 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001016.0004.

CRWMS M&O 2000b. *Data Qualification Report: Water and Mineral Chemistry Data for Use on the Yucca Mountain Project.* TDR-NBS-GS-000024 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001218.0005.

CRWMS M&O 2000c. *In-Drift Microbial Communities.* ANL-EBS-MD-000038 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001213.0066.

Helgeson, H.C.; Delany, J.M.; Nesbitt, H.W.; and Bird, D.K. 1978. "Summary and Critique of the Thermodynamic Properties of Rock Forming Minerals." *American Journal of Science, 278-A,* . New Haven, Connecticut: Kline Geology Laboratory, Yale University. TIC: 220013.

Johnson, J.W.; Oelkers, E.H.; and Helgeson, H.C. 1992. "SUPCRT92: A Software Package for Calculating the Standard Molal Thermodynamic Properties of Minerals, Gases, Aqueous Species, and Reactions from 1 to 5000 Bar and 0 to 1000°C." *Computers & Geosciences, 18,* (7), 899-947. New York, New York: Pergamon Press. TIC: 234273.

King, E.G. and Weller, W.W. 1970. *Low-Temperature Heat Capacities and Entropies at 298.15° K of Goethite and Pyrophyllite.* Report of Investigations 7369. Washington, D.C.: United States Department of the Interior, Bureau of Mines. TIC: 249499.

Morel, F.M.M. and Hering, J.G. 1993. *Principles and Applications of Aquatic Chemistry.* New York, New York: John Wiley & Sons. TIC: 248465.

Morrison, R.T. and Boyd, R.N. 1992. *Organic Chemistry.* 6th Edition. Englewood Cliffs, New Jersey: Prentice Hall. TIC: 245883.

Robie, R.A. and Hemingway, B.S. 1995. *Thermodynamic Properties of Minerals and Related Substances at 298.15 K and 1 Bar (105 Pascals) Pressure and at Higher Temperatures.* Bulletin 2131. Reston, Virginia: U.S. Geological Survey. TIC: 249441.

Robie, R.A.; Hemingway, B.S.; and Fisher, J.R. 1979. *Thermodynamic Properties of Minerals and Related Substances at 298.15 K and 1 Bar (10[superscript]5 Pascals) Pressure and at Higher Temperature.* Bulletin 1452. Denver, Colorado: U.S. Geological Survey. TIC: 230505.

Sargent-Welch Scientific Company 1979. *Periodic Table of the Elements.* Catalog Number S-18806. Skokie, Illinois: Sargent-Welch Scientific Company. TIC: 245069.

Tanger, J.C., IV and Helgeson, H.C. 1988. "Calculation of the Thermodynamic and Transport Properties of Aqueous Species at High Pressures and Temperatures: Revised Equations of State for the Standard Partial Molal Properties of Ions and Electrolytes." *American Journal of Science, 288,* (1), 19-98. New Haven, Connecticut: Yale University, Kline Geology Laboratory. TIC: 248310.

7.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

ASTM A 242/A 242M-00a. 2000. *Standard Specification for High-Strength Low-Alloy Structural Steel.* West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 249501.

ASTM A 307-00. 2000. *Standard Specification for Carbon Steel Bolts and Studs, 60 000 PSI Tensile Strength.* West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 249502.

ASTM A 36/A 36M-00a. 2000. *Standard Specification for Carbon Structural Steel.* West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 249500.

ASTM A 53/A53M-99b. 1999. *Standard Specification for Pipe, Steel, Black and Hot-Dipped, Zinc-Coated, Welded and Seamless.* West Conschohocken, Pennsylvania: American Society for Testing and Materials. TIC: 247689.

ASTM A 572/A 572M-99a. 1999. *Standard Specification for High-Strength Low-Alloy Columbium-Vanadium Structural Steel.* West Conshohocken, Pennsylvania: American Society

for Testing and Materials. TIC: 246273.

ASTM A 709/A 709M-00a. 2000. *Standard Specification for Carbon and High-Strength Low-Alloy Structural Steel Shapes, Plates, and Bars and Quenched-and-Tempered Alloy Structural Steel Plates for Bridges.* West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 249504.

ASTM A 759-85 (Reapproved 1992). *Standard Specification for Carbon Steel Crane Rails.* West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 246309.

ASTM F 432-95. 1995. *Standard Specification for Roof and Rock Bolts and Accessories.* Philadelphia, Pennsylvania: American Society for Testing and Materials. TIC: 241007.

AP-3.12Q, Rev. 0 ICN 4. *Calculations*. Washington D.C.: U. S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20010404.0008.

AP-2.21Q, Rev. 1 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. ACC: MOL.20010212.0018.

7.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER

GS980908312322.008. Field, Chemical, and Isotopic Data from Precipitation Sample Collected Behind Service Station in Area 25 and Ground Water Samples Collected at Boreholes UE-25 C #2, UE-25 C #3, USW UZ-14, UE-25 WT #3, UE-25 WT #17, and USW WT-24, 10/06/97 to 07/01/98. Submittal date: 09/15/1998.

LL980704605924.035. Engineering Material Characterization Report, Volume 3. Submittal date: 07/17/1998.

MO0012MAJIONIS.000. Water-Major Ion and Isotope Data. Submittal date: 12/01/2000.

MO0008THRMODYN.000. Data Qualification Report: Data Qualification Report for Thermodynamic Data File, DATA0.YMP.R0 for Geochemical Code, EQ3/6. Submittal date: 08/03/2000.

MO9909SPAMING1.003. Temperature Dependent Delta G Relationships for Selected Redox Half Reactions Used in MING V1.0. Submittal date: 09/14/1999.

MO9912DTMKCCOF.000. Chemical Compositions of Silica Fume. Submittal date: 12/07/1999.

MO9912SEPMKTDC.000. Chemical Compositions of TYPE E-1 (K) Cement. Submittal date: 12/07/1999.

7.4 SOFTWARE

CRWMS M&O 1998. *Software Code: MING V1.0* . V1.0. 30018 V1.0.

Software Code: SUPCRT92 V1.0. STN: 10058-1.0-00.

7.5 OUTPUT DATA, LISTED BY DATA TRACKING NUMBER

MO0106MWDTDG01.035. Model Warehouse Data for the Development of Temperature Dependent Gibbs Free Energies for Selected Half Reactions Involved in Microbial Metabolism. Submittal date: 06/19/2001.

MO0106SPAIDM01.034. Temperature Dependant Gibbs Free Energy Relationships for Selected Redox Half Reactions for Use in the In-Drift Microbial Communities Model. Submittal date: 06/19/2001.