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NM5507

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET

Complete Only Applicable Items

1. QA: QA

Page: 1 of: 113

☒ 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

Describe use:

See Section 1

3. ☒ Model — Check all that apply

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

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

Describe use:

See Section 1

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In Drift Microbial Communities

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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL REVISION RECORD

Complete Only Applicable Items

1. Page: 2 **of:** 113

Analysis or Model Title:

In Drift Microbial Communities

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

ANL-EBS-MD-000038 Rev 00

4. Revision/Change No.	5. Description of Revision/Change
00	Initial Issue

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FIGURES

TABLES

ACRONYMS

AMR	Analysis/Modeling Report
AP	Administrative Procedure
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
AT	Altered Tuff
BWR	Boiling Water Reactor
CAM	Waste package Corrosion Allowance Material
CD	Carbon Deficient microbial growth media
CDF	Cumulative Distribution Function
CFR	Code of Federal Regulations
CNS	Calcium Naphthalene Sulfonate (superplasticizer)
CRM	Corrosion Resistant Material
CRWMS	Civilian Radioactive Waste Management System
CSCI	Computer Software Configuration Identifier
CSNF	Commercial Spent Nuclear Fuel
DC	Dilute Complete growth media
DHLW	Defense High Level Waste
DOC	Dissolved Organic Carbon
DOE	U. S. Department of Energy
DTN	Data Tracking Number
EBS	Engineered Barrier System
EBSO	Engineered Barrier System Operations
EDA	Enhanced Design Alternative
EMMA	Estimation of Maximum Microbiological Activity
ESF	Exploratory Shaft Facility
FEP	Features, Events, and Processes
FFTF	Fast Flux Test Facility
FR	Federal Register
FW	Formula Weight
GFW	Gram Formula Weight
HLW	High Level Waste
IDGE	In-Drift Geochemical Environment
INEEL	Idaho National Engineering & Environmental Laboratory
INEL	Idaho National Engineering Laboratory (now INEEL)
IRSR	Issue Resolution Status Report
KTI	Key Technical Issues
LADS	License Application Design Selection

LLNL	Lawrence Livermore National Laboratories
M&O	Management and Operations
MIC	Microbial Induced Corrosion
ML	Material Lifetime
NFE	Near Field Environment
NFGE	Near Field Geochemical Environment
NRC	Nuclear Regulatory Commission
PA	Performance Assessment
PD	Phosphate Deficient microbial growth media
PWR	Pressurized Water Reactor
QA	Quality Assurance
QAP	Quality Assurance Procedure
QARD	Quality Assurance Requirements and Description
RH	Relative Humidity
RSDO	Repository Subsurface Design Organization
SQR	Software Qualification Report
SR	Site Recommendation
SR/LA	Site Recommendation/License Application
SZ	Saturated Zone
TBD	To Be Determined
TBV	To Be Verified
TDMS	Technical Data Management System
TH	Thermohydrologic
THC	Thermal-Hydrological-Chemical
TIC	YMP Technical Information Center
TMN	Topopah Spring Tuff Middle Non Lithophysal Unit
TSPA	Total System Performance Assessment
UT	Unaltered Tuff
UZ	Unsaturated Zone
VA	Viability Assessment
WP	Waste Package
WPO	Waste Package Operations
WWF	Welded Wire Fabric
YMC	Yucca Mountain Complete microbial growth medium
YMP	Yucca Mountain Project

1. PURPOSE

As directed by written work direction (CRWMS 1999e), Performance Assessment (PA) developed a model for microbial communities in the engineered barrier system (EBS) as documented here. The purpose of this model is to assist Performance Assessment and its Engineered Barrier Performance Section in modeling the geochemical environment within a potential repository drift for TSPA-SR/LA, thus allowing PA to provide a more detailed and complete near-field geochemical model and to answer the key technical issues (KTI) raised in the NRC Issue Resolution Status Report (IRSR) for the Evolution of the Near Field Environment (NFE) Revision 2 (NRC 1999).

This document will supercede the in-drift microbial communities model as documented in Chapter 4 of the TSPA-VA Technical Basis Document (CRWMS M&O 1998a). This document provides the conceptual framework of the revised in-drift microbial communities model to be used in subsequent performance assessment (PA) analyses.

This model has been developed to serve as a basis for the in-drift geochemical modeling work performed by PA. However, portions of the conceptual model discussed within this report may also apply to near and far-field geomicrobiological processes and can have conceptual application within the unsaturated zone (UZ) and saturated zone (SZ) transport modeling efforts. The outputs from this model feed the microbially induced corrosion (MIC) portions of the waste package corrosion modeling for TSPA-SR/LA and can serve as a source term for microbial colloids in the in-drift colloid modeling.

2. QUALITY ASSURANCE

The Quality Assurance (QA) program applies to the development of this model. The Performance Assessment Department responsible manager has evaluated the technical document development activity in accordance with QAP-2-0, *Conduct of Activities*. The QAP-2-0 activity evaluation, *Conduct of Performance Assessment* (CRWMS M&O 1999a), 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. Preparation of this analysis did not require the classification of items in accordance with QAP-2-3, *Classification of Permanent Items*. This activity is not a field activity. Therefore, an evaluation in accordance with NLP-2-0, *Determination of Importance Evaluations* was not required.

3. COMPUTER SOFTWARE AND MODEL USAGE

3.1 COMPUTER SOFTWARE

The following software is used in this model:

- MING V1.0 (MING V1.0 CSCI 30018 V1.0 MI 30018-M04-001) was obtained from the software configuration management (CM) organization. MING V1.0 is used within the range of validation as described in the users manual and qualification documentation

(CRWMS M&O 1998d and 1998h) and is appropriate for use in this model as a tool for conducting model validation calculations and for estimating microbial growth within a repository drift through time.

- Microsoft Excel 97, a commercially available standard spreadsheet software package. This software was used to tabulate and chart results.
- CorelDRAW 7, a commercially available graphics package. This software was used to create Figure 2 (see Section 6.3.3.1.3).
- SigmaPlot for Windows, Version 4.00, a commercially available graphics plotting software package. This software was used to chart results.

No other software codes or routines besides MING V1.0 were developed for use in this model. Three other pieces of software are mentioned in Section 6.4 of this report (EMMA, AREST-CT, and EQ3/6). These three pieces of software were not used to produce results or output for this model, therefore only the documentation for these codes is cited in Section 6.4.

3.2 MODELS

The previous model used for PA near-field geochemical environment analysis of microbial communities growth is documented in Chapter 4 of the TSPA-VA Technical Basis Document (CRWMS M&O 1998a). This new model is being developed to supercede the old microbial communities model discussed in the technical basis document. The soon to be superceded TSPA-VA near-field geochemical environment (NFGE) microbial communities model is only used in this document as a reference. The old model consists of the documentation found in Chapter 4 of the technical basis document (CRWMS M&O, 1998a) the use of MING V1.0 software [CSCI 30018 V1.0 as documented in CRWMS M&O 1998d, and 1998h] and the input and output files found in the following DTN: MO9807MWDEQ3/6.005.

4. INPUTS

4.1 DATA AND PARAMETERS

For TSPA-Site Recommendation/License Application (SR/LA) analyses, requests were made by PA to the Waste Package Operations (WPO), Engineered Barrier System Operations (EBSO) and Repository Subsurface Design Organization (RSDO) to obtain the appropriate design information for the in-drift geochemical model analyses. Each organization responded using AP-3.14Q *Transmittal of Input* to provide the requested information (CRWMS M&O 1999d, CRWMS M&O 1999g, CRWMS M&O 1999h, CRWMS M&O 1999i, CRWMS M&O 1999k, and CRWMS M&O 1999l). Because these inputs are not all qualified or accepted they are considered TBV inputs. However, these inputs do contain some qualified and/or accepted data (e.g. reference to American Society for Testing and Materials [ASTM] standards).

In addition to the AP-3.14Q *Transmittal of Input* information cited above, the following tables (Tables 1 through 5) list the technical data management system (TDMS) data tracking numbers

(DTN), accepted data, or developed data (within this document) and their qualification status which are used as input values to the modeling runs.

These inputs are considered appropriate for this model.

Table 1. Source Data/Input Information used in Parameter Derivation.

DTN/Source	Description	Location in Text	Q Status
LA000000000086.002	Iron Mineral Types	Attachment I	Qualified
LA000000000086.002	Maximum Mineral % In Repository Horizon Tuff	Attachment I	Qualified
Sargent-Welch (1979)	Gram Formula Weights	Attachment I	Accepted
CRWMS M&O (1999m)	Repository Drift Radius	Attachment I	Qualified
GS960908312231.004	Bulk Density Of TMN	Attachment I	Qualified TBV-Y
GS931208314211.047	Depth Of TMN Horizon	Attachment I	Qualified
MO9909SPAMICRO.001	Microbial Volume	Attachment I	Accepted
MO9909SPAMICRO.001	Microbial Water Content	Attachment I	Accepted
LALH831342AQ96.002	Biomass In ESF	Attachment I	Qualified TBV-Y
MO9909SPABMASS.000	Biomass In Rainier Mesa	Attachment I	Accepted
Weast (1979)	Composition Of Air	Attachment I	Accepted
MO9912SEPMKTDC.000	Composition Of Type K Cement	Attachment II	Not Qualified (Preliminary)
MO9912DTMKCCOF.000	Composition Of Silica Fume	Attachment II	Not Qualified (Preliminary)
MO9911SPAWAP05.010	Stainless Steel General Corrosion Distribution	Section 6.5.3.3	Not Qualified (Preliminary)
MO0003SPASUP02.003	Alloy 22 And Ti7 General Corrosion CDF	Section 6.5.3.3	Qualified
SN9911T0811199.003	Aqueous Dissolution Rates For HLW Glass	Section 6.5.3.3	Not Qualified (Preliminary)
American Society of Metals (1987)	Corrosion Rates For Aluminum	Section 6.5.3.3	Accepted
LL980704605924.035	Aqueous Corrosion Rates For Mild Carbon Steel	Section 6.5.3.3	Qualified TBV-Y
LL980504105924.034	Aqueous Corrosion Rate For Neutronit A978	Section 6.5.3.3	Not Qualified
MO9906RIB00049.000	Neutronit A978 Composition	Attachment III	Not Qualified
MO9912SPADWR90.007	Dimensions And Masses Of HLW Glass And Pour Canisters	Section 6.5.3.3, Attachment IV	Not Qualified

DTN/Source	Description	Location in Text	Q Status
CRWMS M&O (1999g)	Mass Of Steel Sets In Lithophysal Areas Per Meter Of Drift	Attachment II	Not Qualified
CRWMS M&O (1999g)	Mass Of Steel Sets In Nonlithophysal Areas Per Meter Of Drift	Attachment II	Not Qualified
CRWMS M&O (1999g)	Mass Of Rock Bolts In Nonlithophysal Areas Per Meter Of Drift	Attachment II	Not Qualified
CRWMS M&O (1999g)	Mass Of Cement In Rock bolt Grout Per Meter Of Drift	Attachment II	Not Qualified
CRWMS M&O (1999g)	Mass Of Steel Invert Per Meter Of Drift	Attachment II	Not Qualified
CRWMS M&O (1999g)	Mass Of Gantry Rail Per Meter Of Drift	Attachment II	Not Qualified
CRWMS M&O (1999g)	Mass Of Rail Fittings Per Meter Of Drift	Attachment II	Not Qualified
CRWMS M&O (1999g)	Mass Of Conductor Bar Fittings Per Meter Of Drift	Attachment II	Not Qualified
CRWMS M&O (1999g)	Mass Of Communications Cable Per Meter Of Drift	Attachment II	Not Qualified
CRWMS M&O (1999g)	Composition Of Rock Bolt Grout	Attachment II	Not Qualified
CRWMS M&O (1999g)	Composition Of Grout Admixtures	Attachment II	Not Qualified
CRWMS M&O (1999g)	Composition Of Rail Fittings	Attachment II	Not Qualified
CRWMS M&O (1999g)	Composition Of Wire Conductor	Attachment II	Not Qualified
CRWMS M&O (1999g)	Composition Of Communications Cable	Attachment II	Not Qualified
CRWMS M&O (1999g)	Composition Of Wire Mesh(WWF)	Attachment II	Not Qualified
CRWMS M&O (1999g)	Mass Of WWF Per Meter Of Drift In Lithophysal Area	Attachment II	Not Qualified
CRWMS M&O (1999g)	Mass Of WWF Per Meter Of Drift In Nonlithophysal Area	Attachment II	Not Qualified
CRWMS M&O (1999h)	Waste Package Lengths For 21PWR, 44BWR, 5DHLW, And Naval SNF	Attachment III	Not Qualified
CRWMS M&O (1999h)	Length Of Drip Shield Segment	Attachment III	Not Qualified
CRWMS M&O (1999h)	Length Of Waste Package Pallet	Attachment III	Not Qualified
CRWMS M&O (1999h)	Masses Of Materials In Drip Shield Design	Attachment III	Not Qualified
CRWMS M&O (1999h)	Masses Of Materials In Waste Package Design	Attachment III	Not Qualified

DTN/Source	Description	Location in Text	Q Status
CRWMS M&O (1999h)	Masses Of Materials In Waste Package Pallet Design	Attachment III	Not Qualified
CRWMS M&O (1999h)	Waste Package Outer Barrier Thickness	Section 6.5.3.3	Not Qualified
CRWMS M&O (1999h)	Waste Package Inner Barrier Thickness	Section 6.5.3.3	Not Qualified
CRWMS M&O (1999h)	Basket Plate (Neutronit) Thickness	Section 6.5.3.3	Not Qualified
CRWMS M&O (1999h)	Basket Plate (Aluminum) Thickness	Section 6.5.3.3	Not Qualified
CRWMS M&O (1999h)	Basket Guide Thickness	Section 6.5.3.3	Not Qualified
CRWMS M&O (1999d)	Invert Material Thickness	Section 6.5.3.3	Not Qualified
CRWMS M&O (1999d)	Gantry Rail Material Thickness	Section 6.5.3.3	Not Qualified
CRWMS M&O (1999d)	Rail Fittings (Anchor Clips) Material Thickness	Section 6.5.3.3	Not Qualified
CRWMS M&O (1999d)	WWF (Wire Mesh) Material Thickness	Section 6.5.3.3	Not Qualified
CRWMS M&O (1999l)	Drip Shield Material Thickness	Section 6.5.3.3	Not Qualified
CRWMS M&O (1999k)	Waste Package Pallet Steel Tube Material Thickness	Section 6.5.3.3	Not Qualified

Table 2. Parameter Listing and Status to be Used in Future TSPA-SR Calculations.

Parameter	Location in Text	Source	Q Status
Material Lifetimes	Table 28	Section 6.5.3.3	Not Qualified
Breakdown Codes	Table 29	DTN: MO9909SPAMING.002	Not Qualified
Delta G Relationships For Redox Half Reactions	Table 16	DTN: MO9909SPAMING1.003	Not Qualified
Atomic Mass	Table 17	Sargent-Welch (1979)	Accepted
Temperature Cutoff	Table 19	Section 6.3.1.3	Qualified
Humidity Cutoff	Table 19	Section 6.3.3.2.2	Qualified
MING V1.0 Near-Field Porosity	Table 19	CRWMS M&O (1998h)	Qualified
Gas Buttons	Table 19	Section 6.3.1.10	Qualified
Energy Cut Off	Table 19	McKinley et al. (1997)	Accepted
Reactant Compositions	Table V-2	Section 6.5.3.2 and Attachment V	Qualified
Tunnel Length	Table 19	User Selected	Qualified
Tunnel Diameter	Table 19	CRWMS M&O (1999m)	Qualified
Layer Designator	Table 30	Section 6.5.3.5	Qualified

Parameter	Location in Text	Source	Q Status
Elemental Composition Of Type K Concrete	Table II-20	Attachment II	Not Qualified
Elemental Composition Of Superplasticizer	Table II-22	Attachment II	Not Qualified
Elemental Composition Of Rock Bolts	Table II-17	Attachment II: ASTM F 432-95	Accepted
Elemental Composition Of Welded Wire Fabric	Table II-19	Attachment II	Not Qualified
Elemental Composition Of Gantry Rail	Table II-18	Attachment II: ASTM A759-85	Accepted
Elemental Composition Of Rail Fittings	Table II-23	Attachment II	Not Qualified
Elemental Composition Of Steel Set Ground Support	Table II-16	Attachment II: ASTM A572/A572M-99a	Accepted
Elemental Composition Of Conductor Bar Fittings	Table II-16	Attachment II: ASTM A572/A572M-99a	Accepted
Elemental Composition Of Commo Cable	Table II-25	Attachment II	Not Qualified
Masses Of Materials For A One Meter Repository Segment	Table II-26 and Table II-27	Attachment II	Not Qualified
Composition Of PWR CNSF Waste Assembly	Table IV-4	DTN: MO9911SPAAWC68.002	Not Qualified
Composition Of BWR CNSF Waste Assembly	Table IV-5	DTN: MO9911SPAAWC68.002	Not Qualified
Composition Of DHLW Waste Glass	Table IV-3	DTN: SN9911T0811199.003	Not Qualified
Composition Of Waste Package Supports (316L Stainless Steel and Alloy C-22)	Table III-8 Table III-10	Attachment III ASTM A276-91a ASME Section II B SB-575	Accepted
Composition Of Drift Invert	Table II-16	Attachment II: ASTM A572/A572M-99a	Accepted
Composition Of Waste Package Corrosion Resistant Material (CRM) (Alloy C-22)	Table III-10	Attachment III ASME Section II B SB-575	Accepted
Composition Of Waste Package Structural Steel (316NG Stainless Steel)	Table III-9	Attachment III ASTM A276-91a	Accepted
Composition Of Waste Package Thermal Shunts (Aluminum 6061)	Table III-11	Attachment III ASTM B 209M-92a	Accepted
Composition Of Waste Package Absorber Plates (Neutronit A978)	Table III-13	Attachment III MO9906RIB00049.000	Not Qualified
Masses Of Materials For A One Lineal Meter Segment Of Design Waste Canisters	Table III-1 Table III-2 Table III-3 Table III-4	Attachment III	Not Qualified
Abstracted Seepage/Infiltration Into The Drift Through Time	Section 6.5.1.1	Documented during future calculations	TBD*
Abstracted Incoming Water Compositions Through Time	Section 6.5.1.3	Documented during future calculations	TBD*

Parameter	Location in Text	Source	Q Status
Abstracted Temperature/RH At WP Surface Through Time	Section 6.5.1.2	Documented during future calculations	TBD*
Abstracted cumulative Gas Flux Into The Drift Through Time	Section 6.5.1.4	Documented during future calculations	TBD*

* The data discussed in section 6.5.1 below reflect TSPA-VA data, which was the most current available data. It is used only as a placeholder until other TSPA-SR modeling efforts that provide these input data are finalized. The lack of this data will not effect the conclusions of this model. However, it prevents the inclusion of the TSPA-SR calculations in this revision of the model. The TSPA-SR model calculations will be documented in a future calculation document or revision of this model.

Table 3. Referenced Data Used in Model Validation.

DTN	Description	Location in Text	Q Status
MO9911SPAEMMA0.007	EMMA Test Case Results	Section 6.6.1	Not Qualified

Table 4. Parameters and Status used in Ambient Validation Test Cases.

Parameter	Location in Text	Source	Q Status
Infiltration Rates	Table 33	DTN: MO9807MWDEQ3/6.005	Not Qualified
Cumulative Gas Flux	Table 34	DTN: MO9911SPACGF04.000	Not Qualified
Material Lifetimes	Table 33	DTN: MO9807MWDEQ3/6.005	Not Qualified
J-13 Water Compositions	Table 32	DTN: MO9909SPA00J13.006	Not Qualified
Bulk Rock Compositions For Topopah Spring Tuff	Table 13	DTN: LL981209705924.059	Qualified TBV Y
Delta G Relationships For Redox Half Reactions	Table 16	DTN: MO9909SPAMING1.003	Not Qualified
Atomic Mass	Table 17	Sargent-Welch (1979)	Accepted
Temperature Cutoff	Table 19	Section 6.3.1.3	Qualified
Humidity Cutoff	Table 19	Section 6.3.3.2.2	Qualified
MING V1.0 Near-Field Porosity	Table 19	CRWMS M&O (1998h)	Qualified
Gas Buttons	Table 19	Section 6.3.1.10	Qualified
Energy Cut Off	Table 19	McKinley et al. (1997)	Accepted
Reactant Compositions	Table 35	Section 6.6.2.2.1	Qualified
Tunnel Length	Table 19	User Selected	Qualified
Tunnel Diameter	Table 19	CRWMS M&O (1999m)	Qualified
Layer Designator	Table 35	Section 6.6.2.2.1	Qualified

Parameter	Location in Text	Source	Q Status
RH	Section 6.6.2.1	Assumption 5.2	Qualified

Table 5. Parameters and Status used in LLNL Validation Test Cases.

Parameter	Location in Text	Source	Q Status
Flask Volume pH Of Growth Media Mass Of Crushed Tuff Temperature Of Growth Media Volume Of Growth Media In Flask	Table 39	LL000206105924.126	Qualified
Growth Media Compositions	Table 40	LL980608505924.035	Qualified TBV Y
Bulk Rock Compositions For Topopah Spring Tuff	Table 13	LL981209705924.059	Qualified TBV Y
Delta G Relationships For Redox Half Reactions	Table 16	MO9909SPAMING1.003	Not Qualified
Atomic Mass	Table 17	Sargent-Welch (1979)	Accepted
Temperature Cutoff	Table 19	Section 6.3.1.3	Qualified
Humidity Cutoff	Table 19	Section 6.3.3.2.2	Qualified
MING V1.0 Near-Field Porosity	Table 19	CRWMS M&O (1998h)	Qualified
Gas Buttons	Table 19	Section 6.3.1.10	Qualified
Energy Cut Off	Table 19	McKinley et al. (1997)	Accepted
Reactant Compositions	Table 35	Section 6.6.2.2.1	Qualified
Layer Designator	Table 35	Section 6.6.2.2.1	Qualified
RH	Section 6.6.3.2.1	Assumption 5.2	Qualified
Tunnel Length	Table I-10	Attachment I	Qualified
Drift Diameter	Table I-10	Attachment I	Qualified

4.2 CRITERIA

Below is a summary of the applicable NRC review and acceptance criteria outlined in the issue resolution status report (IRSR). These acceptance criteria 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 processes on the chemical environment for radionuclide release, and (c) coupled thermal-hydrologic-chemical processes on radionuclide transport through engineered and natural barriers (NRC 1999).

Also, below is a listing of the applicable features, events and processes (FEP) that are associated with this document.

4.2.1 NRC IRSR Criteria

The exact wording below reflects only the criteria as presented in NRC (1999) Section 4.3.1. However, the wording is similar to those presented below in the other cited sections (i.e. 4.1.1, 4.2.1, 4.4.1, and 4.5.1) and can be used to obtain the general feel of each criteria. The exact wording of these sections can be found by referring to the appropriate section in the IRSR document (NRC 1999). A discussion is found in Section 7.5 below of the IRSR criteria and whether they were addressed in this model as documented in Section 6 of this document.

4.2.1.1 Data and Model Justification Acceptance Criteria

1. Available data relevant to both temporal and spatial variations in conditions affecting coupled THC effects on the chemical environment for radionuclide release were considered. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

2. DOE's evaluation of coupled THC processes properly considered 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 were 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 4.2.1, 4.3.1, and 4.4.1]

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 4.2.1, 4.3.1, and 4.4.1]

6. Sensitivity and uncertainty analyses (including consideration of alternative conceptual models) were 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, and 4.4.1]

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, DOE has identified specific plans to acquire the necessary information as part of the performance confirmation program. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1]

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 are 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 were considered. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

3. DOE's evaluation of coupled THC processes properly considered 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 were consistent with available data. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

5. DOE's performance confirmation program should 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, and 4.4.1]

4.2.1.3 Model Uncertainty Acceptance Criteria

1. Appropriate models, tests, and analyses were 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 cementatious 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, and 4.4.1]

2. Alternative modeling approaches consistent with available data and current scientific understanding were investigated, and their results and limitations were appropriately considered. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

3. DOE provided a reasonable description of the mathematical models included in its analyses of coupled THC effects on the chemical environment for radionuclide release. 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 are 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. DOE appropriately adopted accepted and well-documented procedures 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 are based on the same assumptions and approximations shown to be appropriate for closely analogous natural or experimental systems. Abstracted model results are verified through comparison to outputs of detailed process models and empirical observations. Abstracted model results are 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)

Table 6 below gives a listing of Yucca Mountain Project FEP's (CRWMS M&O 1999m) that are discussed in this document. The YMP FEP # is part of the database search properties and is provided for convenience.

Table 6. A Listing of YMP FEP's that Pertain to Issues Discussed in this Document.

Number	YMP FEP #	FEP Name
1	2.1.09.06.00	Reduction-oxidation potential in waste and EBS
2	2.1.09.13.00	Complexation by organics in waste and EBS
3	2.1.09.18.00	Microbial colloid transport in the waste and EBS
4	2.1.10.01.00	Biological activity in waste and EBS
5	2.1.11.08.00	Thermal effects: chemical and microbiological changes in the waste and EBS
6	2.1.09.05.00	In-drift sorption

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 specified Subparts/Sections of the proposed NRC high-level waste rule, 10 CFR Part 63 (64 FR 8640). Subparts of this proposed rule that are applicable to data include Subpart B, Section 15 (Site Characterization) and Subpart E, Section 114 (Requirements For Performance Assessment). The subpart applicable to models is also outlined in Subpart E Section 114.

4.3.2 ASTM/ASME 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 model.

The following ASTM/ASME Standards were used as a source for accepted chemical compositions of metals and alloys (see Section 8.2 for complete reference citations to these standards). Tables containing these compositions are found in Attachments II and III.

- ASME Section II B SB-575
- ASTM A240/A240M-97a
- ASTM A276-91a
- ASTM A516/A516M-90
- ASTM A572/A572M-99a
- ASTM A759-85
- ASTM B 209M-92a
- ASTM F432-95

The following ASTM standards were used as references to Type K cement and welded wire fabric, respectively.

- ASTM C845-96
- ASTM A185-97

5. ASSUMPTIONS

Assumptions used in each of the attachments are contained within the body of that attachment and are not duplicated here.

5.1 The unsaturated conditions within in the drift wall and in materials within the drift are in equilibrium with the relative humidity in the drift due to the capillary pressure of the unsaturated porous medium in the drift (used in Section 6.4.2.3 below).

This is a conservative bounding assumption as the capillary pressure in the rock and porous materials may not always allow the relative humidity (RH) in the atmosphere to be in equilibrium with the unsaturated conditions within the drift. This assumption is bounding in that it will allow microbial communities to develop under unsaturated conditions in the drift that might otherwise be prohibited due to the lack of water. This assumption allows for the use of Equation 2 (see Section 6.3.3.2.2) where RH becomes a surrogate for water activity (a_w).

5.2 MING V1.0 was designed to calculate microbial growth in both saturated conditions as well as unsaturated conditions. Modeling under these conditions requires the appropriate RH to be input. For saturated cases where the RH is 1, the input parameter value to be used will be 0.999, which approximates 100% RH (used in Sections 4.1, 6.6.2.1, and 6.6.3).

This will not cause any discrepancies, as the RH switch will be set at 0.90. Any value above this threshold whether saturated or unsaturated conditions will not make a difference in the calculation. Additionally, the relative humidity (RH) under ambient unsaturated conditions is calculated to be at 100% (see Figure 5 in Section 6.5.1.3).

5.3 304L stainless steel corrosion rates are assumed similar to 316L/NG stainless steel (used in Section 6.5.3.3).

No 304L specific rates are currently available. A similar assumption (See DTN: SN9911T0811199.003) for using the 316L stainless steel rates as a surrogate for 304L rates has been used in the past in other modeling efforts.

5.4 Median material lifetimes for cement grout, silica fume, and superplasticizer of 10000 years was selected to represent a reasonable lifetime of cement. In addition, minimum and maximum material lifetimes were derived for these materials by taking a factor of five less and greater, respectively (used in Section 6.5.3.3).

No information is available on the material lifetimes of cement grout, superplasticizer or silica fume. Therefore, the 10,000-year median lifetime selected for the material lifetimes of cement grout, silica fume, and superplasticizer is based on TSPA-VA calculations. The TSPA-VA results show that the minimum duration for cement modified water compositions to be affected by the cement and thus be a source of nutrients for microbial growth in the drift is around 10,000 years (CRWMS M&O 1998a, Section 4.7.2). This lifetime would then be a conservative value for the potential materials because the quantities of grout used in the SR design are significantly less than the VA design (CRWMS M&O 1998a and CRWMS M&O 1998g).

5.5 Material lifetimes (minimum, median, and maximum) for the release of Fe^{2+} from biotite of 100,000 1 million, and 10 million years were selected for use in model validation calculations (used in Section 6.6.2.2.1).

The maximum release rate of Fe^{2+} from biotite was determined by assuming that hematite is not a syngenetic mineral (formed at the same time the volcanic tuff was deposited; Vaniman et al. 1989, Section 4.1.3.2) and that all hematite is thought to be an alteration product of biotite. This provides a conservative bound on the rate of oxidation of the iron minerals in the rock because some of the hematite in the rock could be syngenetic. Since the volcanic eruptions that emplaced the tuff at Yucca Mountain occurred at least 10 million years ago and there is approximately 1 percent of each mineral in the current system, a material lifetime of 10 million years for remaining 1 percent of biotite to alter was thought to represent a reasonable bound for the maximum lifetime. The median and minimum lifetimes were selected to be one and two orders of magnitude less than this. These faster rates will allow for the subsequently larger amounts of redox energy available for microbes to grow in the natural system.

5.6 J-13 water and TSw tuff serve as surrogates for the tuff and water at Rainier Mesa. (used in Sections 6.6.2.1 and 6.6.2.2.4)

J-13 water and TSw tuff are similar to the water and rock compositions found at the Rainier Mesa natural analog site located in close proximity to Yucca Mountain. Some discussion on the similarity of fracture water from Rainier Mesa with J-13 water is documented in Section 6.3.2.1.2.1 and is reported in CRWMS M&O (1998a, Section 4.2.3.1.2). The similarity for the TSw tuff is demonstrated where Haldeman and Amy (1993) describe the ash fall tuff that was sampled in Rainier as being both vitric and zeolitic These terms are also used to describe the Topopah Spring and Calico Hills tuffs. The analog comparison of the sites is also referred to in CRWMS M&O (1998a, Section 4.2.3.1.2). Therefore, there should be no significant impact to the results due to the use of this assumption.

5.7 A surface area multiplication factor for glass waste of 30 is used to determine the surface area available for dissolution to account for cracks that form during glass cooling [used in Section 6.5.3.3].

This assumption was made because no actual measurements of surface area for cracked glass are reported in the TDMS. CRWMS M&O (1995) report a range between 10 and 30 for this factor. In order to account for the largest surface area available, the factor of 30 was selected.

5.8 The single corrosion rate value for Bohler A976 SD (Van Konynenburg et al. 1998) was used as a surrogate corrosion rate for Neutronit A978. This rate is found in the following DTN: LL980504105924.034 [used in Section 6.5.3.3].

The rational for this assumption is that for Neutronit A978 there are no project documented corrosion rates available. However, a corrosion rate has been determined and documented for two similar materials, Bohler A976 SD and Nutrosorb Plus. These materials, like Neutronit A978, are both borated stainless steels and have similar corrosion rates. (Van Konynenburg 1998). The use of the A976 SD material as a surrogate should capture the general impacts to microbial communities from the corrosion of the Neutronit A978.

5.9 Material lifetimes for the commo cable of 100, 1,000, and 10,000 were used [used in Section 6.5.3.3].

There are no rates available, therefore a two order of magnitude range of lifetimes were selected to bound the potential range of lifetimes. Because the mass of the commo cable

(0.79 kg/m of drift) is small, lifetimes greater than the assumed values should not produce sufficient nutrients or energy to affect the overall results.

6. ANALYSIS/MODEL

6.1 PREVIOUS WORK

For TSPA-VA, a microbial communities model was developed to assess the possible magnitude of effects on the system's total chemistry by bounding the magnitude of development of microbial communities (CRWMS M&O 1998a). The TSPA-VA model was based on most of the concepts documented in Section 6.3, 6.4 and 6.6 below and was patterned after the models used in the Swiss and Canadian nuclear waste programs (McKinley and Grogan 1991, McKinley et al. 1997, and Stroes-Gascoyne 1989). The VA model used constraints on both the supply rate of nutrients and the limits on total energy available for microbial metabolism.

The constraints on the supply rates of the nutrients were used to build an idealized microbial composition, comprised of carbon, nitrogen, sulfur, and potassium in addition to the water components. The rates of supply of these constituents were input as constant release rates for each introduced material in the system by specifying the mass and composition of the material and its degradation lifetime. The other major constraint evaluated is the energy available for microbes to grow based on the pH corrected, standard state free energy released from oxidation/reduction reactions. Other constraints on microbial growth are temperature and RH thresholds in the model that limit the start of microbial activity until the boiling period is over. Although microbes could be sterilized out of the drifts during the highest temperature period, because they are present in the water-rock system they will return as water drips back into potential drifts. Microbes could also be sterilized in high radiation fields, but microbes would be reintroduced from the geosphere once the radiation field decays to lower levels. The TSPA-VA microbial communities model was not directly used in the TSPA-VA base case (CRWMS 1998a), but provided first-order limits on potential microbial effects.

The results of the TSPA-VA microbial communities model indicated that the TSPA-VA design would result in the growth of about 10-12 grams of microbial mass per year during the first 10,000 years of the repository (Figure 1). This mass is equivalent to approximately 0.6 parts per million. Based on this small mass of microbes being generated, effects to the bulk chemistry in the drift were determined to be negligible. However, the effects of the localized impacts such as biofilm development, colloid formation, and the production of inorganic acids, methane, organic byproducts, carbon dioxide, and other chemical species that could change the longevity of materials and the transport of radionuclides from the near field were not investigated.

Analyses of the TSPA-VA in-drift microbial communities model results indicated that

- The estimates of microbe masses growing in the potential repository system suggest that effects to the bulk in-drift geochemical environment would be negligible.
- Microbial influenced corrosion (MIC) and other localized microbial attack of materials from biofilm formation cannot be precluded.
- Consideration of microbes as colloids could be pursued in future work.

- There is some potential for additional ligands generated locally; however, the radionuclides would have to compete directly with many other available multivalent metals.

Therefore, the conceptual model documented below updates and enhances the concepts outlined in CRWMS M&O (1998a) and sets the stage for future investigation of the concerns listed above.

6.2 IN DRIFT MICROBIAL COMMUNITIES MODEL DISCRIPTION

The in drift microbial communities model is made up of the following parts; first, the conceptual model description as discussed in Section 6.3 below. Second, the use of MING V1.0 software as reported in the software documentation (CRWMS M&O 1998d and 1998h) and discussed in Section 6.4. Finally, the model inputs are derived and discussed in Sections 6.4.3.1, 6.5 and Attachments II to V. These three parts integrated together make up the model. Model validation parameter derivation, exercises, and results are discussed in Section 6.6 and Attachment I.

6.3 CONCEPTUAL MODEL

6.3.1 Environmental Limits on Microbial Activity

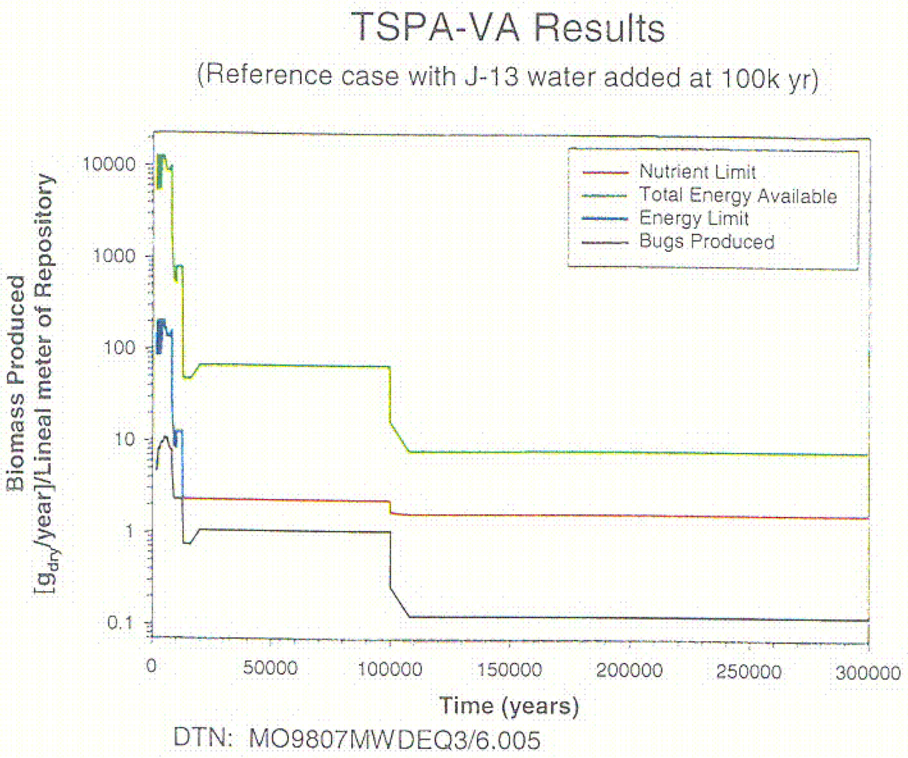
Included below is a summary describing the environmental conditions required to sustain and proliferate microbial life. The following citations were used as general references and are the basis for the majority of the text written in this section unless otherwise indicated: Amy and Haldeman (1997) is the fourth in a series of Chemical Rubber Company Volumes on The Microbiology of Extreme and Unusual Environments that compiles papers covering microbiology in the deep crust; Banfield and Nealson (1997) is the Mineralogical Society of America Reviews in Mineralogy Volume on geomicrobiology; and Pedersen and Karlsson (1995) is a Technical Report from the Swedish Program that assesses the potential importance of microorganisms to performance assessment of a radioactive waste disposal site.

6.3.1.1 Metabolism

Microbes act as catalysts in geochemical processes through their metabolism. The metabolic pathway that a given microorganism will use depends on the energy source (light or chemical) (Amy and Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). Thus, a microorganism is described as either a phototroph or chemotroph, respectively. Among the chemotrophs are those microorganisms that use organic carbon as an energy source (chemoorganotrophs) or those that use an inorganic energy source (chemolithotrophs). If an organism uses organic carbon as its source of carbon, it is referred to as a heterotroph, while if it fixes all of its carbon from CO_2, it is an autotroph. Combinations of these metabolic pathways can give great versatility to organisms in nutrient-limited environments. The types of organisms that exist in the potential Yucca Mountain repository environment (see Section 6.3.2.2) should primarily follow the chemotrophic metabolic pathway.

Bacterial groups are known to use many redox pairs to derive their energy. If chemical kinetic constraints exist such that the rate of a given chemical reaction is sufficiently slow, bacteria can compete; thus, almost any redox couple that yields energy could be exploited (Amy and

Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). The metabolic processes listed below usually define the types of redox processes and input of organic carbon that are available to provide energy and nutrients for growth. They are: aerobic respiration, nitrification and denitrification, methane oxidation, manganese and iron oxidation, sulfur oxidation, manganese and iron reduction, sulfate reduction, and methanogenesis (for a summary discussion on the metabolic processes listed above, see Kieft and Phelps 1997; Pedersen and Karlsson 1995; or Nealson and Stahl 1997). Table 7 gives a listing of possible redox half reaction associated with microbial catalysis. Microbes accumulate at redox interfaces because of the energy that is available to be harvested. Often the metabolic pathways listed above are used to describe the various types of organisms that are present in microbial ecology (i.e., a methanogen is a type of bacteria that uses the redox reactions specific to methanogenesis).


TSPA-VA Results

(Reference case with J-13 water added at 100k yr)

DTN: MO9807MWDEQ3/6.005

Figure 1. Results of TSPA-VA Model for Microbial Communities (see CRWMS M&O 1998a, Figure 4-85).

Additionally, research has demonstrated microbes that are involved in iron reduction can also reduce U(VI) to U(IV) and thus provide energy for their metabolic needs (Lovley et al. 1991, Lovley and Phillips 1992, Lovley et al. 1993, Francis et al. 1994, Abdelouas et al. 1998). This could play a potential role in the growth and sustainment of a microbial population within a high level radioactive waste repository where the majority of the waste emplaced would be spent nuclear fuel.

6.3.1.2 Redox Conditions

Bacteria that are able to grow in the presence of molecular oxygen, either in gaseous or dissolved form, are termed aerobes, whereas those that can grow without oxygen are anaerobes (Amy and

C1

Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). Table 8 shows the terms used to describe the O_2 relations of bacteria. Thus, we see that different microbes can thrive at various redox conditions, including both the oxygenated environments that are at high redox potential and the reducing environments where the oxygen abundance is minimal.

6.3.1.3 Temperature

The temperature of the subsurface environment will greatly affect or limit the type of bacteria present, based on the optimum growth band of the microbe (Amy and Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). There are 5 temperature classifications of bacteria: psychrophiles, facultative psychrophiles, mesophiles, thermophiles, and hyperthermophiles. Table 9 shows the ranges of temperatures that are acceptable to the 5 classes of bacteria. Therefore, during elevated temperatures in the Yucca Mountain repository the microbial population would be dominated by thermophiles and hyperthermophiles; later, as the repository cooled, the repository would be dominated by mesophiles.

Table 7. Redox Half Reactions Associated with Microbial Catalysis.

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**
$CO_3^{2-} + 10H^+ + 8e^- = CH_4 + 3H_2O$	$S + H^+ + 2e^- = HS^-$
$CO_3^{2-} + 6H^+ + 4e^- = CH_2O + 2H_2O$	$S + 2H^+ + 2e^- = H_2S$
$CO_3^{2-} + 8H^+ + 6e^- = CH_3OH + 2H_2O$	$SO_4^{-2} + 9H^+ + 8e^- = HS^- + 4H_2O$
$CO_3^{2-} + 3H^+ + 2e^- = HCOO^- + H_2O$	$SO_4^{-2} + 10H^+ + 8e^- = H_2S + 4H_2O$
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**
$2NO_2^- + 8H^+ + 6e^- = N_2 + 4H_2O$	$O_2 + 4H^+ + 4e^- = 2H_2O$
$NO_3^- + 9H^+ + 8e^- = NH_3 + 3H_2O$	

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Table 8. Terms Used to Describe the O_2 Relations of Bacteria (Modified from Pedersen and Karlsson [1995]).

Group	O_2 Relation
Aerobes	
Obligate	O_2 is required
Facultative	O_2 is not required but growth is better with O_2
Microaerophilic	O_2 is required but at levels lower than atmospheric
Anaerobes	
Aerotolerant	O_2 is not required and growth is not better with O_2
Obligate (strict)	O_2 is harmful or lethal

Table 9. Bacterial Temperature Classes and Their Temperature Ranges. Data are taken from Pedersen and Karlsson (1995) and Horn and Meike (1995).

Temperature Class	Minima	Maxima	Optimum range
Psychrophiles	*	20°C	0 to 15°C
Facultative Psychrophiles	0°C	35°C	20 to 30°C
Mesophiles	15°C	45°C	20 to 45°C
Thermopiles	45°C	70°C	55 to 65°C
Hyperthermophiles	60°C	120°C	80 to 100°C

* No lower bound reported.

6.3.1.4 Radiation

Bacteria are much more resistant to radiation than are most humans (Amy and Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). The acute lethal dosage for many bacteria is approximately 5 to 1,000 krad (Pedersen and Karlsson 1995, p. 48-49). The medical sterilization threshold is about 2,500 krad, and the limit of microbial activity for some species indigenous to the ESF was found to be 200 krad (Pitonzo 1996). Therefore, levels of radiation in the drift thought to be present after waste emplacement at Yucca Mountain as reported by Van Konynenburg (1996) should be low enough to allow microbial growth and catalysis.

6.3.1.5 Hydrostatic Pressure

Although hydrostatic pressure is not thought to be a problem in the proposed Yucca Mountain repository, bacteria are able to withstand and flourish at the highest hydrostatic pressure on the planet (Amy and Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). Ordinary bacteria that have not been challenged by high hydrostatic pressure during their evolution are, nevertheless, remarkably tolerant to such pressure.

6.3.1.6 Water Activity

Water availability seems to be the most limiting condition for microbial growth (Amy and Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). Microbiologists normally use water activity (a_w) to quantify the amount of water available to bacteria. Water activity is normally defined by the ratio of the solution vapor pressure to the vapor pressure of pure water.

Most bacteria cannot exist when a_w falls below about 0.90 and have trouble thriving when a_w is less than 0.95. In order for bacteria to grow well, a_w needs to be around 0.98 (Pedersen and Karlsson 1995). Many fungi and yeast can thrive at lower a_w levels (on the order of 0.7 to 0.85; Pedersen and Karlsson 1995). Water activity in the potential repository will range from about 1 to values approaching zero because of the thermal perturbation.

6.3.1.7 Deep Vadose-Zone Microorganisms

By definition, vadose zones are unsaturated. However, this does not imply that the water found in the vadose zone limits the presence or growth of the microorganisms present. In fact, matric water potentials in most vadose zones are not sufficiently low to cause desiccation stress in microbes (Amy and Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). The microbes found in these unsaturated environments seem to be desiccation resistant (Kieft et al. 1993).

Work done in several vadose zones in arid and semiarid sites indicate that the total numbers of microbes that are considered ambient populations range from 10^4 to 10^7 cells/g dry wt. (Kieft et al. 1993). Kieft et al. (1993) also stated that in the various vadose systems, there are many populations that are growth limited, most by water or organic carbon, but some systems were growth limited by nitrogen or phosphorous.

6.3.1.8 Influence of pH

Bacteria grow over wide ranges of pH, but there are limits to their tolerance (Amy and Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). Bacteria frequently change the pH of their own habitat by producing acidic or basic metabolic waste products. Some bacteria create their own habitats by the formation of biofilms (see Section 6.3.1.14). Each species of microbe has a pH growth range and growth optimum. Table 10 below shows the types of microbes and their pH relationships. In certain areas of the Yucca Mountain repository where the pH is dominated by the cement phases, the repository is favorable to alkalophiles and extreme alkalophiles. In other areas of the repository where other materials would be present, such as iron from WPs, neutrophiles or acidophiles may thrive.

Table 10. pH Ranges of Differing Classes of Microbes. Data Taken from Pedersen and Karlsson (1995) and Horn and Meike (1995).

pH Class	pH Range
Acidophiles	1.0 to 5.5
Neutrophiles	5.5 to 8.5
Alkalophiles	8.5 to 11.5
Extreme Alkalophiles	>10.5

6.3.1.9 Salinity

Bacteria can be affected by changes in the osmotic concentration of their surroundings (Amy and Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). However, there are bacteria that have adapted to highly saline conditions and can grow in high levels of sodium chloride (2.8 to 6.8M; Pedersen and Karlsson 1995). Many bacteria are osmotolerant and thrive in saline solutions with concentrations up to 3M (Pedersen and Karlsson 1995).

6.3.1.10 Nutrition

About 95 percent of the microbial cell dry weight is made up of a few major elements: carbon, oxygen, hydrogen, nitrogen, sulfur, phosphorous, potassium, calcium, magnesium and iron (Amy and Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). Besides these macro-elements, there exists the requirement of several trace elements, namely, manganese, zinc, cobalt, molybdenum, nickel and copper. These trace elements are needed in such low concentrations that they are not thought to be the limiting factors in microbial growth. The requirements for carbon, hydrogen, and oxygen are normally satisfied together, because they are the chief constituents of the molecules that make up the carbon sources for microbes. One source for which this is not true is the autotroph utilization of CO_2 as its principal source of carbon as opposed to the heterotroph utilization of reduced organic carbon. However, the direct utilization of CO_2 is a very energy expensive process. It is far easier for most microbes to utilize the heterotrophic metabolic pathway. Heterotrophs show a great range of flexibility with respect to carbon sources. Some bacteria will degrade almost any reduced carbon source, whereas others will only catabolize a few select carbon compounds.

In order to grow, microbes need to be able to incorporate nitrogen, phosphorous, and sulfur (Amy and Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). Microbes usually employ inorganic sources of these elements. Nitrogen is often used by taking nitrate and reducing it to ammonia, which then can be incorporated via biosynthetic pathways. Some microbes are able to reduce and assimilate atmospheric nitrogen. However, this process is extremely sensitive to oxygen and requires a great deal of available energy. Almost all bacteria use inorganic phosphate as their phosphorous source and incorporate it directly. Most bacteria use sulfate as a source of sulfur and reduce it by assimilatory reduction. Sulfate is available in groundwater and is not usually a limiting nutrient, but quantities of phosphate and nitrogen can be small enough to limit the growth of microorganisms. However, in most conditions, the flux of energy will limit the amount of microbial growth possible. Table 11 shows the nutritional requirements for chemotrophs.

Table 11. Nutritional Requirements for Chemotrophic Organisms.
Modified from Pedersen and Karlsson (1995).

Nutritional type	Carbon sources	Electron sources (reducing power)	Examples of organisms
Chemolithotrophic autotrophy	CO_2	NH_4^+, NO_2^-, Mn^{2+}, Fe^{2+}, H_2S, S, H_2	Ammonium, nitrite, manganese, iron, sulfur, and hydrogen oxidizing bacteria, methanogenic bacteria
Chemoorganotrophic heterotrophy	Organic compound	Organic compound	Most bacteria, fungi, animals

6.3.1.11 Starvation-Survival

Evidence that supports the concept that microbial populations can survive for millions of years in the subsurface has been recently presented (for a detailed explanation of starvation-survival, see Amy [1997] and Morita [1990]). The basic idea is termed starvation-survival and is defined as a state of metabolic arrest, which permits the organisms to survive for long periods without sufficient energy for growth and reproduction (Amy and Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995). This state is the normal state of most microorganisms in nature. Cells exist at this starvation level until there are energy producing substrates present for growth and reproduction (Morita 1990). Following such a growth period, cells can then return to the starvation state when the metabolic substrates are depleted.

6.3.1.12 Size

The size of bacteria varies depending on the species and nutritional status. Growing (thriving) bacteria can be up to several μm long with a volume of several μm^3. The same species in a non-growing state (i.e., a low nutrient or starvation environment) may be as small as 0.2-0.3 μm and have a volume of not more than 0.05 μm^3. This small size is about the smallest possible size of a living organism because of the essential cellular functions that need to take place. This size would tend to be the smallest size involved in bacterial transport in a porous medium and defines the minimum pore size through which bacterial can be transported (Pedersen and Karlsson, 1995; Nealson and Stahl, 1997).

6.3.1.13 Movement in the Subsurface

Microorganisms tend to attach or sorb onto surfaces where they can obtain available redox energy. Once they become attached, microorganisms tend to form biofilms (see Section 6.3.1.14) and thus remain attached. At some point, biofilms grow and reach a steady state where attachment is balanced out by detachment and movement. Both water movement and gravitation are considered the chief mechanisms of transport in the subsurface. Over short distances hydrogeochemical (mineral surface coatings) and cell-associated biological factors (negative microbial surface charge) dominate the transport process. The presence of preferred flow paths can also influence the extent of the transport as well.

Often microbes are thought of as colloids, as they tend to show some of the same behaviors that abiotic colloidal particles do. The movement of microbes is often modeled using either a filtration or an advection-dispersion type model (see Mills [1997] for more detailed discussion on microbial transport).

6.3.1.14 Biofilm Production

After attachment to surfaces, microbes initiate production of slimy adhesive substances, generally exopolysaccharides. These extracellular polymers, which frequently extend from the cell to form a tangled matrix of fibers, provide structure to the microbial assemblage. This structure is normally termed a biofilm. Microorganisms within biofilms are capable of maintaining environments at biofilm/surface interfaces (both liquid/solid and gas liquid interfaces) that are radically different from the bulk in terms of pH, dissolved oxygen, and other organic and inorganic species. In some cases, these interfacial conditions could not be maintained in the bulk medium at room temperature near atmospheric pressure. As a consequence, microorganisms within biofilms produce minerals and mineral replacement reactions that are not predicted by thermodynamic arguments based on the chemistry of the bulk medium (Little et al., 1997). In other words, microbes can create the living conditions (biofilms) to which they are most suited and comfortable even if these conditions are not necessarily the same chemically as the bulk materials that serve as the substrate.

Biofilm accumulation is the result of the following microbial processes: attachment, growth, decay and detachment. Attachment is due to microbial transport and subsequent binding to surfaces. Growth (and biofilm decay) is due to cell division and is generally described by Monod kinetics:

$$\mu = \frac{\mu_{\max} S}{K_s} \qquad \text{(Eq. 1)}$$

where μ_{max} = maximum specific growth rate (t^{-1}), K_s = half saturation coefficient (mole L^{-3}), S = substrate concentration (mole L^{-3}) (Little et al. 1997). Detachment includes two processes: erosion and sloughing. Sloughing happens when large pieces of the biofilm are rapidly removed. Erosion is the continuous removal of individual cells or small groups.

6.3.2 The Ambient System

6.3.2.1 Ambient Environmental Conditions

Besides the presence of water and substrate, the other major necessity for microbial life is the presence in the environment of a few major nutritional elements: carbon, oxygen, hydrogen, nitrogen, sulfur, phosphorous, potassium, calcium, magnesium and iron (see Section 6.3.1.10 above). These elements are the chief building blocks of a microbe. These building blocks are present in the ambient environment in the gas, groundwater and strata that make up the Yucca Mountain site subsurface. The three components (gas, groundwater, and strata) are discussed below. Additionally, the ambient temperature and water activity in the subsurface is not extreme, nor are any of the other environmental limits discussed in Section 6.3.1 above (i.e. pH, salinity, nutrition, etc.) a concern.

6.3.2.1.1 Gas Compositions

As discussed in Section 6.3.1.10 autotrophic organisms can directly assimilate gases. The values of the gases O_2, N_2, and Ar in samples of pore gases from the UZ are all very close to their atmospheric values (CRWMS M&O 1998i, Section 6.2.7.2, pp. 6.2-43). Measurements of gas compositions from various UZ boreholes demonstrate that UZ CO_2 gas concentrations are elevated above atmospheric CO_2 partial pressures (about 350 parts-per-million-by-volume [ppmv]) by about a factor of three (CRWMS M&O 1998i, Section 6.2.7.2, pp. 6.2-43). The values of UZ pore-gas composition analyzed for the site indicate that the CO_2 content of pore gases tends to average about 1000 ppmv (CRWMS M&O 1998i, Section 5.3.4.2.4.6, pp. 5.3-181). These elevated values could be the result of mixing of CO_2-rich gases generated in the soil zone with the rest of the gas volume of the mountain (CRWMS M&O 1998i, Section 5.3.4.2.4.6, p. 5.3-181).

6.3.2.1.2 Water Compositions

As discussed in Section 6.3.1.10 microorganisms can utilize nutrients that are found in groundwater. Analyses of the groundwater compositions at Yucca Mountain are described in detail in the Site Description Document (CRWMS M&O 1998i, Sections 5.3.4, 5.3.5, and 6.2). The ambient water composition could either be defined by analyzed values of saturated-zone water (e.g., Well J-13), or from the analyses performed on pore water extracted from UZ rock samples.

6.3.2.1.2.1 Ambient SZ Water

Harrar et al. (1990) evaluated water from Well J-13 for use as a reference water composition and concluded that it could be used as such for the purpose of a reference case fluid. In addition, the saturated-zone fluids are similar compositionally to both the perched water (CRWMS M&O 1998i, Section 6.2.5.2, p. 6.2-20) and to that collected flowing from fractures at Rainier Mesa (Harrar et al. 1990, pp. 6.5 and 6.6, Table 6.1). At this time, it appears that a reasonable ambient water composition moving through fractures can be represented by the J-13 composition. The average composition of J-13 water from Harrar et al. (1990) is given in Table 12, together with averages for UZ fluids analyzed from boreholes UE-25 UZ-5 and UE-25 UZ-4 (Yang et al. 1988, 1990; Yang 1992).

In an analysis of the groundwater content of dissolved organic carbon (DOC, CRWMS M&O 1997b, Section 4.1), the DOC content of groundwaters from well J-13 and other wells in the Death Valley region show that the standard deviation of DOC falls between 1.48 ppm to 0.36 ppm with the average for J-13 well water at 0.96 ppm.

6.3.2.1.2.2 Ambient UZ Pore water

Analyzed water compositions from the UZ tuffaceous rocks (Yang et al. 1988, 1990; Peters et al. 1992; Yang 1992) indicate that they have pH values in the range of 6.4 to 7.5 and that some constituents (Ca^{2+}, K^+, Mg^{2+}, SO_4^{2-}, Cl^-, and dissolved silica) are more concentrated than found in samples from the SZ tuffaceous aquifer. However, the average HCO_3^- content measured in 83 water samples extracted from UZ nonwelded tuff was lower than that in the saturated-zone samples (Peters et al. 1992). Some of this variability may be caused by the extraction techniques used to remove water from unsaturated samples (Peters et al. 1992). No analyses of the dissolved organic content have been given in the studies of the UZ fluid compositions. Because of the intimate contact between the UZ fluids and the pore gases in the rock, these groundwaters are relatively oxidizing and the oxidation potentials are probably controlled primarily by atmospheric oxygen levels (CRWMS M&O 1998i, Section 6.2.5.2, p. 6.2-21). In the units above the Calico Hills, the pH of the water is thought to be dependent primarily on the carbon dioxide content of the gas, with some degree of Na^+-H^+ ion exchange affecting the values (CRWMS M&O 1998i, Section 6.2.5.2, p. 6.2-20).

There are clearly differences between the J-13 and UZ fluids, primarily higher Ca, Mg, Cl, and SO_4^{2-} in the UZ fluids (see Table 12 and discussion in CRWMS M&O 1998i, Section 6.2.5.2). Whether these differences are meaningful, as well as which fluid composition most closely represents the ambient composition of fluid that moves through Yucca Mountain, is not currently completely understood. There may have been some alteration of UZ pore fluid chemistry from the extraction techniques, as discussed above. In addition, it was thought that the UZ-4 samples had lost water by evaporation, which may account for the generally higher values compared to UZ-5 analyses (Peters et al. 1992; Yang 1992). Because of low sample volumes, the UZ analyses are not as comprehensive as those for the SZ.

Table 12. Average Compositions for Saturated Zone Water Well (J-13) and for Unsaturated Zone Water (UZ-5 and UZ-4) (nr = not reported) (Table taken from CRWMS M&O 1998a, Table 4-2).

Constituent	Units	J-13 AVG	UE-25 UZ-5 AVG	UE-25 UZ-4 AVG
Ca	mg/l	12.9	45.2	99.2
Mg	mg/l	2.0	9.2	17.4
Na	mg/l	45.8	39.1	56.4
K	mg/l	5.0	8.6	14.2
SiO_2	mg/l	61.0	92.4	86.8
NO_3^-	mg/l	8.8	nr	nr
HCO_3^-	mg/l	128.9	nr	nr
Cl^-	mg/l	7.1	53.2	94.0
F^-	mg/l	2.2	nr	nr
SO_4^{2-}	mg/l	18.4	51.0	151.8
Li	µg/l	48.3	nr	nr
Fe	µg/l	~30	49.1	24.3
Mn	µg/l	~45	18.5	38.6
Sr	µg/l	~50	422.6	1196.5
Al	µg/l	~30	nr	nr
Zn	µg/l	nr	62.0	102.1
field Eh	mV	340.0	nr	nr
field O_2	mg/l	5.6	nr	nr
field pH	pH	7.4	7.0	7.5

6.3.2.1.3 Mineralogy of Strata

Microbial cells attach to and interact with associated mineral surfaces. Many nutrients that sustain microbial life are derived from the minerals and redox reactions at mineral surfaces provide metabolic energy. Even in nutrient poor environments such as tuff which contain mostly feldspars, existing microbial populations effectively scavenge the essential macronutrients necessary for survival by looking for inclusions of phosphorous based minerals such as apatite (Rogers et al. 1998). Bulk-rock compositions for Topopah Spring tuff are given below in Table 13.

Table 13. Bulk-rock Compositions for Topopah Spring Tuff.

Element	Unaltered Lower Vitrophyre Concentration wt%	Altered Lower Vitrophyre Concentration wt%
Si	72.2	69.6
Ti	0.07	0.10
Al	14.3	19.5
Fe^{3+}	0.78	1.07
Mn	0.05	0.06
Mg	0.45	1.33
Ca	0.69	3.73
Na	6.43	3.65
K	4.98	0.91
P	0.01	0.02

DTN: LL981209705924.059

By carefully looking at the information provided above for the three components (gas, water, and rock) of the ambient geochemical system, it is obvious that they contain the sufficient nutritional building blocks and provide enough energy to sustain microbial life.

6.3.2.2 Ambient Microbial Populations

As discussed above, the ambient environment has all of the requirements to sustain microbial activity at low levels in the host rock. In fact, microbial analyses conducted in the exploratory studies facility (ESF) have determined the existence of aerobic heterotrophs and autotrophs (Ringelberg et al. 1997). The organisms present include the following types: iron-oxidizing, sulfur oxidizing and nitrifying organisms. Cell counts for autotrophs range between 10 and 500 cells/g dry wt. and for the heterotrophs between 3.2 x 10^4 to 2 x 10^5 cells per gram of tuff. The samples were taken within a month of tunnel boring machine excavation, and sampling precautions were taken to ensure that there were no contamination problems from introduced microbes due to construction activities. Similar investigations were conducted on tuff samples taken from nearby Rainier Mesa and resulted in viable cell counts of about 10^4 per g of crushed tuff (Kieft et al. 1993).

Experiments were also conducted on microbes cultured from tuff collected from the ESF to determine which, if any, nutrients were the limiting factors in microbial growth (Kieft et al. 1997). The collected samples were thought to represent an uncontaminated ambient microbial population. The addition of both water and organic carbon to the cultured microbes caused substantial colony growth. From these experiments, the conclusion was that the potential for microbial growth is large, if nutrients and water are introduced into the environment.

6.3.3 Repository System Conditions and Constraints

Throughout the repository, microbes will use the nutrients and available energy from chemical oxidation and reduction reactions. The construction of the repository will add nutrients and available energy where microbes will be able grow beyond the ambient populations. Table 14 below represents the various materials that the VA design specified. These materials are similar to the materials that will be specified in the LA design. Thus, there will be an increase in nutrient and energy supply above that which the ambient system would provide to sustain its microbial populations.

In addition to the introduced materials, the emplacement of the high level waste will alter the repository environment due to the heating of the repository environment. This will change the ambient conditions, especially the temperature, water, and gas regimes that influence microbial growth.

6.3.3.1 Introduced Materials

As found in Table 14 below, there are three main categories of introduced materials that, as part of the waste package or as structural components, will potentially be abundant post-closure: steels/alloys, cementitious materials, and organic substances. This conceptual model's focus is on microbial interaction with the materials that potentially will be introduced into the drift environment containing some or all of these components. Figure 2 below shows the general locations of most of the major LADS design materials (CRWMS M&O, 1999c) within a repository drift.

6.3.3.1.2 Steels and Alloys

The alteration of metals/alloys in the ground support, waste packages and fuel rods/waste forms will produce metal-oxide and -hydroxide corrosion products within the drift and may form metal-silicate minerals. As the Fe, Mn, U, and other metals in the steel/alloys oxidize, they represent a sink for oxygen and could be a mechanism for generating locally reducing conditions if the oxygen flux into the potential drift is low enough. Such oxidation reactions represent a source of metabolic energy for microbial activity within the potential emplacement drifts. With the shear mass of these materials planned to be emplaced in the repository, abundant energy will be available for microbial catalysis. Additionally, the steels and alloys contain trace elements (i.e. carbon, sulfur, and phosphorous) that can be used for microbial growth.

6.3.3.1.3 Cementitious Materials

Cementitious materials are highly alkaline and have pH's ranging between 11 and 13 (CRWMS M&O 1998a, page 4-17 and Table 4-3). They require organic admixtures to assist in their workability in construction. They are also often high in sulfates and nitrates. In the case of concrete, steels are used as reinforcing agents. Essentially, because of their durability and longevity in the environment, cementitious materials could act as both a nutrient source and as an energy source.

The natural analog to alkaline groundwater is the natural springs in the Maqarin area in NW Jordan, where the groundwaters have pH values as high as 12.9. These springs contain diverse microbial populations, therefore the high alkalinity of the cementitious material and water in equilibrium with it will not preclude the growth of microorganisms (Pedersen 1999). The types of microorganisms residing in this environment would be alkalophiles and extreme alkalophiles (see Section 6.3.1.8, Table 10). Even the extreme alkaline pH environments will not preclude microbial colonization where biofilms have been known to form on concretes The biofilms create very low pH environments and can rapidly degrade the concrete (Diercks et al. 1991, Horn and Meike 1995).

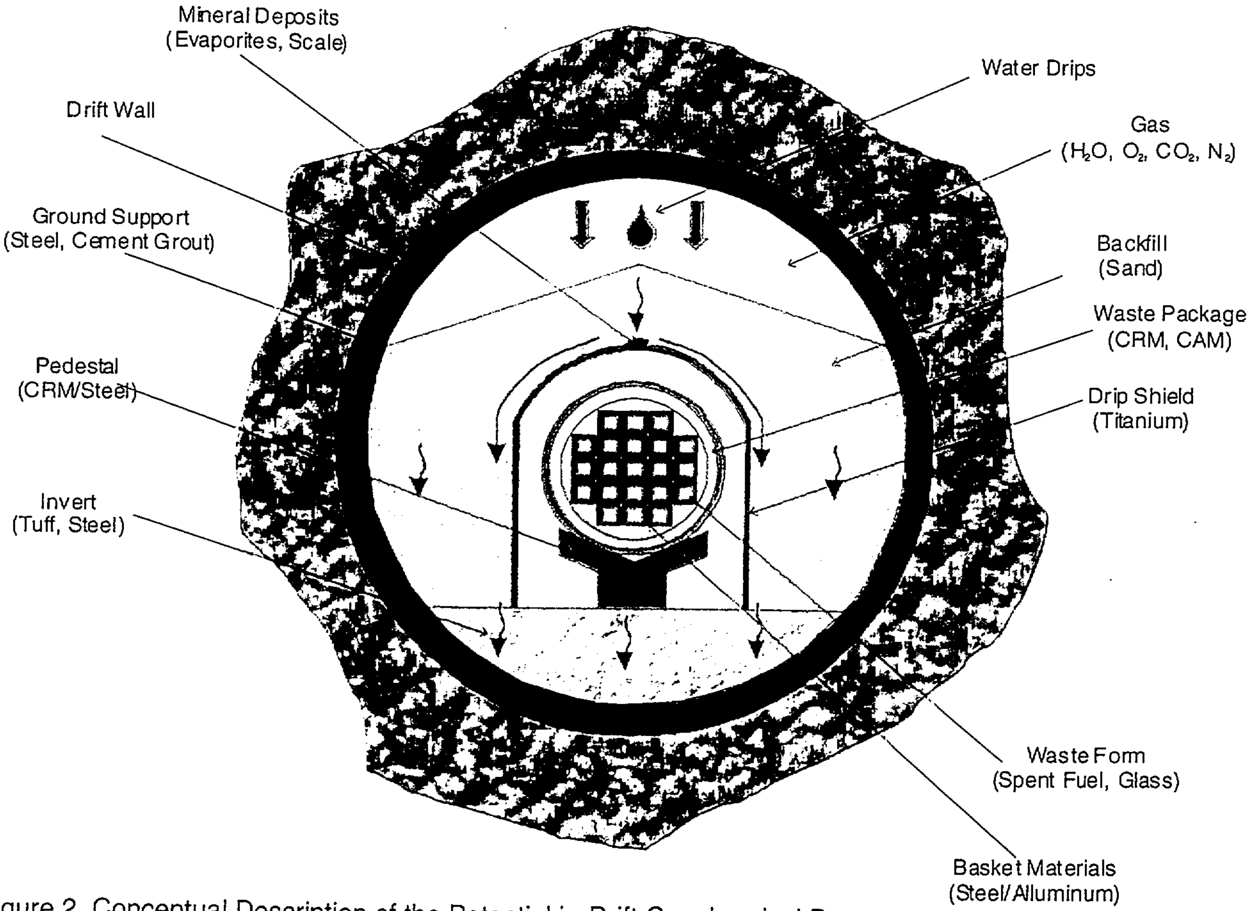


Figure 2. Conceptual Description of the Potential in-Drift Geochemical Processes and the Interaction with the Materials of the EDA II Design (CRWMS M&O 1999c, Rail and Gantry System not Depicted).

Table 14. Materials, Quantities and Compositions of the Various Design Materials and Waste Package Types. Values are Calculated or Documented in Attachments II, III and IV.

Material Name	Quantity kg/m (per WP)**	Element composition and Wt %						
		Fe	*Mn*	*C*	*P*	*S*	*N*	*Other*
304L Stainless Steel	651	65.045	2.0	0.03	0.045	0.03	0.10	Bal.
316L Stainless Steel	128	61.795	2.0	0.03	0.045	0.03	0.10	Bal.
316NG Stainless Steel	2106	61.805	2.0	0.02	0.045	0.03	0.10	Bal.
Alloy C-22	1456	6.0	0.5	0.015	0.02	0.02	-	Bal.
Aluminum 6061	63	0.7	0.15	-	-	-	-	Bal.
ASTM A572 Steel	587.2	97.48	1.65	0.23	0.04	0.05	-	Bal.
ASTM A759-85 Steel	133.9	97.59	1	0.82	0.04	0.5	-	Bal.
ASTM F432-95 Steel	48	99.022	-	0.79	0.058	0.13	-	Bal.
C Steel ASTM A516	1073	97.91	1.3	0.27	0.035	0.035	-	Bal.
Commo Cable	0.79	-	-	27	-	-	-	Bal.
CSNF Waste PWR	32.56	95.73	2.54	0.59	0.66	0.07	0.38	*
CSNF Waste BWR	34.36	95.598	2.974	0.675	0.176	0.106	0.472	*
DHLW Waste	2190	7.35	1.55	-	0.014	0.13	-	Bal.
Neutronit A978	387	66.66	-	0.04	-	-	-	Bal.
Rail Fittings	13.4	73.11	-	0.1725	0.03	0.0375	-	Bal.
Silica Fume	3.35	0.21		1.3		0.32		Bal.
Superplasticizer	0.67	-	-	16.12	-	4.28	-	Bal.
Ti Grade 7	563	0.30	-	0.1	-	-	-	Bal.
Type K Cement	63.50	1.96	-	-	-	2.76	-	Bal.
WWF Steel	70	98.8	-	1.0	0.1	0.1	-	Bal.

*Values were normalized to the quantity of the seven elements reported here and does not reflect the actual masses or complete radionuclide inventory. **Quantities generally represent PWR waste packages and a repository design representing the nonlythophasae host rock. Items like 304L, alloy C-22 and A572 are taken from the designs that apply or are summed from various tables found in the attachments.

6.3.3.1.4 Organic Substances

The introduction of organic substances into the drifts will promote microbial activity and may have an impact on performance through changes in the concentrations of organic acids and organic colloids which can increase WP corrosion, increase radionuclide solubility-limits and transport properties, and enhance silicate mineral dissolution (Choppin 1992; Minai et al. 1992; Bennett et al. 1993; Meike and Wittwer 1993). In addition, organic substances can take part in oxidation/reduction reactions and may therefore contribute to generation of locally reducing conditions, possibly reducing metal solubilities.

Depending on the amount of degradable organic carbon, heterotrophic bacteria will mineralize the organic carbon into inorganic nutrients and carbon dioxide. Under aerobic conditions the organic molecules are generally degraded completely into carbon dioxide. In anaerobic conditions the organic byproducts of one microbial community serves as a substrate for a different community. In these environments the organic carbon can be mineralized either to carbon dioxide by combined oxidative processes or to methane by oxidation-reduction processes, depending on the availability of inorganic electron acceptors in the system (Pedersen and Karlsson, 1995).

6.3.3.2 Thermal Perturbation

With the introduction of waste into the repository environment, there will be an increase in the temperature of the drifts and surrounding host rock. The four sections below describe the potential effects that this perturbation will have on microbial populations–whether they are indigenous species or introduced via construction.

6.3.3.2.1 Temperature

As discussed in Section 6.3.1.3 microorganisms are sensitive to the temperature of their environment. However, hypothermophiles can survive in high temperature regimes up to about 120°C (see Table 9). In the thermally perturbed environment, in-drift repository temperatures will likely rise above boiling for a substantial amount of time and could certainly be >120°C during some of that time. It would only be during this period of time (T>120°C) that the potential for microbial growth could be suspended. Otherwise, microbial growth is not limited by the temperature of the drift environment.

6.3.3.2.2 Water

Water entering the drift will have variable composition as a function of time as a result of the heating of the system driving processes such as boiling/condensation and reaction of both heated and condensate waters with minerals and gases in the fractures of the host rocks (Arthur and Murphy 1989; Glassley 1994; Murphy 1993; Wilder 1996; Lichtner and Seth 1996; Glassley 1997; Hardin 1998, Section 6.2.2). These reacted, or thermally perturbed, fluid compositions may flow down fracture pathways and enter potential emplacement drifts where they could undergo reaction with introduced materials or be boiled again and deposit mineral precipitates containing salts (Glassley 1994; Murphy and Pabalan 1994; Wilder 1996; Lichtner and Seth

1996). However, the different water compositions and water-rock reactions should have limited impact to microbial growth.

The real concern with the water is its availability. As discussed in Section 6.3.1.6, water activity is the limiting condition for microbial growth. Without water, microbes can not exist. Water activity in the unsaturated repository environment is then tied to the thermohydrology of the system. Thus, the elevated temperatures of the emplaced waste packages will tend to dry out the repository and dry up the atmosphere. If the porous medium in the near field and within the drift is in equilibrium with the atmosphere in the drift, then the water activity will be controlled by the relative humidity in the drift environment (see assumption 5.1). This allows us to relate the relative humidity in the atmosphere to the availability of moisture for microbial survival and growth by the following equation

$$a_w \approx \frac{RH}{100} \qquad \text{(Eq. 2)}$$

Where a_w is the water activity and RH is the relative humidity in the drift. If microbes do not thrive below an a_w of 0.90 then when the drift atmosphere falls below a RH of 90 there should be a suspension of microbial growth.

Because boiling of fluids will occur, mineral precipitates including salts will form in the region of boiling. Water undergoing boiling/evaporation or reacting with precipitated salts will become concentrated in a number of dissolved constituents either in close proximity to, or within, potential emplacement drifts (Hardin 1998, Section 6.2.2). However, unless the concentrations of the saline solutions are greater than 3M there should not be an impact from these fluids (see Section 6.3.1.9).

6.3.3.2.3 Gas

The thermally driven perturbations to the system will also affect the flux and composition of gas entering the potential emplacement drifts (Murphy 1991; Glassley 1994; Codell and Murphy 1992; Murphy and Pabalan 1994; Lichtner and Seth 1996; Wilder 1996; Glassley 1997; Hardin 1998, Section 5.7.1). One major process affecting the in-drift gas composition is the boiling of the pore water, which is expected to drive out most of the air component of the gas from the drift environment (CRWMS M&O 1998b). The changes in the air mass-fraction of the gas will drive changes in the redox system and pH in the environment. However there are no real limitations to microbial communities from this perturbation. Microbes can thrive in very different redox and pH environments as discussed in Sections 6.3.1.2 and 6.3.1.8.

6.3.3.2.4 Mineral Precipitation

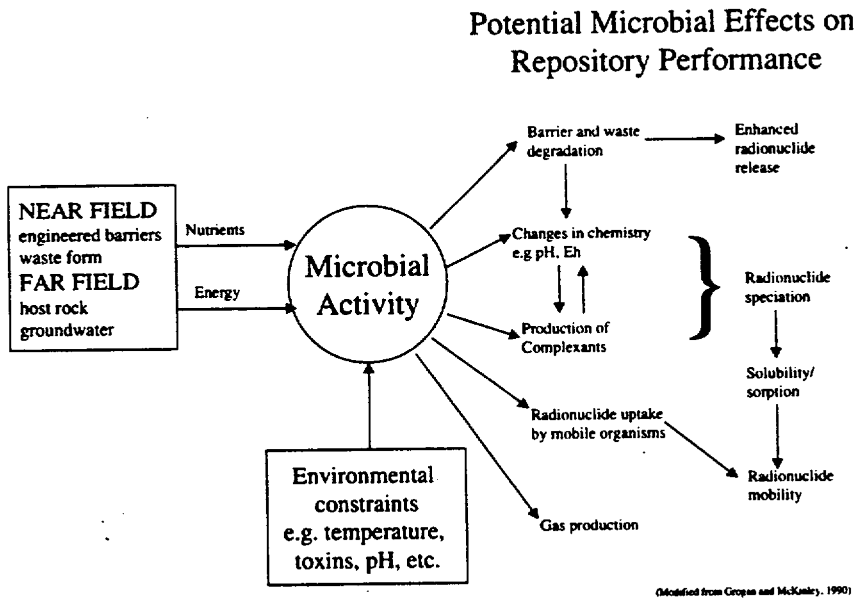
The increased temperatures will vaporize much of the water in the near-field as an above-boiling zone forms in the very near-field (Glassley 1994). This transition will increase the capacity of the system to transport moisture as volatiles and will result in precipitation of all dissolved solids from boiling fluids in the near-field. Condensation of steam as water in cooler regions above the potential repository horizon will dissolve new material, which could be transported through fractures back down into the boiling zone with subsequent boiling and phase precipitation. This refluxing could produce porosity and permeability changes that may impact the near-field hydrology (Glassley 1994; Hardin 1998, Section 5.6). However, mineral precipitation should not effect greatly the ability of microbes to thrive in the system.

6.3.4 Microbial Effects on EBS Performance

The EBS is one of the primary barriers to radionuclide release. The potential degradation of this barrier is of primary concern to the long term performance of the repository. A workshop conducted to examine the potential effects of microbial activity in the potential geologic repository at Yucca Mountain resulted in the following hypotheses (Horn and Meike 1995).

- Microbes can compromise the integrity of WPs (and other repository materials)
- Microbes can modify water chemistry outside the bounds predicted by abiotic chemical calculations
- Microbes can alter the rate of radionuclide transport from breached WPs.

In addition to these three potential effects of microbial populations on a radioactive waste disposal system, some additional concerns have been previously raised: degradation of concrete support structures (Perfettini et al. 1991), production of gas within a repository (Bachofen 1991), alteration of pH and redox conditions within a repository (Hersman 1997), and the disruption of surfaces, e.g. oxide surfaces on metals (West et al., 1985). These effects among others are depicted in Figure 3.



(Modified from Grogan and McKinley, 1990)

Figure 3. Simplified Flow Diagram of the Potential Effects of Microbial Activity on Repository Performance.

Figure 3 also depicts two major classifications of effects on the proposed repository due to the presence of microbial communities, that of impacts to EBS performance and effects on radionuclide transport. Because changes in aqueous chemistry, colloid generation and the production of complexants are integral to transport issues and in order to avoid duplicative discussion in this section, they will be discussed in Section 6.3.5 below.

6.3.4.1 Barrier and Waste Degradation

Perhaps the biggest impact to the proposed repository safety would be the premature degradation of the EBS. This event will cause the release of radionuclides into the transport environment at a much earlier time via degradation of the waste package/drip shield thus allowing entrance of drift seepage into the waste package, cladding, waste form, etc. As far as microbial communities are concerned, the direct way this would be accomplished is via MIC. However, there are other general impacts that would influence the in-drift geochemical environment and enhance the corrosion of metals, namely the changes to chemistry and the production of complexants. These areas are discussed in other sections of this report (see Section 6.3.5).

MIC generally manifests itself as localized corrosion via pitting on metal surfaces. This is usually a result of biofilm formation (see Section 6.3.1.14). Biofilms lead to the formation of electrochemical cells characterized by the physical separation of cathodic and anodic areas. This separation and the depletion of the cathodic reactant enhances the anodic dissolution of the area, promoting acidification as a result of the hydrolysis of the metal cations, increasing the concentration of the aggressive anions such as chloride, and fostering the oxidative dissolution of detrimental species from the metal (Geesey 1993). This in turn tends to increase the rate of anodic dissolution.

The localized environments in these areas are far more complex in the case of MIC than those present under abiotic conditions in crevices or beneath deposits. This complexity is the result of the multiple biochemical reactions associated with the generation of metabolic products through bacterial activities. With the possibility of MIC enhancing the degradation of all metals used in the construction of the repository drift and on the waste package and drip shield, MIC can influence the premature release of radionuclides from the repository. For a more detailed discussion of these processes, in both general and Yucca Mountain specific terms, the reader is referred to Geesey (1993) and Horn et al. (1998a and 1998b).

6.3.4.2 Gas Generation

In the relatively open atmosphere in the planned repository, the generation of gas from microbial metabolism does not seem to be a great concern. However, microbes do generate and consume various gases. All of these are found in the atmosphere and are members of the biogeochemical cycles of carbon, hydrogen, nitrogen, oxygen and sulfur (Bachofen 1991). Perhaps during the time of highest repository heating where the air mass fraction would be mostly water vapor, the generation of gas could be an important geochemical process. However, it is during this time that microbial growth would be limited by the elevated temperatures in the drift. Therefore, the bulk impacts should be negligible.

6.3.5 Potential Microbial Effects on Transport

Radionuclide transport is a performance issue that is continually being investigated. Thus, the effects of microbial populations are of concern to repository performance. Microbial processes affecting radionuclide transport are varied and significant (see Figure 4). The processes include, but are not limited to, sorption/precipitation, complexation/ chelation, dissolution, oxidation/reduction reactions, and colloidal agglomeration. Additionally microorganisms create microenvironments of nutrient and chemical gradients that are capable of altering radionuclide solubilities. The basis for the majority of the information in this section was taken from Hersman (1997).

6.3.5.1 Microbial Sorption

Microorganisms can affect sorption/desorption reactions with the minerals on the surface of the matrix. Attached microbial populations occupy portions of the matrix surface area with cells and or exopolymers. Both have different sorption characteristics than the bare matrix. The outer cellular membranes of microbes have net negative charges and would tend to bind heavy metal cations. These cell walls have various surface functional groups such as carboxyl, phosphate and hydroxyl groups (Daughney et al. 1998, Fein et al. 1997). These are efficient metal building agents and are of importance in metal removal from solution (Hersman 1997). Therefore, with respect to sorption, microorganisms may decrease the amount of radionuclides in solution, thus reducing potential for transport as a dissolved species, yet increase potential for transport as a microbial colloid.

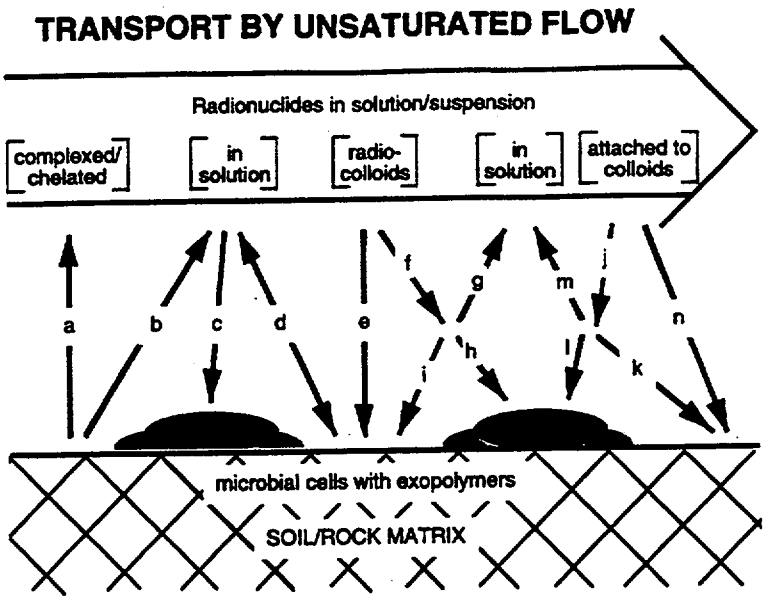
6.3.5.2 Complexation/Chelation

Microorganisms also perturb the geochemical speciation of metallic elements by releasing inorganic and organic chemicals into the surrounding extracellular environment (Stone 1997). These chemicals contain a variety of functional groups that complex strongly with metals. When a chemical attaches to a metal with two or more functional groups forming a ring structure, then this complexation is called chelation.

Two groups of microbial compound are considered complexing agents: by-products of microbial metabolism and degradation, and microbial exudates. The first group consists of simple organic compounds such as low molecular weight organic acids and alcohols and macromolecular humic and fulvic acids. The second group includes microbial exudates induced by metals ions. Iron-binding siderophores are produced in response to low iron concentrations and toxic-metal binding proteins.

6.3.5.2.1 By-products of Microbial Metabolism

Depending on the types of organic materials introduced into the repository drift and the environmental conditions there could be variable abundances of the small molecular weight complexing agents. Additionally, the large macromolecular humates are limited without the introduction of repository materials in the drift environment. The interactions with these materials can a) include altering adsorption, bioavailibility and toxicity, b) reduce Np(V), Pu(V), and Pu (VI), and solubilize ^{241}Am and Th (Hersman 1997).



Note the following legend: (a) adsorbed radionuclides are complexed/chelated; (b) dissolution occurs; (c) radionuclides are sorbed by microorganisms; (d) various redox reactions result in solubilization or precipitation; (e and n) agglomeration of colloids; dissolution of (f) radiocolloids or (j) radionuclides attached to colloids, leading to (g and m) solubilization, (h and l) sorption, or (i and k) adsorption/precipitation. Figure taken from Hersman (1997).

Figure 4. Interactions Between Radionuclides in Solution/Suspension and Indigenous Microorganisms.

6.3.5.2.2 Microbial Exudates (Siderophores)

Microbes require Fe for DNA synthesis, electron transfer proteins, and nitrogen fixation. However, Fe suffers from extreme insolubility in aerobic environments at physiological pH. Aerobic and facultatively anaerobic microorganisms have developed a system where they can acquire Fe(III). This is done by the generation of siderophores. Siderophores are low molecular-mass, ferric-specific ligands that are induced at low iron concentration for the purpose of biological assimilation of Fe(III). The most common siderophores contain the hydroxamic acid functional group -R-CO-N(OH)-R', which forms a five membered chelate ring with Fe^{3+} (Hersman 1997). Because Fe(III) and Pu(IV) are similar in their charge/ionic radius ratio, Pu(IV) might serve as an analog to Fe(III) (Hersman et al. 1993). Complexation/chelation would increase the amount of radionuclides in solution, thus increasing their availability for transport.

6.3.5.3 Redox Reactions

The solubility of a radionuclide is generally related to its oxidation state. Therefore, if microorganisms affect the redox chemistry of radionuclides then they would also affect the solubility of radionuclides. The redox cycling of metals by microorganisms is the foundation of microbial growth as the redox cycles provide both nutrients and energy (see Sections 6.3.1.1, 6.3.1.2 and 6.3.1.10 above). Thus microorganisms are able both directly and indirectly to affect redox changes in metals. Direct effects are the oxidation of the metal as a source of energy and the use of a metal as a terminal electron acceptor, thus reducing the metal. The indirect effects are the nonspecific oxidation of metals at the outer surface of the bacterial envelope and the reductions of secondary metals caused by the presence of a microbially reduced primary metal. Because the effect of redox on solubility varies with each radionuclide, the overall effect on total radionuclide solubility is unknown (Hersman 1997).

6.3.5.4 Biodegradation of Organic/Radionuclide Complexes

Hersman (1997) reports that complexed/chelated radionuclides may become subject to microbial degradation as the transport regime moves the complexed/chelated radionuclides into areas of the drift and unsaturated zone that have lower nutrient concentration. Low molecular weight organic acid, alcohols and siderophores could all serve as nutrients for indigenous microbial populations. The biodegradation could generally result in the precipitation of the released ion as water-insoluble hydroxide or salts and thus retard transport.

6.3.5.5 Dissolution

Due to similarities between Fe and Mn and radionuclides, evidence indicates that microorganisms will affect the dissolution rates of radionuclides (Hersman 1997). Microbially enhanced dissolution reactions will affect the stability of radionuclides in radiocolloids and radionuclides attached (either sorbed or precipitated) to natural colloidal particles, to the matrix surface, or to the surfaces of microorganisms. However, the overall results are difficult to predict (Hersman 1997). Radionuclides removed by dissolution would be available to be complexed or chelated by microbial metabolites, thus increasing the transport of radionuclides. However, radionuclides may precipitate onto surfaces or be reabsorbed. Also removal of the adsorbed/precipitated radionuclides from colloids or the dissolution of radionuclides, both of which have the potential to be mobile, can have a negative effect on transport rate.

6.3.5.6 Colloidal Agglomeration

In the presence of microorganisms colloidal movement through a rock matrix could be reduced because of an overall increase in the size of colloidal particle agglomerates (Hersman 1995). There are several general interactions between microorganisms and solid surfaces (including colloidal particles) and the affects of microbial adhesion on colloids. These interactions include attraction processes: adhesion, adsorption and flocculation.

6.3.5.6.1 Attraction of Bacteria to Solid Surfaces

Solid surfaces are potential sites for concentrating nutrients and for promoting microbial activity. Besides movement of water across a solid surface, there are many physico-chemical and biological attraction mechanisms at solid surfaces. These attraction mechanisms include chemotaxis, Brownian motion, electrostatic attraction, van der Waals interaction, electrical double layer effects, and cell surface hydrophobicity (for a more detailed discussion on these processes see Hersman 1995, page 2-4). Depending on the nature of the particulate matter, fabric organization, clay type, etc., the availability of the substrate may be either enhanced or reduced by the presence of particulates. If substrates were concentrated on the surface of clay minerals, this would enhance the colonization of microbes on those surfaces. These interactions can lead to the formation of multiple bacterial-colloidal particle agglomerates (Hersman 1997). In addition, Hersman (1995) indicates that clay colloids can be adsorbed onto the surfaces of microbes.

6.3.5.6.2 Adhesion

Adhesion of microorganisms is involved in fouling of man-made surfaces, in microbial influenced corrosion, and in syntrophic and other community interactions between microorganisms in natural habitats. Bacteria appear to adhere to surfaces by means of surface polymers, including cellular lipopolysaccharides, extracellular polymers and capsules, pili, fimbriae, and flagella. These materials are the same components that are used in biofilm production as described in Section 6.3.1.14. The composition and quantity of bacterial surface polymers vary considerably and are influenced by growth and environmental conditions (Hersman 1997).

6.3.5.6.2 Enhanced Flocculation

Hersman (1995) and Hersman (1997) discuss the processes that have been patented for the flocculation of clays. They include microbial polysaccharides and nucleoproteins. These processes have the potential to inhibit colloidal transport.

6.3.6 Conceptual Model Summary

In the repository environment, many different microbes could grow and provide a plethora of potential chemical processes that may affect the bulk chemistry within the emplacement drifts (Hardin 1998, Section 7). Large sources of potential nutrients for microbes are the materials used in the construction of the ground support. The waste-package materials represent reduced metals that can be oxidized to provide energy for microbes to thrive, and the waste forms themselves contain both nutrient and energy sources for microbes. This process conceptual model for microbial communities is meant to conceptualize the factors that limit the growth of microbes and to identify what are the potential chemical effects to the in-drift geochemical environment from the microbial community that would grow. Such growth would be a direct result of perturbing the ambient environment and adding potential nutrients (e.g., steel, concrete, and other repository materials) for bacterial catalysis and growth.

Microbes can thrive over a wide range of pH, under high hydrostatic pressures, in highly saline conditions, and in high radiation conditions that would normally be lethal to humans. Microbes live in nutrient starved environments and can be expected to continue to live even if the nutrient supply of introduced repository materials becomes exhausted. In these nutrient starved environments, some microbes even metabolize CO_2, N_2 and CH_4 directly from the gas phase via autotrophic behavior or methanogenic metabolic processes. Microbes will alter their environment by creating biofilms. Biofilms make it possible for anaerobic microbes to live in aerobic conditions by isolating them from the normal atmospheric conditions in which they would not survive. Biofilms also initiate pitting corrosion on metals via MIC. Therefore, all microbial influenced redox mineral transformations are possible in a Yucca Mountain repository. Microbes will adhere to mineral surfaces where they are able to utilize available nutrients and energy; otherwise they can act as colloidal particles and move through the subsurface via advective-dispersive mechanisms.

Over time, the repository environment will have environmental conditions that will favor certain bacteria over others (i.e., thermophiles over mesophiles or acidophiles over neutrophiles).

However, with the exception of the period in time when the temperature of the repository is >120°C and the water activity is <0.90, microbes should be able to grow and produce their metabolic byproducts.

Microbes will either attach (accumulate) themselves to surfaces in the in-drift environment, thus affecting the chemical environment in the repository or they will be available to act as colloids, thus affecting radionuclide transport. Microbial processes affecting radionuclide transport are varied and significant. The processes include but are not limited to, sorption/precipitation, complexation/chelation, dissolution, oxidation/reduction reactions, and colloidal agglomeration. Additionally, microorganisms create microenvironments of nutrient and chemical gradients that are capable of altering radionuclide solubilities.

6.4 MING SOFTWARE CODE

MING 1.0 [CSCI 30018 V1.0] has undergone a software verification and validation process (with the code having passed all its validation tests), as documented in CRWMS M&O (1998h), the finalized SQR (software qualification report, CSCI 30018 V1.0, 30018-2003). MING 1.0 is used in this report to evaluate potential impacts that the committed repository would have on microbial populations and their associated impacts to radionuclide release and facilitated transport. The MING code as discussed in Section 6.4.1 and 6.4.2 below, is based on the Swiss and Canadian models for estimating microbial production in potential repositories in the saturated-zone (McKinley et al., 1997; Stroes-Gascoyne, 1989; West et. al., 1989; Capon and Grogan, 1991; and Grogan and McKinley 1990).

The Swiss and Canadian models were enhanced for Yucca Mountain site-specific conditions (unsaturated zone, thermal perturbation, and specific design materials) and implemented in the MING code. Thus, MING accounts for growth thresholds based on (a) temperature (<120°C) and water activity (via relative humidity, where a_w=[RH/100] > 0.90), (b) flux of gas-phase constituents, (c) pH- and temperature-dependent redox couples, and (d) design-specific materials descriptions and degradation rates as discussed in Section 6.4.1 and 6.4.2 below.

MING uses the supply of constituents from design materials and constituent fluxes into the drift to perform two separate mass-balance calculations as a function of time. The first (nutrient limit) assesses the available nutrients (C, N, P and S) and calculates how many microbes can be produced based on a microbe stoichiometry of $C_{160}(H_{280}O_{80})N_{30}P_2S$. The second (energy limit) calculates the energy available from optimally combined redox couples (see Table 16 in Section 6.4.3.1 below for half reactions considered), for the temperature, and pH at that time. This optimization maximizes those reactions that produce >15kJ/mol (limit on useable energy, McKinley et al. 1997) using an iterative linear optimization technique. The final available energy value is converted to microbial mass at a rate of 1 kg of biomass for every 64 MJ of energy (Grogan and McKinley, 1990). These two values (nutrient limit and energy limit) are then compared and the smaller value represents the number of microbes that can be produced for that time. This code and the associated conceptual model for microbial activity (see Section 6.3) does not attempt to quantify the effects of individual microbial colonies or biofilms that may be present on repository materials, but attempts to quantify the overall global bulk effect of microbes on the in-drift geochemical environment (IDGE).

6.4.1 Code Development Concepts

The purpose for developing MING was to provide a tool to implement the applicable concepts in Section 6.3 to assess the microbial growth in a potential drift and the potential for microbial effects to bulk water compositions. MING can also provide a basis for discussing the other potential IDGE chemistry effects for the needs of performance assessment, given that microbial activity will occur in the proposed repository. The magnitude of such activity needs to be quantitatively analyzed. Three basic approaches are possible and have been previously documented in McKinley and Grogan (1991). They are as follows:

- Mass balance approach–the biomass will inherently be limited by the inventory and/or supply rate of some essential element (e.g., C, N, P, and S) which may represent a very significant constraint. If the biomass is very low, it may be possible to justify neglecting microbial processes in comparison with competing purely inorganic reactions.
- Thermodynamic approach–in addition to nutrients, constraints set by the available energy sources can be evaluated.
- Kinetic approach–the evolution of a population of organisms in a particular evolving chemical system is explicitly modeled using either empirical or mechanistically derived kinetic data.

The kinetic approach is mathematically possible and in fact, other near field geochemical model computer codes (EQ3/6, Wolery 1992; AREST-CT, Chen et al. 1995), used in PA analyses could potentially be modified and used to simulate the kinetic approach. However, it is not possible to obtain the required information about all the relevant microbial processes at the resolution that is required to interface directly with these codes at this point in time. Thus, we chose to use the more simplistic approaches, similar to those used by the Canadian High-Level Waste Repository program (Stroes-Gascoyne 1989) and the Swiss Low/Intermediate-Level Waste Repository program (Capon and Grogan 1991; McKinley and Grogan 1991; McKinley et al. 1997; and West et al. 1989, a natural analog study for the Swiss program) which use both mass balance and thermodynamics to quantify the impacts of microbial populations. Subsequently, these two approaches are used as the basis for the development of MING. In the first aspect of this, abiotic processes are used to determine the rate at which nutrients become available to microorganisms, which is used as the rate that the microorganisms convert those nutrients to the products (i.e., instantaneously in this mass balance approach). The second uses limiting guidelines of energy availability and the availability of all the required nutrients in the proper ratio to get the rate at which this occurs (thermodynamics approach).

Different design options can be examined by assessing various cases in which all of the available nutrients (derived from WP materials, ground support materials, gas flux, water flux, etc.) are converted into the appropriate products. All of the possible combinations of these parameter values will be used as input into MING in order to conduct sensitivity analyses of the various repository design options, temperatures, relative humidities, gas fluxes, and water chemistries, etc., that are derived from other TSPA and process level modeling efforts. The objective is to be as transparent (i.e. to integrate inputs and output so that all PA calculations and models are consistent) as possible considering the multiple time dependent inputs. However, obtaining degradation rates of all the introduced materials in the near field (e.g. concrete, steel, polymers, etc.) is not a realistic goal at this time.

6.4.2 Software Development

The starting point for the MING software model development was based on documentation for the software routine titled Estimation of Maximum Microbiological Activity, also known as EMMA (Capon and Grogan 1991), and is also based on the documented approach to modeling the Swiss Low/Intermediate Level Waste Repository found in Grogan and McKinley (1990) and McKinley and Grogan (1991). MING contains the same basic modeling approach and structure of calculating the nutrient and energy limitations described in Grogan and McKinley (1990) and McKinley and Grogan (1991).

Early on, it was determined that EMMA would not be able to serve as the vehicle to do the calculations without some major modifications. Many of the concepts to which modifications to EMMA were derived are documented in the Near-Field Geochemical Environment Abstraction/Testing Workshop Results (CRWMS M&O 1997a). However, as programming developed, other requirements were added and the original concept was refined.

Essentially, there are two main components that were brought forward into MING from the Swiss modeling approach: (a) the numerical solution for the amount of energy available for microbial growth; and (b) the general method for calculating nutrient availability. However, smaller pieces of the approach were also maintained and used in MING (see Table 15 below) including the average empirical microbial formula $[C_{160}(H_{280}O_{80})N_{30}P_2S]$ with a dry weight 3998.1 g mol^{-1} (McKinley et al. 1997). This formula represents the ratio of elements needed to form a microbe (e.g., 160 carbon atoms for every sulfur atom). In addition, the implementation in MING also uses an average microbial water content of 99 percent and an average microbial volume of 1.5×10^{-13} ml (McKinley et al. 1997). Multiplying this latter value by the density of water (1 g/cm^3, Weast 1979) produces an average microbe mass of 1.5×10^{-13} g (see Attachment I).

Like the EMMA code, MING utilizes the same basic approach to thermodynamic modeling, where microbes use redox couples in order to supply the energy required to carry out their basic metabolic functions (i.e., aerobic respiration, nitrification and denitrification, methane oxidation, etc.). Because microbes tend to utilize specific, well-documented metabolic pathways (Amy and Haldeman 1997; Banfield and Nealson 1997; Pedersen and Karlsson 1995), a list of appropriate redox half reactions was derived (see Table 7, Section 6.3.1.2) based on the available nutrients in the system that will maximize energy production. MING uses the same values used by EMMA on the limits of usable energy available from a given full redox reaction, where 15 kJ per mole of electrons transferred is the lower limit of energy needed to create biomass (i.e. only those full reactions that produce >15kJ/mol are considered). The final available energy value is converted to microbial mass at a rate of 1 kg of biomass for every 64 MJ of energy limit on useable energy (Grogan and McKinley 1990, Appendix 3, p. AIII-1).

Table 15. Accepted Mass Balance Modeling Parameters used as Conversion Factors.

Parameter	Value
Microbial Composition	$C_{160}(H_{280}O_{80})N_{30}P_2S$
Average Water Content	99% by weight
Average Microbial Volume	1.5×10^{-13} ml

MO9909SPAMICRO.001

The EMMA model is based on a simplified thermodynamic system where the pH is fixed at 12; the temperature in the repository is set to 25° C; and the Gibbs free energies (ΔG) used to calculate the available energy for microbial production were fixed at standard temperature (25° C) and pressure (1 atmosphere). For example, any redox reaction can be written in the general form

$$A + ae^- + bH^+ = cB + dH_2O \qquad \text{(Eq. 3)}$$

for which a standard free energy of reaction ($\Delta G_r°$) can be specified. The $\Delta G_r°$ can be derived from standard free energies of formation ($\Delta G_f°$):

$$\Delta G_r^\circ = \sum \Delta G_f^\circ\,(\text{products}) - \sum \Delta G_f^\circ\,(\text{reactants}) \qquad \text{(Eq. 4)}$$

or from an equilibrium constant (K):

$$\Delta G_r^\circ = -RT \ln K \qquad \text{(Eq. 5)}$$

where R stands for the gas constant and T represents the absolute temperature. The calculations are made by combining independent half reactions and calculating the overall $\Delta G_r°$ for the reaction.

EMMA's simplified model is certainly not realistic in the sense that the repository environment will undergo temperature changes due to the hot WPs. For MING, in order to account for a chemically variable system, the time dependent temperatures, gas fluxes, and water chemistries need to be accounted for over the time frame of the calculations. With the incorporation of these variables, the calculations should end up being as transparent as possible with other calculations being derived from other TSPA abstractions.

6.4.3 Site-Specific Additions to the Software

Some of the features built into MING that extend its capabilities beyond those of EMMA are as follows:

- The addition of temperature dependencies on the ΔG calculations

- The stipulation that nutrient dependencies are calculated from the time dependent gas flux into the repository drift (to address autotrophic and aerobic behavior) as well as the presence of other repository materials

- The addition of time dependent water chemistries entering the drift

- The addition of pH dependence on the governing redox equations (EMMA used a single fixed pH value of 12 for all calculations)

- The ability to degrade one repository material before another becomes available (such is the case with a layered WP design where the CAM degrades well before the CRM)

- The addition of physical limitations to microbial growth as a result of temperature and RH

6.4.3.1 Corrections to ΔG_r° for pH and Temperature

It is important to note that within MING, only the standard-state free energies are used and these are not corrected for either Eh or the activity of dissolved species to derive the actual nonstandard-state free energies. By not calculating the nonstandard-state free energies, the calculation of available energy is not precise, but only represents a rough estimate of this value. Because the half-reactions are written as simple reduction reactions, the free energy of a full reaction constraint applies slightly more generally than purely standard-state conditions. It is actually constrained such that the ion activity ratios of the redox pairs are at isoactivities, which could be possible for ion activities different than unity (the standard-state conditions). For each full reaction, correcting for the actual pH brings the free energies of reaction further from the standard state values. However, using this simplified model should allow increased understanding of the complexity of the microbiological system and provide a mechanism to understand the bulk system at an approximate (order-of-magnitude) level.

Within a biofilm or an individual microbe, the pH (and speciation) can certainly be completely different than the bulk chemistry imposed by the in-drift or near-field environment. However, the bulk chemistry is the major influence on the types of nutrients and energy that can be provided for a given microbe or biofilm. Microenvironments do exist, however this model can not analyze those localized conditions. In order to gain the detail needed to correct ΔG_r° for the activity of dissolved species in the fluids and analyze microscale processes, a much greater effort must be made than is possible at this time. Only the first step in this process has currently been completed, which is to correct for the actual pH of the bulk system. To truly incorporate the localized system water chemistry effects, the effort would require iterative solution of changes to the activities of dissolved species for localized microbial processes. This iterative effort can be done, but would involve an enormous effort to collect the dissolved species data for the calculations

Because the temperature of the repository will not be fixed over time, a method to incorporate temperature effect on reaction free energies was derived in order to build into the MING results the transparency required to incorporate the thermohydrologic temperature histories provided from other modeling efforts (e.g., see Figure 5 below).

Regression analyses were performed on ΔG_r° values at various temperatures (0°, 25°, 50°, 60°, 75°, 100°, 125°, and 150°C) for a selected group of half reactions to define temperature dependent curves that could be incorporated into the energy calculations. The regression analyses are documented in CRWMS M&O (1998f) with the results shown on Table 16 below. The derived regression variables are used to calculate the temperature dependent ΔG_r° that is used in the derivation of the available energy for a given reaction. The temperature dependent regression variables are used in MING in the following way:

$$\Delta G^\circ_{r\,(\mathrm{temp})} = B_0 + B_1 T + B_2 T^2 \qquad \text{(Eq. 6)}$$

where B_0, B_1 and B_2 are the second order regression coefficients. Thus, both the effects of variable pH and temperature (°C) are accounted for in the calculations.

6.4.3.2 Nutrient Supply

As documented in the microbial modeling approach for the Swiss Low/Intermediate-Level Repository (Grogan and McKinley 1990), MING only considers the major elements essential for cell growth (C, N, S, and P). Other nutrients will be considered freely available (i.e., Na, K, Ca, and Cl) except for water.

The mass balance calculations conducted in MING consider three sources of nutrient supply: first, the time dependent flux of groundwater into the repository; second, the degradation of repository materials including the multilayered effects of WPs (see Section 6.3.3.1 for a description of materials considered), and third, the time-dependent flux of gasses (CO_2, N_2, O_2, and perhaps CH_4) into the repository. The nutrient limits will be calculated by determining the appropriate ratio (relative molar concentration) of material (determined by available nutrient flux) needed to create the typical organism having a stoichiometry of $C_{160}(H_{280}O_{80})N_{30}P_2S$.

6.4.3.3 Temperature and RH Effects on Microbial Growth

The availability of water for microbial growth in the UZ at Yucca Mountain will be dependent on the thermohydrological conditions within the repository. In order to account for periods where there is not enough moisture to allow microbial growth (a_w <0.90, see Section 6.3.3.2.2) the relationship between RH and a_w, is assumed (see Equation 2, Section 6.3.3.2.2, and assumption 5.1) and used to allow for the unsaturated conditions in the repository.

Temperature will also affect the ability of a microbe to reproduce. The temperature dependency of microbial activity is set by the temperature within the repository environment where microbes are not allowed to reproduce and grow above temperatures of 120°C.

6.4.4 Other Code Features

MING is designed to consider all of the committed (not intended to be removed before permanent closure) materials that are included in the current repository and WP designs, as well as the potential to evaluate any alternate design options that are relevant to microbial behavior. Section 6.3.3.1 above lists the various design materials, quantities, and compositions that are to be emplaced in the repository and are evaluated herein. For example, in MING, a committed material (e.g., steel sets, drip shield, etc.) is broken down into its individual chemical composition and allowed to enter the nutrients available in a time step based on a fractional corrosion rate (1/estimated material lifetime) for that given material.

In calculating nutrient availability, MING also will allow a sequential introduction of committed materials. This means that a sequential layered model of the WP can be defined, where the CRM and other internal WP materials are not allowed to mutually degrade and be released into the nutrient stream until the drip shield is completely used up.

Another tool that MING can utilize is a "special reactant" flag where the intermediate breakdown products (other than the basic chemical composition) can be identified. Potential items that fall into this area are substances such as organic admixtures, which are common components of cement mixtures and tend to be resistant to biodegradation. These items can then have their releasable compositional quantities split among the several associated species that are included in the redox model.

MING is also designed to incorporate variable gas flux calculations and incoming water chemistries and provide these inputs to both the nutrient and energy calculations.

6.4.4.1 MING Parameter Inputs

The use and format of the MING input needs are documented with in the MING V.1.0 code and associated users manual (CSCI 30018 V1.0, CRWMS M&O 1998d) Any case specific inputs will be documented in Section 6.5 for each modeling case presented. However, four general types of inputs are needed for a MING model run. They are as follows:

6.4.4.1.1 Fixed Inputs

The most important of these is the redox reaction table and the associated temperature-dependent coefficients for each selected half reaction (see Table 16). Also included is Table 17 below, which is needed in the code to do various calculations but remains a fixed value.

Table 16 represents the redox half reactions and associated temperature dependant coefficients as described above that have been selected to represent generalized microbial catalysis reactions. They include selected half reactions that cover the following known microbial metabolic pathways: aerobic respiration, nitrification and denitrification, methane oxidation, manganese and iron oxidation, sulfur oxidation, manganese and iron reduction, sulfate reduction, and methanogenesis. The thermodynamic data used to derive this table are documented in CRWMS M&O (1998f).

6.4.4.1.2 Environmental Inputs

These include time-dependent temperature and RH values, time-dependent water chemistries (includes pH and infiltration rates) and time-dependent gas fluxes (includes CO_2, O_2, and N_2). These results are provided from other modeling efforts (TH calculations, NFGE THC incoming water, IDGE in-drift gas, seepage flux into the drift).

6.4.4.1.3 Design materials

These inputs include the proper formatting and documenting of quantities and elemental compositions of all the repository and WP design materials that may be placed into the repository. This also includes designation of expected material lifetimes and the designation of breakdown codes and specifying of material reactants necessary for utilization of the redox half reactions that are used to calculate the model energetics.

Table 16. Temperature Dependant Δ*G* Relationships for Selected Redox Half Reactions used in MING V1.0.

Redox half reaction		Δ*Gr*° (cal/mol) vs. *T*(°C)				Δ*Gr*° (kJ/mol) vs. *T*(°C)		
Carbon	**RXN #**	**B0**	**B1**	**B2**	**r^2**	**B0**	**B1**	**B2**
CO2 + H+ + 2e- = HCOO-	C1	9688.3396	27.9163	0.02913	0.9999	40.5554	0.1169	0.0001
CO2 + 4H+ + 4e- = CH2O + H2O	C2	18992.513	-5.888	-0.0623	0.9999	79.5027	-0.0246	-0.0003
CO2 + 6H+ + 6e- = CH3OH + H2O	C3	-4582.1156	5.4553	-0.0696	0.9996	-19.1807	0.0228	-0.0003
HCOO- + 3H+ + 2e- = CH2O + H2O	C4	-8475.1508	-7.7987	-0.0291	0.9999	-35.4770	-0.0326	-0.0001
CO2 + 8H+ + 8e- = CH4 + 2H2O	C5	-27359.7546	2.1845	-0.1187	0.9995	-114.5279	0.0091	-0.0005
CH2O + 2H+ + 2e- = CH3OH	C6	152221.87	-63.2114	-0.0798	0.9969	637.2007	-0.2646	-0.0003
HCOO- + 7H+ + 6e- = CH4 + 2H2O	C7	-37048.093	-25.7317	-0.1478	0.9998	-155.0833	-0.1077	-0.0006
CH2O + 4H+ + 4e- = CH4 + H2O	C8	126179.023	-100.3702	-7.35E-03	0.9988	528.1854	-0.4201	0.0000
CH3OH + 2H+ + 2e- = CH4 + H2O	C9	-22777.761	-3.2642	-0.0491	0.9998	-95.3477	-0.0137	-0.0002
CO32- + 10H+ + 8e- = CH4 + 3H2O	C10	-53532.1136	-95.1347	-0.1906	0.9999	-224.0854	-0.3982	-0.0008
CO32- + 6H+ + 4e- = CH2O + 2H2O	C11	-21683.8211	-50.6762	-0.1471	0.9999	-90.7685	-0.2121	-0.0006
CO32- + 8H+ + 6e- = CH3OH + 2H2O	C12	197588.961	-0.6827	-0.1204	0.9986	827.1074	-0.0029	-0.0005
CO32- + 3H+ + 2e- = HCOO- + H2O	C13	-13213.1388	-43.613	-0.10746	0.9999	-55.3102	-0.1826	-0.0004
Nitrogen								
N2 + 6H+ + 6e- = 2NH3	N1	-16395.0184	-28.7196	9.55E-03	0.9998	-68.6295	-0.1202	0.0000
N2 + 8H+ + 6e- = 2NH4+	N2	-41509.2762	-32.7202	0.0324	0.9996	-173.7578	-0.1370	0.0001
NO2- + 7H+ + 6e- = NH3 + 2H2O	N3	-111389.762	-24.6314	-0.1072	0.9999	-466.2775	-0.1031	-0.0004
NO3- + 2H+ + 2e- = NO2- + H2O	N4	-37615.91	-10.1959	-0.0169	0.9999	-157.4602	-0.0427	-0.0001
NO3- + 10H+ + 8e- = NH4+ + 3H2O	N5	-161590.028	-35.9487	-0.1181	0.9999	-676.4159	-0.1505	-0.0005
NO2- + 8H+ + 6e- = NH4+ + 2H2O	N6	-123974.113	-25.7531	-0.1011	0.9999	-518.9556	-0.1078	-0.0004
NO3- 6H+ + 5e- = 0.5N2 + 3H2O	N7	-140816.478	-20.2528	-0.1301	0.9999	-589.4578	-0.0848	-0.0005
2NO2- + 8H+ + 6e- = N2 + 4H2O	N8	-206401.155	-20.1139	-0.2264	0.9998	-863.9952	-0.0842	-0.0009
NO3- + 9H+ + 8e- = NH3 + 3H2O	N9	-149007.022	-35.1673	-0.1199	0.9999	-623.7434	-0.1472	-0.0005
Oxygen								
O2 + 4H+ + 4e- = 2H2O	O1	-113792.702	17.5605	-0.0416	0.9999	-476.3363	0.0735	-0.0002
Sulfur								
S + H+ + 2e- = HS-	S1	3107.4736	-10.5365	0.03688	0.9999	13.0079	-0.0441	0.0002
S + 2H+ +2e- = H2S	S2	-127020.088	-2.6852	-0.1192	0.9998	-531.7061	-0.0112	-0.0005
SO4-2 + 9H+ + 8e- = HS- + 4H2O	S3	-44105.4889	-71.3428	-0.1525	0.9999	-184.6256	-0.2986	-0.0006
SO4-2 + 10H+ + 8e- = H2S + 4H2O	S4	-53361.3532	-80.989	-0.2362	0.9999	-223.3706	-0.3390	-0.0010
HSO4- + 7H+ + 6e- = S + 4H2O	S5	-45083.4335	-38.7462	-0.1117	0.9999	-188.7193	-0.1622	-0.0005
SO4-2 + 8H+ + 6e- = S + 4H2O	S6	-47183.5454	-60.636	-0.1924	0.9999	-197.5103	-0.2538	-0.0008
SO2 + 4e- + 4H+ = S + 2H2O	S7	-41304.2847	-3.7158	0.0072	0.9991	-172.8997	-0.0156	0.0000
SO32- + 7H+ + 6e- = HS- + 3H2O	S8	-49176.8092	-66.8302	-0.1392	0.9999	-205.8541	-0.2798	-0.0006
2SO4-2 + 10H+ + 8e- = S2O3-2 + 5H2O	S9	-50416.0002	-79.053	-0.2149	0.9999	-211.0414	-0.3309	-0.0009
Hydrogen								
H+ + e- = 0.5H2	H1	387.1731	-15.3815	-4.99E-03	0.9999	1.6207	-0.0644	0.0000
Iron								
Fe2O3 + 6H+ + 6e- = 2Fe + 3H2O	F1	9142.5147	-41.3104	-0.0465	0.9999	38.2706	-0.1729	-0.0002
Fe2+ + 2e- = Fe	F2	22648.6398	-30.7865	-0.0188	0.9999	94.8072	-0.1289	-0.0001
Fe3+ + e- = Fe2+	F3	-16752.7104	-39.2684	-0.0344	0.9999	-70.1268	-0.1644	-0.0001
Fe3O4 + 8H+ + 8e- = 3Fe + 4H2O	F4	17107.4431	-50.4332	-0.0608	0.9999	71.6118	-0.2111	-0.0003
FeOOH + 3H+ + e- = Fe2+ + 2H2O	F5	-14875.6231	-86.2999	-0.0302	0.9999	-62.2694	-0.3613	-0.0001
Manganese								
MnO2 + 4H+ + 2e- = Mn2+ + 2H2O	M1	-58994.1105	64.9218	-0.2417	0.9168	-246.9493	0.2718	-0.0010
Mn3O4 + 8H+ + 2e- = 3Mn2+ + 4H2O	M2	-29541.3246	-7.0738	4.8045	0.9807	-123.6600	-0.0296	0.0201

DTN: MO9909SPAMING1.003

6.4.4.1.4 Model Specific Inputs

These include the following single-value items that are required to implement the conceptual model: temperature cutoff, humidity cutoff, tunnel diameter, tunnel length, porosity, and the energy cutoff.

6.4.4.2 Model Output

Output from MING is designed to define only the bulk system redox chemistry of the near-field system given the variable temperature and pH of the system, it does not reflect the actual chemical speciation or reactions that might occur at a more localized scale. The chemical output is designed to capture molar quantities of the production of byproducts (such as CO_2, H_2S, and H^+ ions) over one linear meter of repository drift. Output is also designed to enable the evaluation of the quantities of microbes produced, the limits to microbial growth from both nutrients and energy, and the stipulation of which nutrient is limiting growth in the repository.

MING V1.0 produces several output tables. The descriptions of these files are found in Section 1.4 of the MING V1.0 users manual (CRWMS M&O 1998d; pp. 36-40). The most used of these files are the "Time Output", "Reactions for Plot" and "Limiting Nutrients Tables". The time output table records a) the output year, b) the number of microbes that could be produced in the output year based on the available nutrient mass balance calculation, c) the total amount of free energy available in that year to create microbes, d) the number of microbes that could be produced in that year based on the available energy, and e) the actual number of microbes that are actually produced based on the lower value of items b and d above. For example, each test case reported in Table 36 (Section 6.6.2.2.1.2 below) is typical of any given year's output.

The reactions for plot table records the reactions that were used in each energy calculation, the ΔG that the particular reaction contributes to the total energy available, the pH of the incoming water, and the temperature at that timestep. Note: although the reactions are balanced, the code does not divide through the reaction to determine the smallest possible stoichiometric coefficients for each of the chemical species before generating the table.

Often, the terms "energy limited" or "nutrient limited" will be used to describe the conditions that limit microbial growth. Energy limited indicates that although there are sufficient nutrients available for growth, the redox conditions within the calculation constrain the amount of microbial growth that can happen. On the other hand, when something is termed nutrient limited, it means that there are not enough nutrients available to produce further microbial growth.

The limiting nutrients output table contains the starting and ending year in which a given nutrient (i.e. carbon, phosphorous, sulfur or nitrogen) is (or could limit if the results indicate that it is energy limiting) limiting microbial growth. In addition, the table may report whether the calculations are being limited by surpassing the thresholds for microbial activity of either RH (<90) or temperature (>120°C). These results may be reported either as a tabular result or in the written text depending on the complexity of the calculation. For most results presented below, the results are not reported in tabular form but can be verified by looking at the output table of interest.

Table 17. Atomic Masses for Each Element (Sargent-Welch 1979).

Element	Atomic Mass	Element	Atomic Mass	Element	Atomic Mass	Element	Atomic Mass	Element	Atomic Mass
Ar	40	Co	59	In	115	Pa	231	Sr	88
Ac	227	Cr	52	Ir	192	Pb	207	Ta	181
Ag	108	Cs	133	K	39	Pd	106	Tb	159
Al	27	Cu	64	Kr	84	Pm	145	Tc	98
Am	243	Dy	163	La	139	Po	209	Te	128
As	75	Es	252	Li	7	Pr	141	Th	232
At	210	Er	167	Lu	175	Pt	195	Ti	48
Au	197	Eu	152	Mg	24	Pu	244	Tl	204
B	11	F	19	Mn	55	Ra	226	Tm	169
Ba	137	Fe	56	Mo	96	Rb	85	U	238
Be	9	Fm	257	Md	258	Re	186	V	51
Bi	209	Fr	223	N	14	Rh	103	W	184
Bk	247	Ga	70	Na	23	Rn	222	Xe	131
Br	80	Gd	157	Nb	93	Ru	101	Y	89
C	12	Ge	73	Nd	144	S	32	Yb	173
Ca	40	H	1	Ne	20	Sb	122	Zn	65
Cd	112	He	4	Ni	59	Sc	45	Zr	91
Ce	140	Hf	178	Np	237	Se	79		
Cf	251	Hg	201	O	16	Si	28		
Cl	35	Ho	165	Os	190	Sm	150		
Cm	247	I	127	P	31	Sn	119		

6.5 MODEL INPUTS

Table 2 above documents the required inputs for TSPA-SR model calculations. Because there are four specific inputs (see Section 6.5.1 below) that were not finalized at the time of documentation, these parameters and the TSPA-SR calculations will need to be included in the next revision of this documentation.

6.5.1 Environmental Inputs

The values required for the environmental inputs are being generated by other modeling efforts for TSPA-SR and have not been finalized prior to the due date of this model. The values reported below are from TSPA-VA calculations MO9807MWDEQ3/6.005 and are only included for reference purposes.

6.5.1.1 Seepage or Infiltration

MING requires input for infiltration rate and/or seepage into the drift through time. The values being generated by other modeling efforts for TSPA-SR and have not been finalized prior to the due date of this model. Figure 5 below depicts the values used in the TSPA-VA calculations documented in MO9807MWDEQ3/6.005. The values but not the timing are also shown on Table 33 below. They are presented here in order to give the reader reference to the type of data used in MING V1.0. The values in Figure 5 are not to be used for TSPA-SR calculations. Prior to using this model for TSPA-SR calculations, the proper infiltration inputs need to be obtained and documented in the specific TSPA-SR calculations.

6.5.1.2 Thermohydrology

MING requires input for combined temperature, and RH values for the WP surface (or another relevant location in the drift) that correspond to the selected infiltration rate and/or seepage into the drift through time. The values being generated by other modeling efforts for TSPA-SR and have not been finalized prior to the due date of this model. Figure 5 below depicts the values used in the TSPA-VA calculations found in MO9807MWDEQ3/6.005. They are presented here in order to give the reader reference to the type of data used in MING V1.0. The values in Figure 5 are not to be used for TSPA-SR calculations. Prior to using this model for TSPA-SR calculations, the proper infiltration inputs need to be obtained and documented in the specific TSPA-SR calculations.

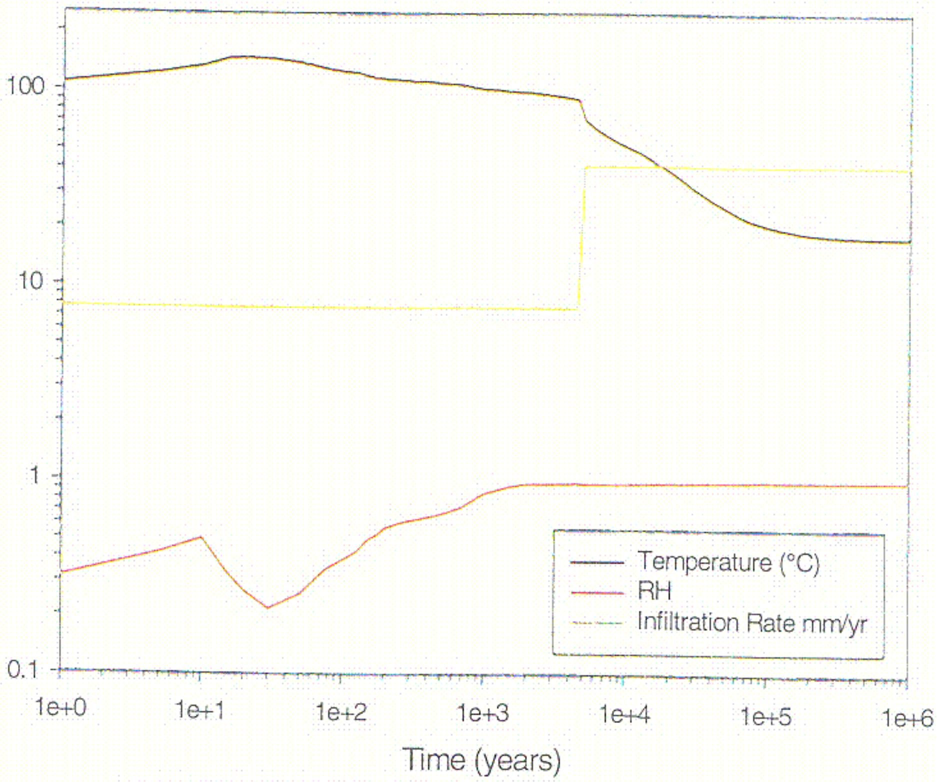
6.5.1.3 Incoming Water Compositions

MING requires input for time varying drift boundary groundwater compositions that correspond to combined temperature, and RH values for the WP surface (or another relevant location in the drift) and to the selected infiltration rate and/or seepage into the drift through time. The values being generated by other modeling efforts for TSPA-SR and have not been finalized prior to the due date of this model. Table 18 below depicts the values used in the TSPA-VA calculations documented in MO9807MWDEQ3/6.005. They are presented here in order to give the reader reference to the type of data used in MING V1.0. The values in Table 18 are not to be used for TSPA-SR calculations. Prior to using this model for TSPA-SR calculations, the proper infiltration inputs need to be obtained and documented in the specific TSPA-SR calculations.

Table 18. Water Compositions Entering the Drift used in MING TSPA-VA Calculations.

Groundwater Constituent ($kmol/m^3$)	**Period A (0-200yr)**	**Period B (200-2000yr)**	**Period C (1000-2000 yr)**	**Period D (2000-4000 yr)**	**Period E (4000-10000 yr)**	**Period F (10000-100000 yr)**
NO_3^-	1.42E-04	1.42E-04	1.42E-04	1.42E-04	1.42E-04	1.42E-04
SO_4^{2-}	1.92E-04	1.92E-04	1.92E-04	1.92E-04	1.92E-04	1.92E-04
Fe^{2+}	4.05E-17	3.29E-18	2.22E-18	1.72E-16	1.73E-16	2.15E-15
PO_4^{3-}	3.80E-06	3.80E-06	3.80E-06	3.80E-06	3.80E-06	3.80E-06
ΣCO_3^{2-}	5.02E-04	2.76E-09	1.23E-04	7.54E-05	1.44E-04	0.00
pH	9.72	10.2	10	8.94	8.2	8.12

DTN: MO9807MWDEQ3/6.005



DTN: MO9807MWDEQ3/6.005

Figure 5. Temperature, Relative Humidity, and Infiltration Rate Histories used in TSPA-VA MING Calculations.

6.5.1.4 In Drift Gas

MING requires input for time varying cumulative influx of O_2, N_2 and CO_2 (CH_4 if available) based on and corresponds with the repository temperature history derived from the thermohydrological calculations presented above. The values being generated by other modeling efforts for TSPA-SR and have not been finalized prior to the due date of this model. Figure 6 below depicts the values used in the TSPA-VA calculations documented MO9807MWDEQ3/6.005. They are presented here in order to give the reader reference to the type of data used in MING V1.0. The values in Figure 6 are not to be used for TSPA-SR calculations. Prior to using this model for TSPA-SR calculations, the proper infiltration inputs need to be obtained and documented in the specific TSPA-SR calculations.

6.5.2 Design Materials

6.5.2.1 Repository Design Materials

These inputs are documented in Attachment II below. Values include both the masses of proposed materials as well as the composition of those materials. These materials represent a synthesis of preliminary design inputs transmitted via AP-3.14Q transmittals as well as use of

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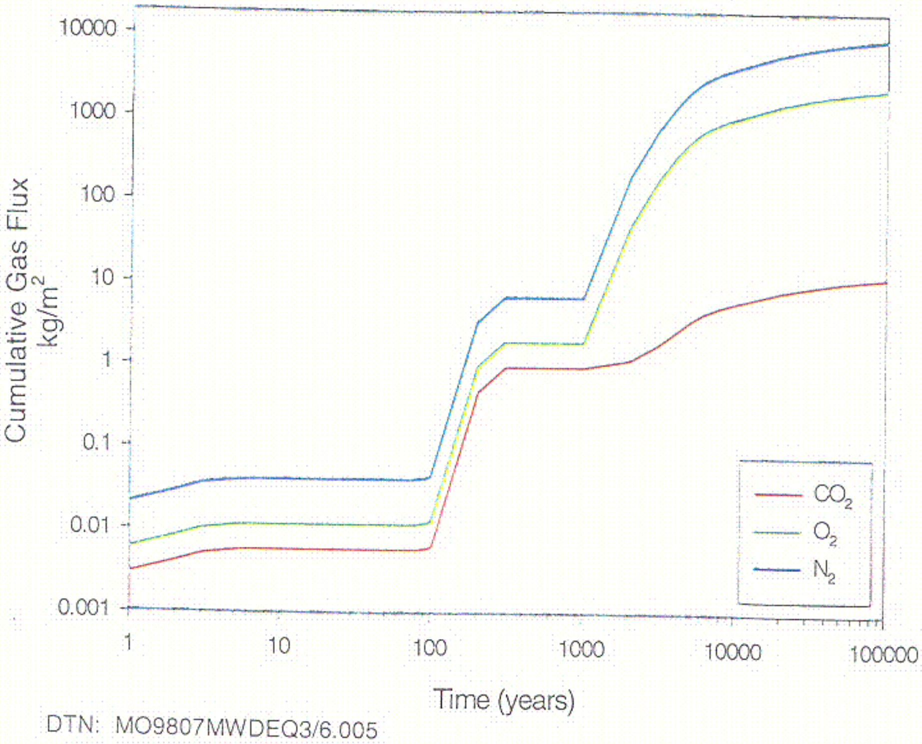
other qualified and unqualified input to generate the appropriate inputs. The input tables are reported in Attachment II, Sections II-5.1 and II-5.2.



DTN: MO9807MWDEQ3/6.005

Figure 6. The Cumulative Fluxes of CO_2, O_2, and N_2 into the Drift to 100,000 Years used in TSPA-VA MING Calculations.

6.5.2.2 Waste Package Design and Waste Form Materials

These inputs are documented in Attachments III and IV below. Values include both the masses of materials proposed materials as well as the composition of those materials. These materials represent a synthesis of preliminary design inputs transmitted via AP-3.14Q transmittals as well as use of other qualified and unqualified input to generate the appropriate inputs. The input tables are reported in Attachment III, Sections III-4.1, III-4.2, and Attachment IV, Section IV-5.

6.5.3 Model Specific Inputs

6.5.3.1 "Default Inputs"

Table 19 includes the user-elicited inputs that are required to make the modeling runs. These values are generally set as default parameters, but can be modified to run a specific sensitivity calculation. Table 19 not only reports the "default value" but also reports the source for the value selected. These values unless otherwise specified are used for all calculations within this report.

C3

In the MING code, there is an option to turn on or off the availability of gas as both a nutrient and as an energy source. This is done by selecting or deselecting the appropriate button(s) on the main form of MING where the inputs are entered. Due to the availability of gas in the repository (see Section 6.5.1.4 above) and the discussion on gas utilization by microbes as nutrients in Section 6.3.1.10 above, these buttons will be placed in the on position as the default input.

Table 19. Standard Default Input Parameters Used in MING Calculations.

Default MING Input Parameters	Value	Source
Temperature Cut off	120° C	See Section 6.3.1.3
Humidity Cut off	0.90	See Section 6.3.3.2.2
Tunnel Diameter	5.5 m	CRWMS M&O (1999m)
Tunnel length	1 m	Standard length of interest
MING V1.0 Near-Field Porosity	0	CRWMS M&O (1998h, p. 53)
Gas Buttons (N_2, CO_2, O_2)	On	See Section 6.3.1.10
Energy Cut Off	15 kJ/mol e^-	McKinley et al. (1997)

6.5.3.2 Reactant Compositions

Each repository or WP material modeled using MING has a given elemental composition, but that elemental composition has to be related to a given redox state and associated with the selected redox equations that represent the microbial metabolic pathways. Attachment V reports the derivation of the reactant composition values. These are reported on Table V-2 (Attachment V). These values represent the associated species for all of the materials that are documented in Section 6.5.2

6.5.3.3 Material Lifetime

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 28. The reference case values (median lifetimes) are thought to be a reasonable lifetime of the given material based on the calculations below.

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 largest minimal dimension of all the items of the given material. Information for these inputs were taken from the AP-3.14Q input transmittals (CRWMS M&O 1999d, 1999g, and 1999h) and from an accepted data source (AISC 1989).

Table 20. Selected Material Thickness of Repository Materials

Material	Item	Thickness (mm)	Source
Alloy 22	Waste package outer barrier	25	CRWMS M&O (1999h)
316NG	Waste package inner barrier	50	CRWMS M&O (1999h)
316L	Pallet tube	9.25	CRWMS M&O (1999k)
Ti Grade 7	Drip Shield plate	15	CRWMS M&O (1999l)
Neutronit A978	Basket plate	7	CRWMS M&O (1999h)
Aluminum 6061	Basket plate	5	CRWMS M&O (1999h)
A516 Carbon Steel	Basket guide	10	CRWMS M&O (1999h)
ASTM F432-95	Rock Bolts	28.5	CRWMS M&O (1999g)
Unspecified	Welded wire fabric	4.95	CRWMS M&O (1999d)
ASTM A572 Steel	Invert	23.8	CRWMS M&O (1999d) AISC (1989)
ASTM A759-85 Steel	Gantry Rail	74.6	CRWMS M&O (1999d) AISC (1989)
Unspecified	Rail Fittings (Anchor Clips)	19.05	CRWMS M&O (1999d)

Values for general corrosion of Ti grade 7 and Alloy 22 were taken from Figures 7 and 8. In this case, the minimum, median and maximum values correspond to the 5th, 50th and 95th percentiles. These are shown on Table 21. Material lifetimes are then determined by dividing the material thickness as shown on Table 20 by the rates shown in Tables 21. The results are found on Table 28.

Table 21. Minimum, Median and Maximum General Corrosion Rates for Alloy 22 and Ti Grade 7.

Percentile	Alloy 22 (mm/yr)	Ti Grade 7 (mm/yr)
5th	3.8e-6	5.3e-6
50th	2.9e-5	2.5e-5
95th	1.1e-4	2.6e-4

DTN: MO0003SPASUP02.003

Stainless Steel corrosion rates are presented in Table 22. The median was determined using the following equation taken from Journel (1989, Equation 20). This equation is used to determine the median of a log normal distribution.

$$Y_p Y_{p\text{-}1} = M^2 \qquad \text{(Eq. 7)}$$

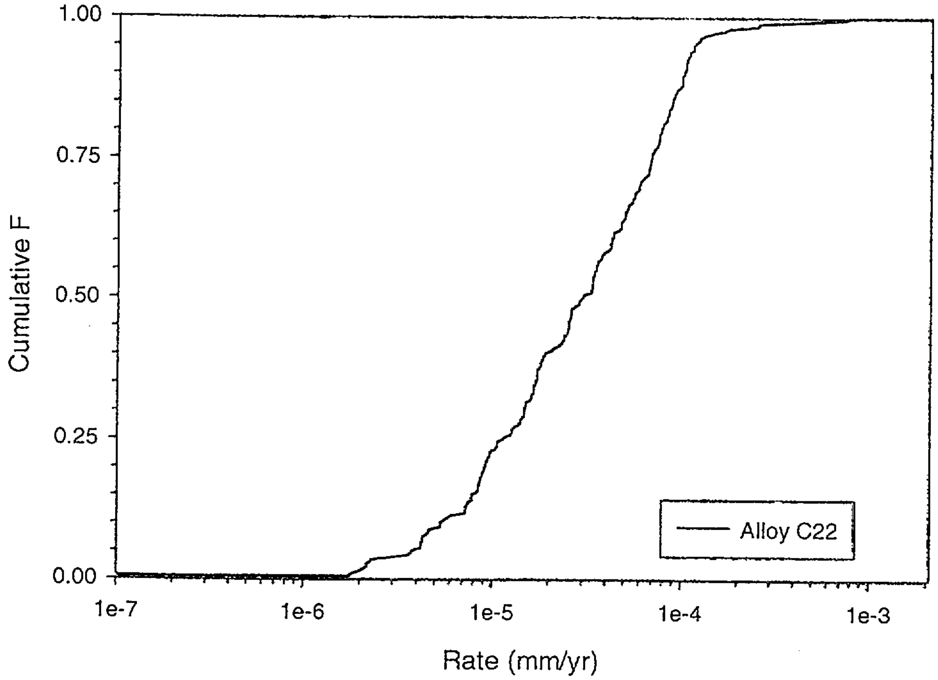
where:

Y_p = Lower bound
$Y_{p\text{-}1}$ = Upper bound
M = Median

Table 22. General Aqueous Corrosion Rates for 316L Stainless Steel.

Material	Lower Bound (mm/yr)	Upper Bound (mm/yr)	Median (mm/yr)
316L	8.79×10^{-5}	4.55×10^{-2}	2.0×10^{-3}

DTN: MO9911SPAWAP05.010

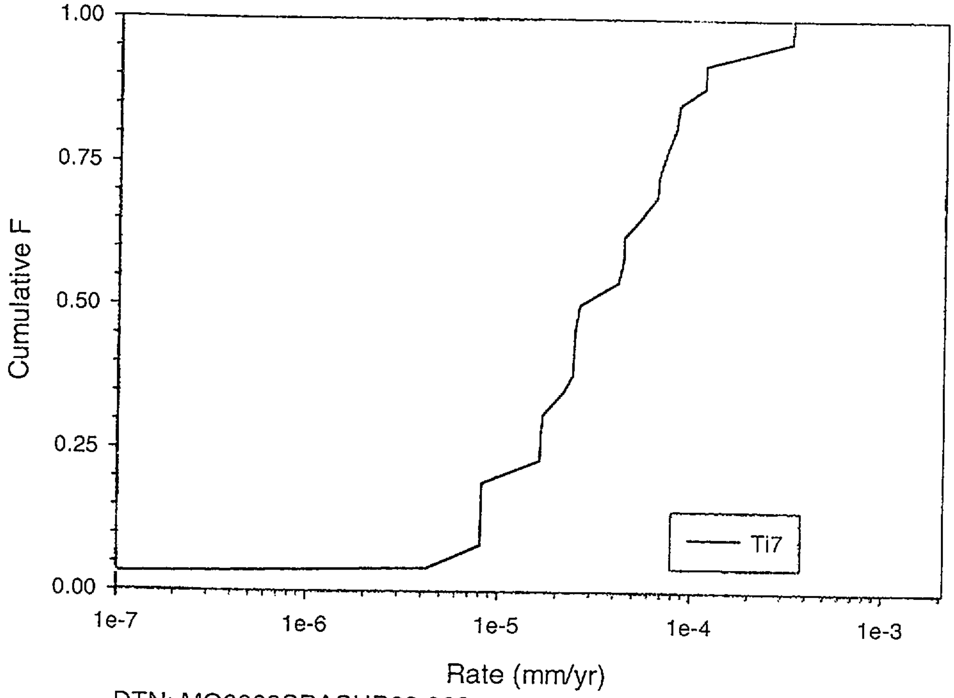


DTN: MO0003SPASUP02.003

Figure 7. Cumulative CDF for General Corrosion of Alloy 22.

Material lifetimes for 316L and 316NG are then determined by dividing the material thickness as shown on Table 20 by the rates from Table 22. The results are found on Table 28. These same results were then applied to 304L stainless steel (see Assumption 5.3) using the thickness of the canister wall as reported on Table 23.

Material lifetimes for DHLW glass are derived by taking the values from Table 23, determining the inner diameter [$2r = 6.1$ m - 2(0.0095 m) = 0.591 m], then calculating the surface area of the glass waste (area=$2\pi rh$) in a 1 meter length of pour canister. This value is obtained by multiplying the surface area by the number of pour canisters (5) per waste package to get the total surface area (9.28 m^2). The total surface area is then modified by a factor of 30 to account for the fracturing of glass during cooling (see Assumption 5.7). This results in a total surface area of 278.50 m^2. The surface area is multiplied by the dissolution rate shown on Table 24 to obtain the number of grams per day. This value is then multiplied by 0.365 to convert g/day to kilograms per year as shown on Table 24. The mass of glass per meter of waste package found on Table IV-6 is divided by the rate to determine the material lifetime. These values are shown on Table 28.



DTN: MO0003SPASUP02.003

Figure 8. Cumulative CDF for General Corrosion of Titanium Grade 7.

Table 23. 304L Stainless Steel Pour Canister Properties From Savanna River HLW.
(Values taken from Table 3.1.1, DOE 1992
as Directed by CRWMS M&O 1999h)

Parameter	Value
Outside Diameter of HLW pour canister	0.61 m
Canister wall thickness	0.95 cm

DTN: MO9912SPADRW90.007

Table 24. Aqueous Dissolution Rates for HLW Glass.

Rate (g/m^2day)	Rate (kg/year)
1.00E-04	1.02E-02
3.00E-02	3.05E+00
3.00E-03	3.05E-01

DTN: SN9911T0811199.003

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 25. These rates are applied to the following materials: ASTM A572 Steel, ASTM A759-85 Steel, ASTM F432-95 Steel, C Steel ASTM A516, WWF Steel, and Rail Fittings. These rates will be divided by the average thickness of the material as shown on Table 20 and the results will be provided on Table 28.

Table 25. 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

For Neutronit A978 there are no documented corrosion rates available. However, a corrosion rate has been determined and documented for two similar materials, Bohler A976 SD and Nutrosorb Plus. These materials are both borated stainless steels. (Van Konynenburg, 1998). The single value is for Bohler A976 SD was used (see Assumption 5.8). The minimum and maximum values shown below were derived by taking an ±1 order of magnitude on the single (median) value. These values are shown on Table 26. The material thickness from Table 20 are then divided by these rates and added to Table 28 below.

Table 26. Surrogate General Aqueous Corrosion Rates for Neutronit A978 Borated Steel.

Material	**Median (mm/yr)**	**Lower Bound (mm/yr)**	**Upper Bound (mm/yr)**
Neutronit A978 (Bohler A976 SD)	0.04	0.004	0.4

DTN: LL980504105924.034

For Aluminum 6061, accepted data values for 10 and 20 year atmospheric corrosion rates on various types of aluminum have been reported in American Society for Metals (1987, p. 601, Table 11). The median rate was determined by taking the average for the reported 10-year rates. The high rate was determined by taking the aggressive values for alloy 6061 from American Society for Metals (1987, Table 8). The low value was taken from the 20-year desert atmosphere rate (American Society for Metals 1987, p. 601, Table 11). These values are shown on Table 27. The material thickness from Table 20 are then divided by these rates and added to Table 28 below.

Table 27. General Aqueous Corrosion Rates for Aluminum 6061.

Material	Median Rate (μm/yr)	Low Rate (μm/yr)	High Rate (μm/yr)
Aluminum 6061	0.35	0.076	422

For CSNF, calculations have shown that aqueous dissolution of spent fuel can occur in 500 years or less (CRWMS M&O 1998a, Figure 4-57). In order to account for some range due to the potential for humid air corrosion, five fold increases to the minimum and median lifetimes will also be included. These values are shown on Table 28.

For Superplasticizer, Type K Cement and Silica Fume an assumption was made (see Assumption 5.4) for the median lifetimes shown, as no other information is known at this time. Minimum and maximum lifetimes are assumed to be a factor of 5 less and greater, respectively, than the median lifetime.

For the commo cable, no rates are available so the lifetimes are assumed so as to span the probable lifetime of the material (see Assumption 5.10).

Table 28. Minimum, Median and Maximum Material Lifetimes (years) used in the MING Calculations.

Material Name	Minimum Lifetime	Median Lifetime	Maximum Lifetime
304L Stainless Steel	208	4750	108077
316L Stainless Steel	203	4625	105233
316NG Stainless Steel	1099	25000	568828
Alloy C-22	227272	862068	6578947
Aluminum 6061	11.8	14286	65789
ASTM A572 Steel	250	401	1013
ASTM A759-85 Steel	782	1255	3174
ASTM F432-95 Steel	299	480	1213
C Steel ASTM A516	105	168	426
Commo Cable	100	1000	10000
CSNF Waste	500	2500	12500
DHLW Waste	718	7180	214705
Neutronit A978	17.5	175	1750
Rail Fittings	200	321	811
Silica Fume	2500	10000	50000
Superplasticizer	2500	10000	50000
Ti Grade 7	57692	600000	2830189
Type K Cement	2500	10000	50000
WWF Steel	52	83	211

6.5.3.4 Breakdown Codes

Some materials used in the design evaluated below contain complex organic compounds that are known to be resistant to biodegradation (i.e., superplasticizer admixtures in the grout formulation) as well as composite materials which contain organics, that are made up of more than one substance (i.e., communications cable). These materials cannot be directly broken down into their basic elemental compositions and fed into the nutrient and energy stream. MING allows for a special reactant flag that allows for partial breakdown and/or multiple reactant compositions (see Section 6.4.3). The input used below (Table 29) was previously documented in CRWMS M&O (1998e).

Table 29. Reactant Compositions, Breakdown Codes and Molecular Masses for the Release of Organic Materials.

Reactant Composition	Breakdown Code	Molecular Mass
Superplasticizer		
CH_2O	0.96	1990.9
SO_3^{2-}	1	
Wire Conductor		
CH_2O	8.53	3264.5
CH_3OH	0.02	
Commo Cable		
CH_2O	3.95	174.8

DTN: MO9909SPAMING.002

6.5.3.5 Material Layer Designators

Until the drip shield and waste package outer barrier materials are penetrated, internal WP materials are not expected to be affected by microbial activity. This is primarily due to the lack of water availability. In order to account for the absence of water in waste packages, the values for the layer flag (see Section 6.4.3) in MING need to be entered to allow the sequential degradation of the materials in question. Table 30 provides input values for the case where there is no corrosion of the waste package internals until drip shield and outer barrier materials are breached (no drip case) and for the case where the drip shield does not divert the water from the waste package surface (drip case). Other values may be selected on a case by case basis to look at various issues that may arise. Note: the lower the layer number the sooner the material degrades.

Table 30. Material Layer Designators Used in MING V1.0 for the Sequential Degradation of Waste Package and Repository Materials.

Material Name	Drip Case Layer	No Drip Case Layer	Material Name	Drip Case Layer	No Drip Case Layer
304L Stainless Steel	1	2	CSNF Waste	1	2
316L Stainless Steel	0	1	DHLW Waste	1	2
316NG Stainless Steel	1	2	Neutronit A978	1	2
Alloy C-22	0	1	Rail Fittings	0	0
Aluminum 6061	1	2	Silica Fume	0	0
ASTM A572 Steel	0	0	Superplasticizer	0	0
ASTM A759-85 Steel	0	0	Ti Grade 7	0	0
ASTM F432-95 Steel	0	0	Type K Cement	0	0
C Steel ASTM A516	1	2	WWF Steel	0	0
Commo Cable	0	0			

6.6 MODEL VALIDATION TEST CASES

The analyses presented below represent model validation tests designed to insure that the conceptual model, software and inputs can be used to assess the microbial growth that may occur within a potential repository at Yucca Mountain. This will allow evaluation of whether or not microbes should be an issue within the overall bulk geochemistry affecting the water composition within the drift, or if the microbial aspects of the system should be treated further only as they affect localized chemical conditions.

Presented below are three different test sets. The first represents our duplication of the results in the Swiss repository program (see Section 6.6.1). The second set of tests represent a depiction of ambient conditions found in the ESF and at Rainier Mesa (a natural analog) are shown in Section 6.6.2 and the third test set represents the duplication of independent lab experiments conducted at LLNL (Horn et al. 1998a and 1998b; Davis et al. 1998) and are shown in Section 6.6.3.

Our presentation of the Swiss case (Section 6.6.1) demonstrates that MING V1.0 code functions adequately when compared to previous modeling activities using the same type of conceptual model and software code. The ambient tests (Section 6.6.2) demonstrate that the selection of redox equations (Table 16) and how we handle the elemental breakdown of materials (Table V-2) are adequate to produce results that are reasonable when compared to the actual measured system at Yucca Mountain. Finally, duplication of the LLNL lab experiments (Section 6.6.3) will give us a feeling of how much uncertainty can be associated with the modeled results.

6.6.1 Swiss Low-Level Test Case

To build confidence that MING was incorporating the portions of the Swiss LLW/ILW model correctly (Grogan and McKinley 1990, Capon and Grogan 1991), we ran MING using the Swiss model input parameters. Both Grogan and McKinley (1990), and Capon and Grogan (1991) can be used as the source of parameter inputs. For detailed information on how the Swiss model parameter inputs were incorporated into a MING calculation, refer to CRWMS M&O (1998h).

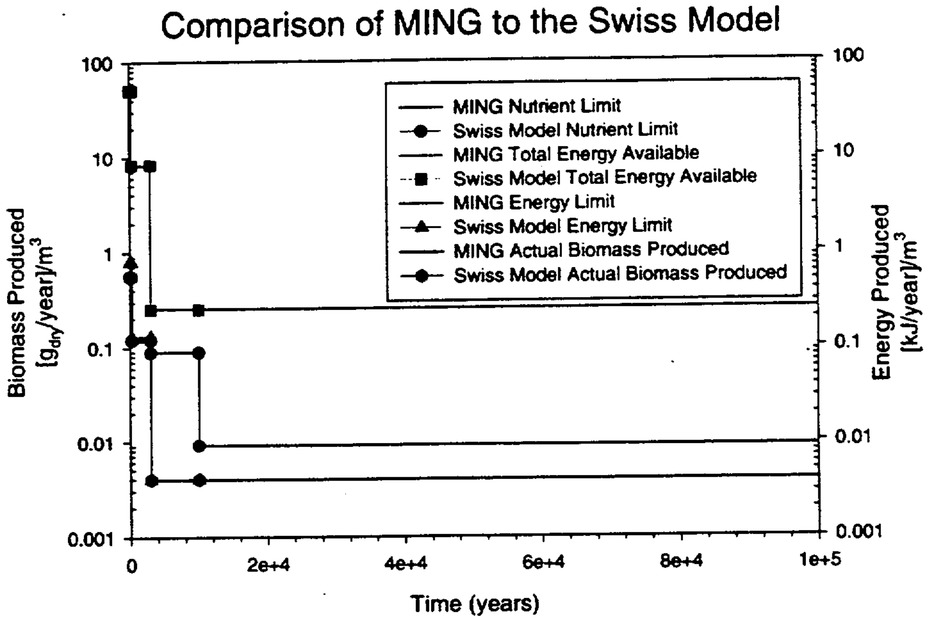
Before results of the benchmark calculation are presented below, two model differences should be spelled out that cause our results to differ very slightly from those reported in Grogan and McKinley (1990) and Capon and Grogan (1991). First, MING does not divide the Swiss calculation into an oxic and an anoxic phase. Therefore, the initial oxygen conditions are not reported in our results. The Swiss model limited this period to the time required to consume the oxygen, which was introduced into a normally anoxic environment due to construction. If we were to incorporate the early oxic phase, the results would be limited to the first year of the calculations, and would not show up in a significant way on our results plots. Second, MING does not incorporate radiolytic products that are generated within the WP. Early on during MING model development, a decision was made not to incorporate this type of effect as there is little evidence that it would be of concern in a Yucca Mountain repository. This was based on the assessment that radiolysis outside WP should be negligible for the given design thickness (Van Konynenburg 1996; see Section 6.3.1.4 above).

The results indicate that the portions of the nutrient and energy models used in the Swiss model and which are used in MING are operating correctly. Figure 9 shows a result comparison for both the energy and nutrient calculations reported by Capon and Grogan (1991) with those calculated with MING. From Figure 9, it can be seen that the results are virtually identical. However, examination of a table of results (Table 31) indicates that there is a slight difference in the energy calculations during the 271- to 3,030-year period. The difference is attributed to not incorporating into MING the radiolytic products produced in the Swiss repository. This indicates that not incorporating those radiolytic effects for the Swiss case resulted in only very minor changes to the results.

Table 31. Comparison of the Swiss Model Results Using EMMA with that of the Same Swiss Model Parameters Used in MING.

Time Period (a)	Maximum Energy (kJ/a)		Maximum Biomass (g/a)	
	EMMA	MING	EMMA	MING
0-270	50.6	50.6	0.79	0.791
271-3,030	8.3	8.14	0.13	0.127
3,031-10,000	2.5E-01	2.53E-01	4.0E-03	3.97E-03
10,001+	2.5E-01	2.53E-01	4.0E-03	3.97E-03

DTN: MO9911SPAEMMA0.007



DTN: MO9911SPAEMMA0.007

Figure 9. Comparison of Swiss Model Results (Capon and Grogan 1991) with MING Calculations of the Swiss Model.

6.6.2 Ambient ESF and Natural Analog Test Cases

To compare the modeled results of the ambient system in MING with the measurements presented in Section 6.3.2, the ambient populations have to be converted to the equivalent unit of measurement that is reported by MING. Table I-9 reports the grams (dry wt) of microbes in a one-meter length segment of TSw2 tuff having a repository drift radius of 2.55 m. Documentation of this calculation is found in Attachment I. Therefore, based on the ESF measurements, the mass of microbes in one linear meter of repository drift ranges between 0.12 to 1.34 grams (dry). If we were to do an equivalent calculation for low and high values for the Rainier Mesa natural analog site (see assumption 5.6), the value would be as low as 0.36 to 1.81 grams (dry) per linear meter of repository drift.

6.6.2.1 General Ambient Test Case Inputs

Eighteen ambient calculations were done using MING to build confidence in the model and to bound the overall way that MING handles nutrient and energy calculations. The general intent of these calculations is to show that MING gives a reasonable answer. Then we can assume that it would provide estimates that are at least in the order-of-magnitude range for the potential microbial abundance in the near field. These sorts of estimates form the starting point for evaluating which pieces of the system microbial-driven chemistry could have some capacity to influence in drift geochemistry. Three separate test case sets were developed, each dependant on the nutrient and energy sources that were likely to be encountered: biotite, altered tuff and unaltered tuff.

In all 18 ambient case calculations the following input parameters were utilized: the average composition of J-13 water (Table 32); an average cumulative influx of O_2, N_2 and CO_2 (Table 34) ; a repository temperature of 25°C; and a RH of 0.99. The average J-13 water chemistry values were taken from Harrar et al. (1990). These values are found on Table 32. Also included with the J-13 water composition was the addition of 1 ppm dissolved organic carbon ([DOC]; converted to the appropriate units and represented as CH_2O in our simplified redox model; see Table V-2) which seems to be the approximate value for DOC in the groundwater at Yucca Mountain (CRWMS M&O 1997b).

Table 32. J-13 Water Compositions
Used in MING Calculations.

Groundwater Constituent	Concentration (kmol/m^3)
Na^+	1.99E-03
Si	1.02E-03
Ca^{2+}	3.25E-04
K^+	1.28E-04
Mg^{2+}	8.38E-05
Li^+	6.90E-06
HCO_3^-	2.12E-03
O_2	1.75E-04
F^-	1.15E-04
Cl^-	2.03E-04
NO_3^-	1.42E-04
SO_4^{2-}	1.92E-04
B	1.22E-05
Al	1.80E-06
Mn^{2+}	8.00E-07
Fe^{2+}	5.80E-07
Sr^{2+}	6.00E-07
PO_4^{3-}	3.80E-06
DOC	3.30E-05
pH	7.4

DTN: MO9909SPA00J13.006

Each of the three test case sets differed by altering two inputs that were thought to be the biggest factors to natural microbial variability. They are the water infiltration rate and the material lifetime of the rock.

Due to cyclic climatic change, the water infiltration rate at the surface of Yucca Mountain is thought to fluctuate. Therefore, two cases were used to look at the variability that infiltration has on the ambient system. The values selected were identical to the values used in TSPA-VA calculations (CRWMS M&O 1998a) as shown on Table 33.

In addition to the infiltration rate, the material lifetime for the alteration of the repository host rock seems to be the most uncertain parameter. Because this rate can provide different quantities of nutrients and energy, this parameter was varied.

Each of the three test cases below were run using the matrix of infiltration rates and material lifetimes as shown on Table 33.

Table 33. Infiltration Rates and Material Lifetimes used in TSPA-VA Ambient Test Cases (see Assumption 5.5).

Test Case	Material Lifetime (years)	Infiltration Rate (mm/yr)
1	10,000,000	7.8
2	1,000,000	7.8
3	100,000	7.8
4	10,000,000	42.06
5	1,000,000	42.06
6	100,000	42.06

DTN: MO9807MWDEQ3/6.005

Cumulative gas flux into the drift values used in the TSPA-VA ambient test cases (CRWMS M&O 1998a) were also used and are shown on Table 34 below.

Table 34. Cumulative Gas Flux Values (kg/m^2) used in the Ambient Test Case Calculations.

Year	CO_2	O_2	N_2	CH_4
1	2.00E-5	4.64E-3	1.85E-2	0
50	1.00E-3	2.32E-1	9.25E-1	0
200	4.00E-3	9.28E-1	3.70E-0	0
3,000	6.00E-2	1.39E+1	5.55E+1	0
5,000	1.00E-1	2.32E+1	9.25E+1	0
27,560	5.55E-1	1.27E+2	5.10E+2	0
28,000	5.60E-1	1.30E+2	5.17E+2	0
50,000	1.00E-0	2.32E+2	9.25E+2	0
100,001	2.00E-0	4.64E+2	1.85E+3	0
1,000,000	2.00E+1	4.64E+3	1.85E+4	0

DTN: MO9911SPACGF04.000

6.6.2.2 Ambient Case Calculations

These analyses are presented in terms of the resultant growth of microbial mass. The mass of microbes that could be produced based on the limiting nutrient or the energy limitations of the system are given in the figures and tables shown below.

6.6.2.2.1 Biotite as Energy Source Test Cases

The first test case set uses the long-term release rate of Fe^{2+} from biotite dissolution (see assumption 5.5). The determination of the maximum mass of biotite that could be potentially found within a 1-meter repository drift volume (460 kg/m) and the available quantity (wt. percent) of Fe that could be released from that amount of biotite (32.7 percent) are documented in Attachment I and are used in these calculations.

In order to utilize biotite as well as the altered and unaltered tuff in the model the biotite parameters from Table 35 need to be entered into MING. These parameters are based on the same premise used to develop the layer designators and reactant compositions found on Table 30 and Table V-2 respectively, as discussed in Sections 6.4.3.1.3 and 6.5.

Table 35. Reactant Compositions and Layer Designator for Biotite (Table I-7, Attachment I), Altered, and Unaltered Tuff (Table 13).

Material Name	Reactant Compositions	Layer Designator
Altered tuff	Fe, Mn^{2+}	0
Unaltered tuff	Fe, Mn^{2+}	0
Biotite	Fe^{2+}	0

6.6.2.2.1.1 Test Specific Conditions

Case 1: This calculation was run in MING using a material lifetime on the biotite (Table I-7) of 10,000,000 years and an infiltration rate of 7.8 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 2: This calculation was run in MING using a material lifetime on the biotite (Table I-7) of 1,000,000 years and an infiltration rate of 7.8 mm/ Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 3: This calculation was run in MING using a material lifetime on the biotite (Table I-7) of 100,000 years and an infiltration rate of 7.8 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 4: This calculation was run in MING using a material lifetime on the biotite (Table I-7) of 10,000,000 years and an infiltration rate of 42.06 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 5: This calculation was run in MING using a material lifetime on the biotite (Table I-7) of 1,000,000 years and an infiltration rate of 42.06 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 6: This calculation was run in MING using a material lifetime on the biotite (Table I-7) of 100,000 years and an infiltration rate of 42.06 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

6.6.2.2.1.2 Test Results

Table 36 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. However, the system is limited by phosphorous.

Table 36. Results from MING for Biotite Test Cases 1 to 6.

Test Case	Mass of microbes from available nutrients (g dry)	Energy available in system (kJ mol^{-1})	Mass of microbes from available energy (g dry)	Calculated Mass of microbes (g dry)
1	0.3018745	0.1036498	0.001619529	0.001619529
2	0.3018745	0.8705462	0.01360228	0.01360228
3	0.3018745	8.53951	0.1334298	0.1334298
4	1.6278	0.1846402	0.002885003	0.002885003
5	1.6278	0.9515365	0.01486776	0.01486776
6	1.6278	8.6205	0.1346953	0.1346953

6.6.2.2.2 Altered Tuff Test Cases

6.6.2.2.2.1 Test Specific Conditions

Case 1: This calculation was run in MING using a altered tuff material lifetime (Table 13) of 10,000,000 years and an infiltration rate of 7.8 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 2: This calculation was run in MING using an altered tuff material lifetime (Table 13) of 1,000,000 years and an infiltration rate of 7.8 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 3: This calculation was run in MING using an altered tuff material lifetime (Table 13) of 100,000 years and an infiltration rate of 7.8 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 4: This calculation was run in MING using an altered tuff material lifetime (Table 13) of 10,000,000 years and an infiltration rate of 42.06 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 5: This calculation was run in MING using an altered tuff material lifetime (Table 13) of 1,000,000 years and an infiltration rate of 42.06 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 6: This calculation was run in MING using an altered tuff material lifetime (Table 13) of 100,000 years and an infiltration rate of 42.06 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

6.6.2.2.2.2 Test Results

Table 37 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. However, the system is limited by phosphorous.

Table 37. Results from MING for Altered Tuff Test Cases 1 to 6.

Test Case	Mass of microbes from available nutrients (g dry)	Energy available in system (kJ mol^{-1})	Mass of microbes from available energy (g dry)	Calculated Mass of microbes (g dry)
1	0.3569763	0.7591901	0.01186235	0.01186235
2	0.8528919	7.44353	0.1163052	0.1163052
3	2.28205	101.9634	1.593177	1.593177
4	1.682902	0.8316002	0.01299375	0.01299375
5	2.178818	7.51594	0.1174366	0.1174366
6	7.137974	74.35934	1.161865	1.161865

6.6.2.2.3 Unaltered Tuff Test Cases

6.6.2.2.3.1 Test Specific Conditions

Case 1: This calculation was run in MING using an unaltered tuff material lifetime (Table 13) of 10,000,000 years and an infiltration rate of 7.8 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 2: This calculation was run in MING using an unaltered tuff material lifetime (Table 13) of 1,000,000 years and an infiltration rate of 7.8 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 3: This calculation was run in MING using an unaltered tuff material lifetime (Table 13) of 100,000 years and an infiltration rate of 7.8 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 4: This calculation was run in MING using an unaltered tuff material lifetime (Table 13) of 10,000,000 years and an infiltration rate of 42.06 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 5: This calculation was run in MING using an unaltered tuff material lifetime (Table 13) of 1,000,000 years and an infiltration rate of 42.06 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

Case 6: This calculation was run in MING using an unaltered tuff material lifetime (Table 13) of 100,000 years and an infiltration rate of 42.06 mm/yr from Table 33, the gas compositions found on Table 34, and J-13 water (Table 32).

6.6.2.2.2.3 Test Results

Table 38 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. However, the system is limited by phosphorous.

Table 38. Results from MING for Unaltered Tuff Test Cases 1 to 6.

Test Case	Mass of microbes from available nutrients (g dry)	Energy available in system (kJ mol^{-1})	Mass of microbes from available energy (g dry)	Calculated Mass of microbes (g dry)
1	0.3294254	0.5592371	0.008738079	0.008738079
2	0.5773832	5.444	0.0850625	0.0850625
3	2.28205	74.50928	1.164207	1.164207
4	1.655351	0.6316471	0.009869485	0.009869485
5	1.903309	5.51641	0.0861939	0.0861939
6	4.382887	54.36403	0.849438	0.849438

6.6.2.2.4 Ambient Case Results

Figure 10 compares the results provided in the three test cases above with the actual measurements taken at Rainer Mesa and in the ESF. They show that all of the measurements are within an order of magnitude and seem reasonable in comparison to the inputs.

Two factors may affect the variability of the results. First there could be some sort of nutrient contamination (not accounted for before sampling) or enhanced growth that allowed the measured ESF and Rainer Mesa tunnel values to be elevated because the sampling took place well after the tunnels were constructed (Kieft et al. 1993, Haldeman and Amy 1993). Second, our model is simplified, and therefore, we may not have included a measurable quantity of an energy-providing nutrient, especially in the Rainier Mesa tests, because TSw2 tuff and J-13 water serve as approximations to the composition of *in situ* materials (see assumption 5.6).

Even with the above factors in mind, the ambient case results seem to indicate that we are modeling the ambient system adequately. The results also indicate the dependence of groundwater composition and flux on microbial growth, especially since the ESF experiments indicate that water is the limiting nutrient in the ambient system (Kieft et al. 1997).

To some extent, the modeling results also indicate that the composition and material lifetime of the altered and unaltered tuff can also play a role in the abundance of microbes. Phosphorous is less abundant in the unaltered tuff and its availability is generally limited to the concentrations found in the tuff. This point is also discussed in the Lawrence Livermore National Laboratory (LLNL) experiments modeled in Section 6.6.3 below. Therefore, the ambient case allows us to have increased confidence that MING can produce reasonable modeling results for the repository system.

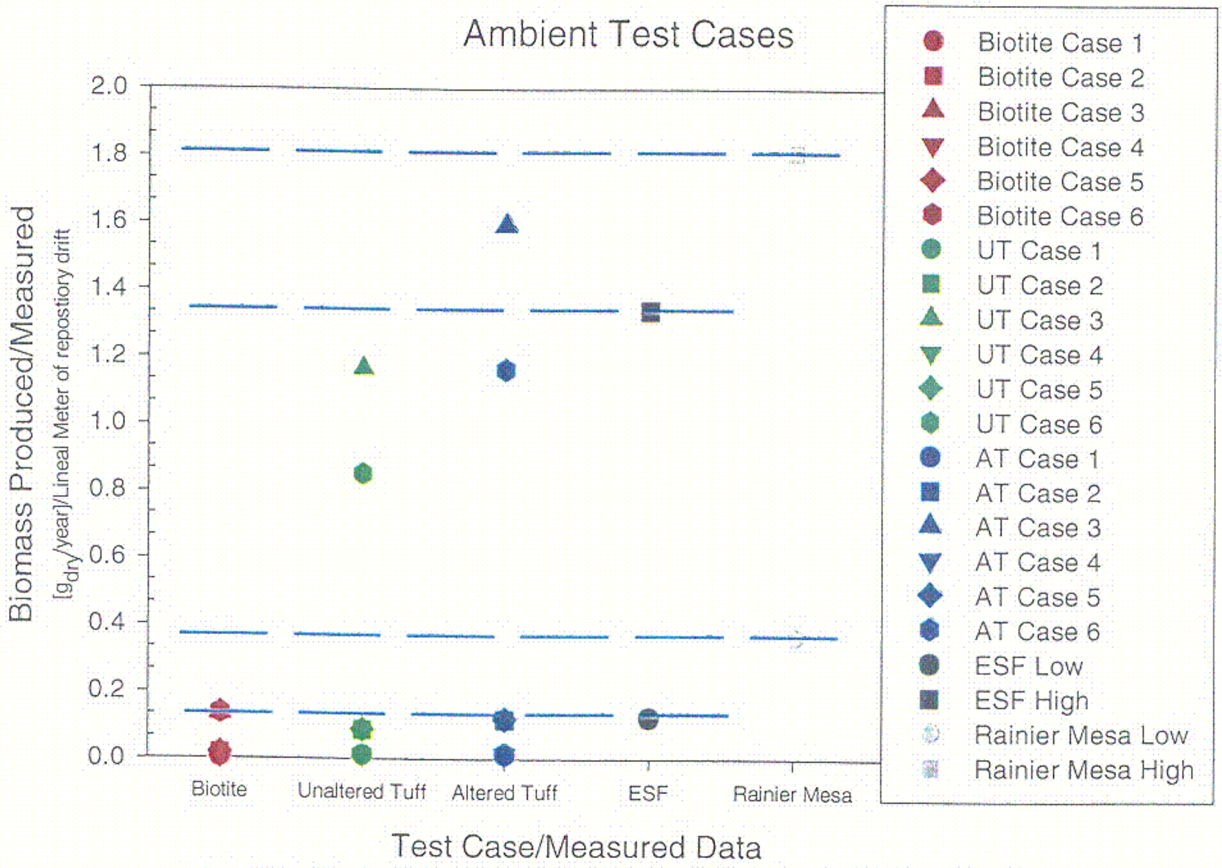


Figure 10. Comparison of Modeled Results to Ambient Measurements. ESF and Rainier Mesa Low and High Values are Taken from Table I-9.

6.6.3 LLNL *In Situ* Limiting Nutrient Experiment Test Cases

Experiments conducted at LLNL to determine limiting nutrients to microbial growth in the YMP environment and to give bounds on MIC on waste packages are utilized in this model to assist in model validation. These experiments were conducted independent of model development and are intended to be a "blind test" on the results of the simulated tests calculated from MING V1.0. A description of these results are reported in Horn et al. (1998a and 1998b) and Davis et al. (1998). Positive test results using this "blind testing" method should determine to what "level of certainty" this model is valid.

C4

6.6.3.1 Experimental Description

The experiments reported in Horn et al. (1998a and 1998b) and Davis et al. (1998) utilize several different growth media to grow microbes (see Table 39). Each of these media was selected to determine the limiting nutrients in the host rock at YM. Each media shown on Table 40 below was specifically selected to enable the determination of limiting nutrients in the repository environment. The reader is referred to Horn et al. (1998a and 1998b) and Davis et al. (1998) for more detailed descriptions of the experiments.

Each of these media was placed in a flask in addition to a known quantity of Topopah Spring tuff (see Table 13) and was cultured for approximately seven days to determine the optimum growth rates. Growth rates were determined by taking samples of the media and periodically subjecting them to live plating.

Two different types of tests were conducted. First, a set of microcosm experiments where the crushed tuff was exposed to a continuous feed of growth media and second, a set of batch experiments where the crushed tuff was exposed to a single aliquot of growth media. The experiments that best fit the setup of MING V1.0 to model are the batch experiments as they use easily duplicated conditions. Table 39 reports the specifics of the batch experiments that are required by MING to duplicate the batch tests. The results of the growth tests for both the batch and microcosm tests are shown below in Figures 11 and 12 respectively.

Table 39. Details of LLNL Batch Experiments used as Inputs to MING V1.0 (Horn et al. 1998a).

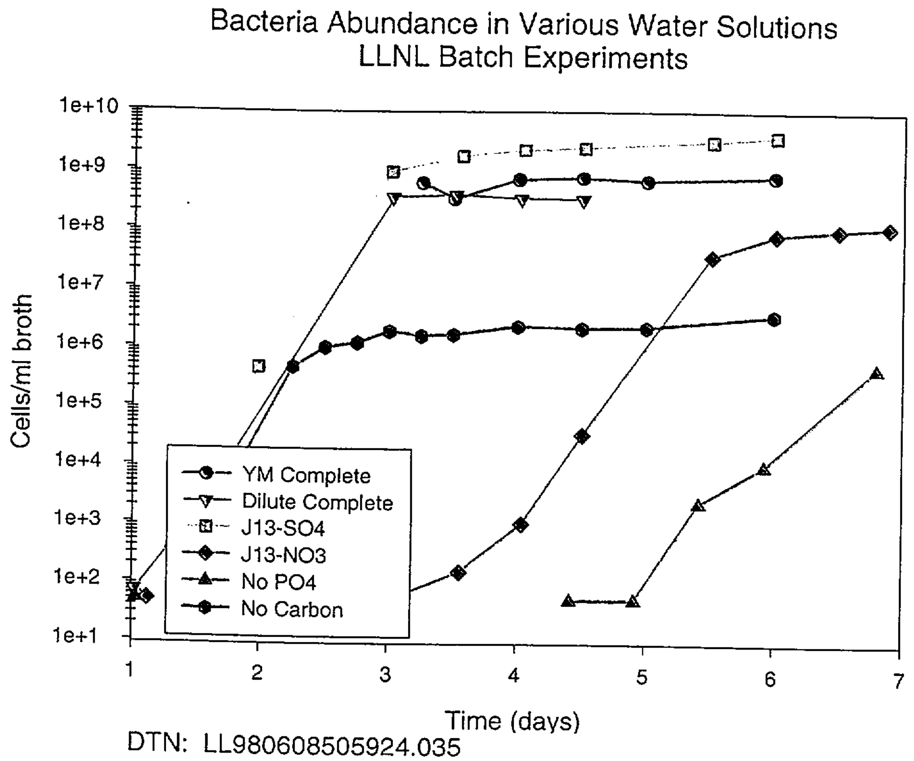
Input Item	Value
Flask Volume	125 ml
pH of Growth Media	7.2
Mass of Crushed Tuff	5 g
Temperature	30°C
Volume of Growth Media	20 ml

DTN: LL000206105924.126

Table 40. Growth Media Compositions (mmol) from the LLNL Lab Experiments.

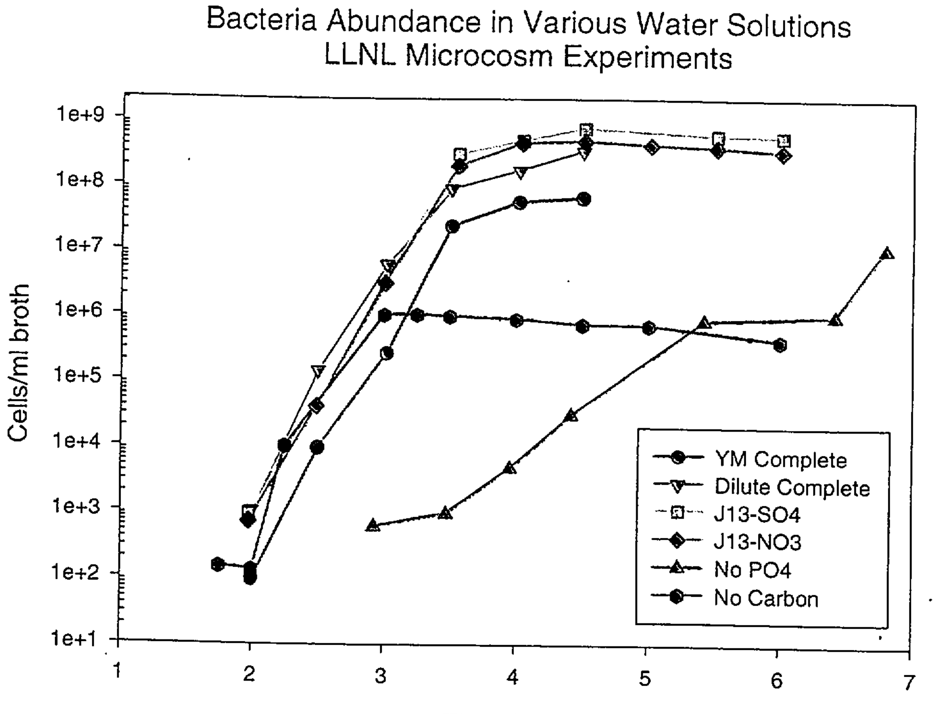
Component	YM complete	Dilute Complete	J13-NO3	J13-SO4	Phosphate deficient	Carbon deficient
NH_4^+	3.75E-03	3.80E-04	0.00E+00	0.00E+00	1.90E-02	3.75E-03
NO_3^-	1.50E-02	1.50E-03	1.00E-04	1.96E-02	1.00E-03	1.50E-02
SO_4^{2-}	9.74E-03	9.70E-04	9.98E-03	1.70E-04	5.79E-02	9.74E-03
PO_4^{3-}	5.71E-02	5.71E-03	6.40E-02	6.40E-02	0.00E+00	5.71E-02
HCO_3^-	1.89E-02	1.89E-03	1.90E-02	1.90E-02	1.90E-02	1.89E-02
Glucose	5.55E-03	5.60E-04	5.55E-03	5.55E-03	5.55E-03	0.00E+00

DTN: LL980608505924.035



DTN: LL980608505924.035

Figure 11. Results of LLNL *In Situ* Limiting Nutrient Batch Test Growth Experiments.



DTN: LL980608505924.035

Figure 12. Results of LLNL *In Situ* Limiting Nutrient Microcosm Test Growth Experiments.

6.6.3.2 Input Development

6.6.3.2.1 General MING Inputs

The following general inputs were used in the test calculations: Tables 16, 17 and 19 with the exception of the values that are substituted on Table 19 as discussed in Section 6.6.3.2.2. Two other parameters that have no consequence on these calculations but have to be entered are the RH value (0.999, equivalent to saturated conditions, see Assumption 5.2 above) and the layer designator parameters for the altered and unaltered tuff (Table 35 above).

6.6.3.2.2 Test Specific Inputs

6.6.3.2.2.1 Lab Values

In addition to the inputs specifically discussed in the sections below the following tables were used as inputs: Table 13 (composition of altered and unaltered tuff), Table 40 (compositions of the various growth media), and Table 39 (various required inputs used to simulate the lab experiments). The same method as discussed in Attachment V was used to generate the "reactant compositions" for the altered and unaltered tuff. They are shown on Table 35.

Any parameters that were altered for sensitivity cases are presented as part of the discussion in Sections 6.6.3.4.2 and 6.6.3.4.3.

6.6.3.2.2.2 Scaling of Time

MING V1.0 uses a year as its standard time unit; however, to scale the MING calculation all time units need to be scaled to days. This is a simple fix as the only real time dependant variable that gets entered as an input is the material lifetimes from which are calculated the material degradation rates. These yearly rates can be simply modified by multiplying the material lifetime by 365 to get the rate in days. Therefore, if the parameter "material lifetime" of altered tuff (AT) were determined to be 10 years, the value 3650 would be entered into the appropriate input table in MING. Additionally, the groundwater "infiltration rate" is usually entered in mm/year; however, with the batch experiment there is only a one-time addition of media to the flask so the time dependence does not interfere with the calculation.

6.6.3.2.2.3 Scaling of Volume

MING V1.0 requires that you input a "tunnel length" and a "tunnel diameter" as default input parameters to all model calculations. In order to account appropriately for gas flow, the scaling of the 125 ml flasks used in the LLNL microcosm experiments (Horn et al. 1998a, 1998b, and Davis et al. 1998) needs to be calculated.

Attachment I documents the development of necessary volume input parameters for model validation test case inputs that are used to replace the default input parameters (tunnel diameter and tunnel length) shown in Table 19. In order to simulate the lab experiments appropriate volume had to be defined. Sections I-2.3, I-4.3, and I-5.3 document the derivation of appropriate volume conditions within the flasks. The results of the derivation that are direct inputs into MING are found on Table I-10.

6.6.3.2.3 Gas Input

MING V1.0 requires gas flux into the drift in units of kg/m^2 year. However, to scale the lab experiments properly, the values entered in MING need to be scaled on the order of days and not years. When scaling MING, as long as all time units are input as the same unit there are no conversion problems.

Attachment I documents the development of necessary gas input parameters for model validation test case inputs. In order to simulate the lab experiments appropriate gas conditions had to be defined. Sections I-2.3, I-4.3 and I-5.3 document the derivation of appropriate gas conditions within a 125 ml flask. The results of this derivation used as direct inputs into MING are found on Table I-11.

6.6.3.3 Test Results

Results calculated in MING using the inputs above are reported in grams (dry weight) of microbes per unit volume. In order to compare the MING results to the growth experiments, the values calculated in MING need to be converted to the number of cells per ml of growth media. This is done using the following two formulas.

$$\mu/\alpha=\phi \tag{Eq. 8}$$

$$\phi/\lambda=\beta \tag{Eq. 9}$$

where:

μ = MING result $(g)_{dry}$ per flask
α = Mass of average microbe $(g)_{dry}$ (see value from Table I-2)
ϕ = # of microbes in flask
λ = Volume of growth media in flask (ml) (See value from Table 39)
β = # of microbes per ml growth media

Equations 8 and 9 are used to create the results tables presented in the sections below. These tables are used in creating the figures shown below. The calculated results presented on these tables are plotted against both the batch and microcosm results shown in Figures 11 and 12 above.

6.6.3.3.2 YM Complete Test

6.6.3.3.2.1 Test Specific Conditions

This calculation was run in MING using a material lifetime on the altered tuff (Table 13) of 10 years (3650 days), the gas compositions found on Table I-11, and the YM-Complete (YMC) growth media composition from Table 40.

6.6.3.3.2.2 Test Results

Table 41 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. Applying equations 8 and 9 to the calculated mass reported on Table 41 gives the values shown on Table 42. This calculated concentration (1.89E+09 cells/ml) is plotted against the batch and microcosm results and shown on Figure 13.

Table 41. Results from MING for YMC Test.

Mass of microbes from available nutrients (g dry)	Energy available in system (kJ mol^{-1})	Mass of microbes from available energy (g dry)	Calculated Mass of microbes (g dry)
0.006077383	0.3621332	0.005658332	0.005658332

Table 42. Calculated Abundance of Microbes per ml of YMC Growth Media using Equations 8 and 9.

Calculated Mass (g dry) (μ)	Mass of Average microbe (α)	# of Microbes in Flask (ϕ)	ml of growth media in flask (λ)	# of Microbes per ml of broth (β)
5.66E-03	1.50E-13	3.77E+10	20	1.89E+09

6.6.3.3.3 Dilute Complete Test

6.6.3.3.3.1 Test Specific Conditions

This calculation was run in MING using a material lifetime on the altered tuff (Table 13) of 10 years (3650 days), the gas compositions found on Table I-11, and the Dilute Complete (DC) growth media composition from Table 40.

6.6.3.3.3.2 Test Results

Table 43 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. Applying equations 8 and 9 to the calculated mass reported on Table 43 gives the values shown on Table 44. This calculated concentration (1.92E+08 cells/ml) is plotted against the batch and microcosm results and shown on Figure 14.

Table 43. Results from MING for DC Test.

Mass of microbes from available nutrients (g dry)	Energy available in system (kJ mol^{-1})	Mass of microbes from available energy (g dry)	Calculated Mass of microbes (g dry)
0.0007697311	0.03683817	0.0005755964	0.0005755964

Table 44. Calculated Abundance of Microbes per ml of DC Growth Media using Equations 8 and 9.

Calculated Mass (g dry) (μ)	Mass of Average microbe (α)	# of Microbes in Flask (ϕ)	ml of growth media in flask (λ)	# of Microbes per ml of broth (β)
5.76E-04	1.50E-13	3.84E+09	20	1.92E+08

6.6.3.3.3 J-13-NO_3 Test

6.6.3.3.3.1 Test Specific Conditions

This calculation was run in MING using a material lifetime on the altered tuff (Table 13) of 10 years (3650 days), the gas compositions found on Table I-11, and the J-13-NO_3 growth media composition from Table 40.

6.6.3.3.3.2 Test Results

Table 45 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. Applying equations 8 and 9 to the calculated mass reported on Table 45 gives the values shown on Table 46. This calculated concentration (1.85E+09 cells/ml) is plotted against the batch and microcosm results and shown on Figure 15.

Table 45. Results from MING for J-13-NO_3 Test.

Mass of microbes from available nutrients (g dry)	Energy available in system (kJ mol^{-1})	Mass of microbes from available energy (g dry)	Calculated Mass of microbes (g dry)
0.007665622	0.3549707	0.005546418	0.005546418

Table 46. Calculated Abundance of Microbes per ml of J-13-NO_3 Growth Media using Equations 8 and 9.

Calculated Mass (g dry) (μ)	Mass of Average microbe (α)	# of Microbes in Flask (φ)	ml of growth media in flask (λ)	# of Microbes per ml of broth (β)
5.55E-03	1.50E-13	3.69E+10	20	1.85E+09

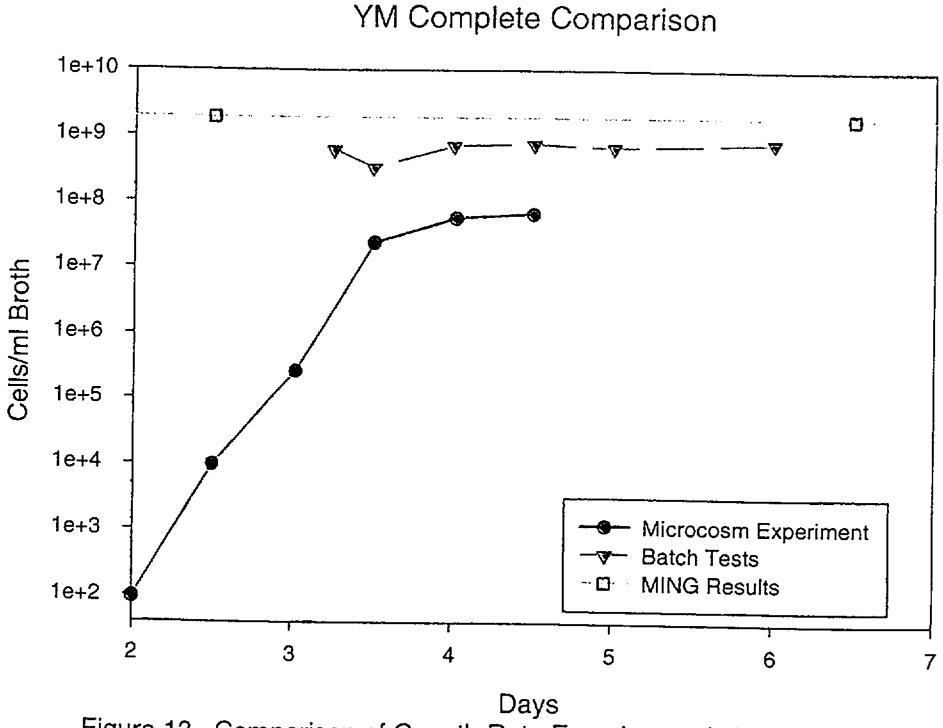


Figure 13. Comparison of Growth Rate Experiments in YMC Growth Media with Calculated Values in MING V1.0.

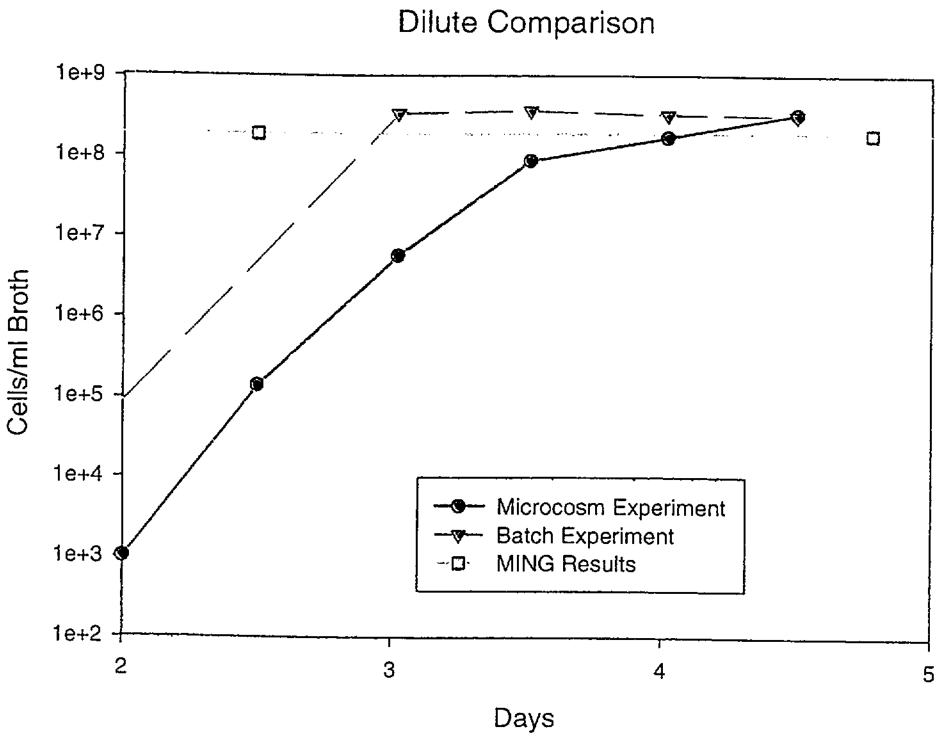


Figure 14. Comparison of Growth Rate Experiments in DC Growth Media with Calculated Values in MING V1.0.

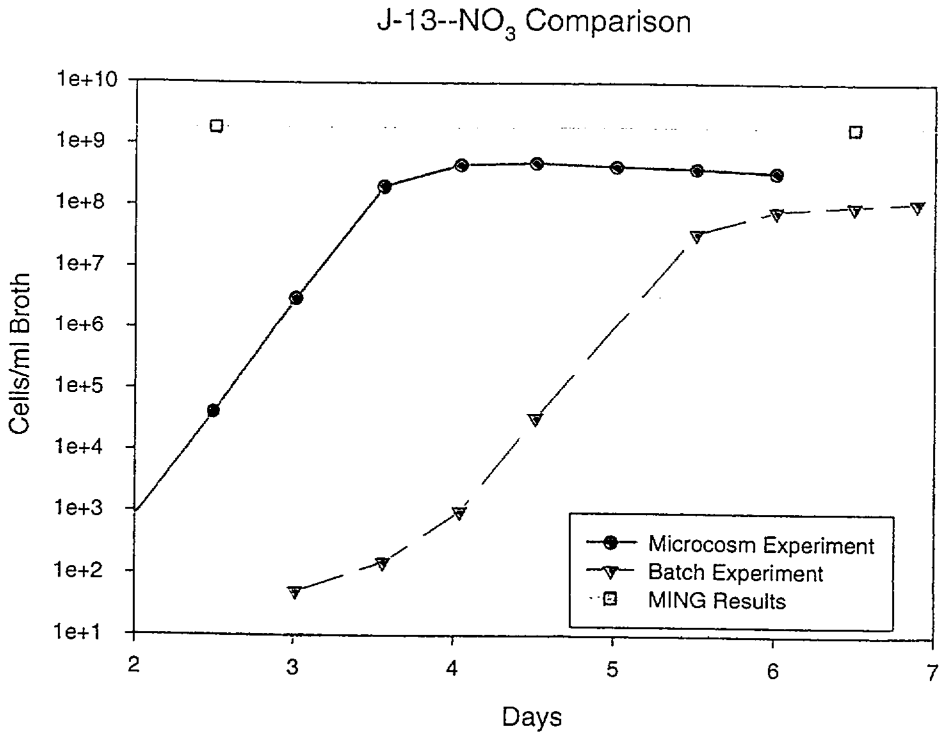


Figure 15. Comparison of Growth Rate Experiments in J-13-NO_3 Growth Media with Calculated Values in MING V1.0.

6.6.3.3.4 J-13-SO_4 Test

6.6.3.3.4.1 Test Specific Conditions

This calculation was run in MING using a material lifetime on the altered tuff (Table 13) of 10 years (3650 days), the gas compositions found on Table I-11, and the J-13-SO_4 growth media composition from Table 40.

6.6.3.3.4.1 Test Results

Table 47 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. Applying equations 8 and 9 to the calculated mass reported on Table 47 gives the values shown on Table 48. This calculated concentration (1.85E+09 cells/ml) is plotted against the batch and microcosm results and shown on Figure 16.

Table 47. Results from MING for J-13-SO_4 Test.

Mass of microbes from available nutrients (g dry)	Energy available in system (kJ mol^{-1})	Mass of microbes from available energy (g dry)	Calculated Mass of microbes (g dry)
0.007665622	0.3549707	0.005546418	0.005546418

Table 48. Calculated Abundance of Microbes per ml of J-13-SO_4 Growth Media using Equations 8 and 9.

Calculated Mass (g dry) (μ)	Mass of Average microbe (α)	# of Microbes in Flask (ϕ)	ml of growth media in flask (λ)	# of Microbes per ml of broth (β)
5.55E-03	1.50E-13	3.70E+10	20	1.85E+09

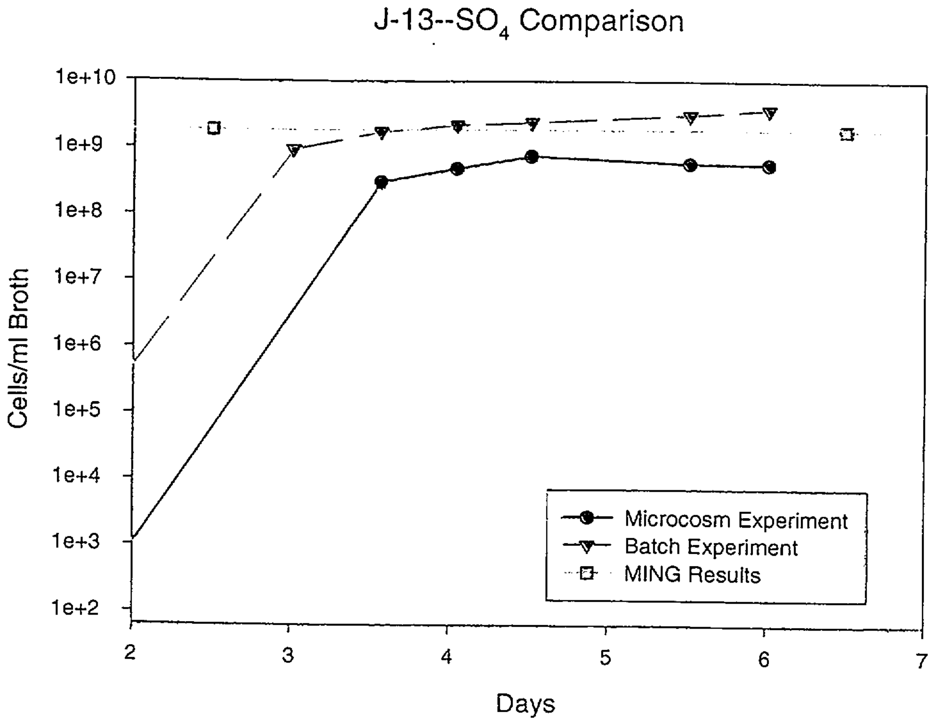


Figure 16. Comparison of Growth Rate Experiments in J-13-SO_4 Growth Media with Calculated Values in MING V1.0.

6.6.3.3.5 Phosphate Deficient Test

6.6.3.3.5.1 Test Specific Conditions

This calculation was run in MING using a material lifetime on the altered tuff (Table 13) of 10 years (3650 days), the gas compositions found on Table I-11, and the Phosphate Deficient (PD) growth media composition from Table 40.

6.6.3.3.5.2 Test Results

Table 49 shows that the system is nutrient limited. There is sufficient energy to produce more microbes. Applying equations 8 and 9 to the calculated mass reported on Table 49 gives the values shown on Table 50. This calculated concentration (1.47E+05 cells/ml) is plotted against the batch and microcosm results and shown on Figure 17.

Table 49. Results from MING for PD Test.

Mass of microbes from available nutrients (g dry)	Energy available in system (kJ mol^{-1})	Mass of microbes from available energy (g dry)	Calculated Mass of microbes (g dry)
4.412285E-07	0.4114369	0.006428701	4.412285E-07

Table 50. Calculated Abundance of Microbes per ml of PD Growth Media using Equations 8 and 9.

Calculated Mass (g dry) (μ)	Mass of Average microbe (α)	# of Microbes in Flask (ϕ)	ml of growth media in flask (λ)	# of Microbes per ml of broth (β)
4.41E-07	1.50E-13	2.94E+06	20	1.47E+05

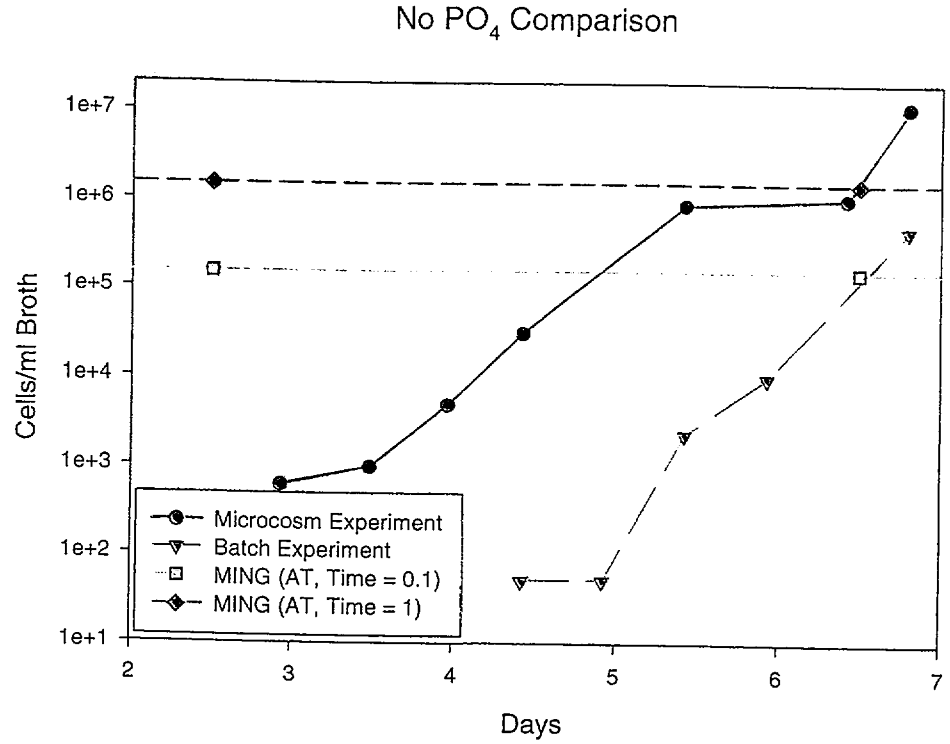


Figure 17. Comparison of Growth Rate Experiments in PD Growth Media with Calculated Values in MING V1.0. A Sensitivity Calculation (see Section 6.6.3.4.2 below) using a Modified Material Lifetime for Altered Tuff of One Year (365 Days) is also Shown.

6.6.3.3.6 Carbon Deficient Test

6.6.3.3.6.1 Test Specific Conditions

This calculation was run in MING using a material lifetime on the altered tuff (Table 13) of 10 years (3650 days), the gas compositions found on Table I-11, and the Carbon Deficient (CD) growth media composition from Table 40.

6.6.3.3.6.2 Test Results

Table 51 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. Applying equations 8 and 9 to the calculated mass reported on Table 51 gives the values shown on Table 52. This calculated concentration (1.88E+09 cells/ml) is plotted against the batch and microcosm results and shown on Figure 18.

Table 51. Results from MING for CD Test.

Mass of microbes from available nutrients (g dry)	Energy available in system (kJ mol^{-1})	Mass of microbes from available energy (g dry)	Calculated Mass of microbes (g dry)
0.00590302	0.3614834	0.005648179	0.005648179

Table 52. Calculated Abundance of Microbes per ml of CD Growth Media using Equations 8 and 9.

Calculated Mass (g dry) (μ)	Mass of Average microbe (α)	# of Microbes in Flask (φ)	ml of growth media in flask (λ)	# of Microbes per ml of broth (β)
5.65E-03	1.50E-13	3.77E+10	20	1.88E+09

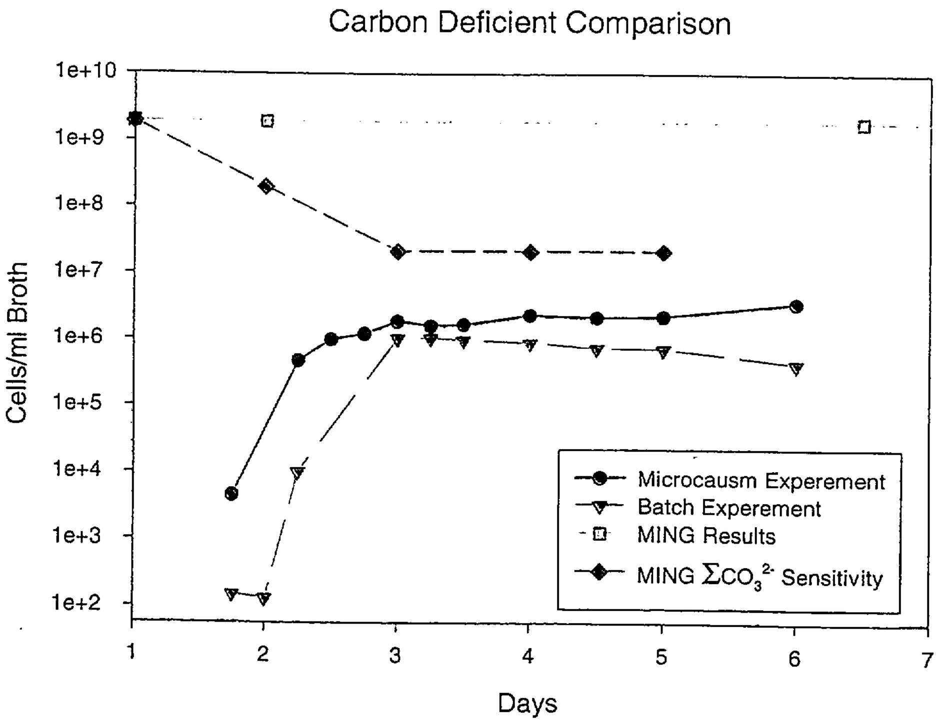


Figure 18. Comparison of Growth Rate Experiments in CD Growth Media with Calculated Values in MING V1.0. A Sensitivity Calculation using Modified Aqueous Carbonate Compositions from Table 40 Spanning Two Orders of Magnitude Decrease is also Shown.

6.6.3.4 Sensitivities to Inputs

6.6.3.4.1 Gas Sensitivity Tests

6.6.3.4.1.1 Test Specific Conditions

These sensitivity calculations were run in MING using a material lifetime on the altered tuff (Table 13) of 10 years (3650 days), the gas compositions found on Table I-11, and the CD growth media composition from Table 40. Each sensitivity calculation was done using a different gas composition. In MING, this is done by turning on or off the various gas switches in the code then proceeding with the calculation. Figure 19 below shows the various gas switches that were selected for each run.

6.6.3.4.1.2 Test Results

Seven separate calculations were done in addition to the calculation presented in Section 6.6.3.3.6. Applying equations 8 and 9 to the calculated masses reported on Table 53 gives the values shown on Figure 19.

6.6.3.4.2 Material Lifetime Sensitivity Tests

6.6.3.4.2.1 Test Specific Conditions

These sensitivity calculations were run in MING using a variable material lifetime on altered (AT) and unaltered tuff (UT) (Table 13) ranging from 1 year to 10,000 years, the gas compositions found on Table I-11, and the YMC and PD growth media composition from Table 40. Each sensitivity calculation was done using a different material lifetime, growth media composition or rock type. Figures 20 and 21 below show the various parametric selections used in each calculation. YMC media and PD media were selected to observe the affects of a nutrient vs. energy limited system. A nutrient-limited system should show an incremental increase in microbial abundance but an energy-limited system should show no effects of the additional nutrients available to the system.

6.6.3.4.2.2 Test Results

Twelve separate calculations were done in addition to the calculations presented in Section 6.6.3.3.1 and 6.6.3.3.5 Applying equations 8 and 9 to the calculated masses reported on Table 54 gives the values shown on Figures 20 and 21.

The results are essentially identical for all cases run. In all of these calculations, the results indicate that the mass of microbes produced is limited by the available energy. However, there is a slight increase when the redox energy from the O_2 is available. The difference in the calculations with and without the oxygen gas (0.00002 grams) indicates that the calculations are insensitive to the nutrients and energy that the gas inputs provide.

Table 53. Results of Gas Sensitivity Calculations.

Gas Switches on in Sensitivity Test	Calculated Mass of microbes (g dry)
N_2 and O_2	5.65E-03
CO_2 and O_2	5.65E-03
N_2 and CO_2	5.63E-03
N_2	5.63E-03
O_2	5.65E-03
CO_2	5.63E-03
All	5.65E-03
None	5.63E-03

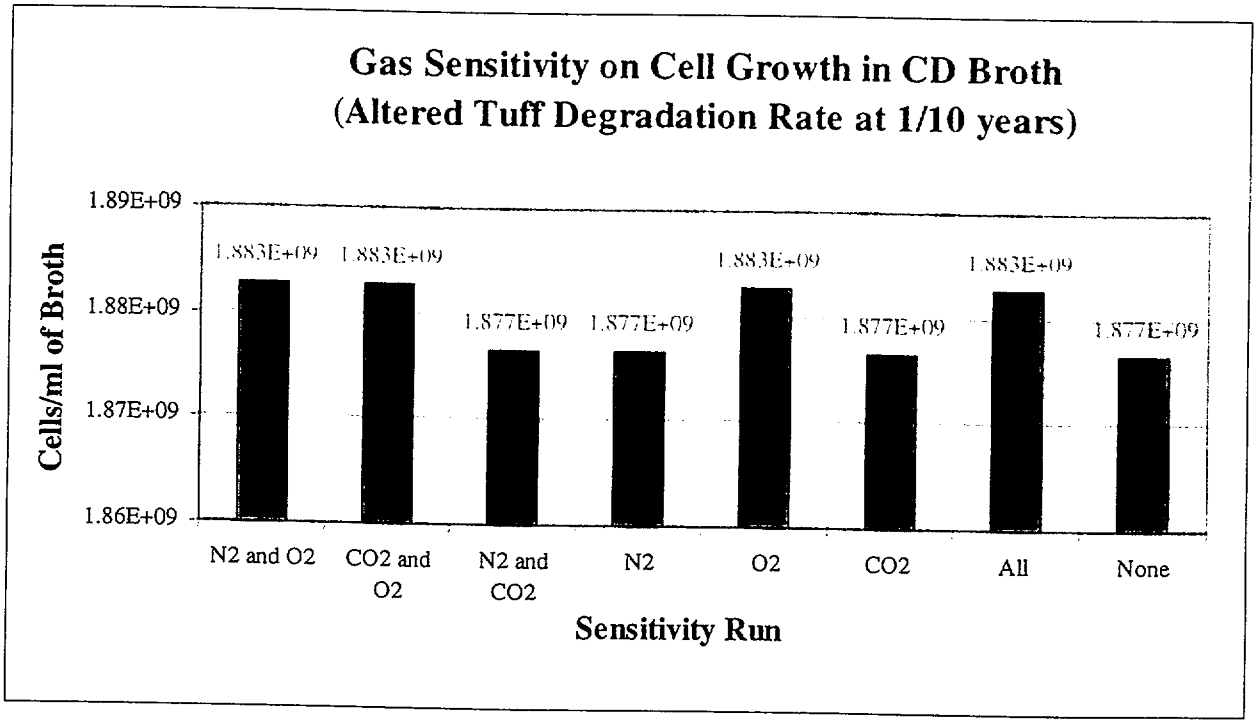


Figure 19. Comparison of Gas Sensitivity on Cell Growth using Modeled Results from the CD Growth Media.

Table 54. Results of Material Lifetime Sensitivity Calculations.

Parameters Selected	Calculated Mass of microbes (g dry)
YMC, AT, ML=1	5.66E-03
YMC, AT, ML=10	5.66E-03
YMC, AT, ML=1,000	5.66E-03
YMC, AT, ML=10,000	5.66E-03
YMC, UT, ML=10	5.66E-03
YMC, UT, ML=1,000	5.66E-03
YMC, UT, ML=10,000	5.66E-03
PD, UT, ML=10	2.21E-07
PD, UT, ML=1,000	2.21E-09
PD, UT, ML=10,000	2.21E-10
PD, AT, ML=1	4.41E-06
PD, AT, ML=10	4.41E-07
PD, AT, ML=1,000	4.41E-09
PD, AT, ML=10,000	4.41E-10

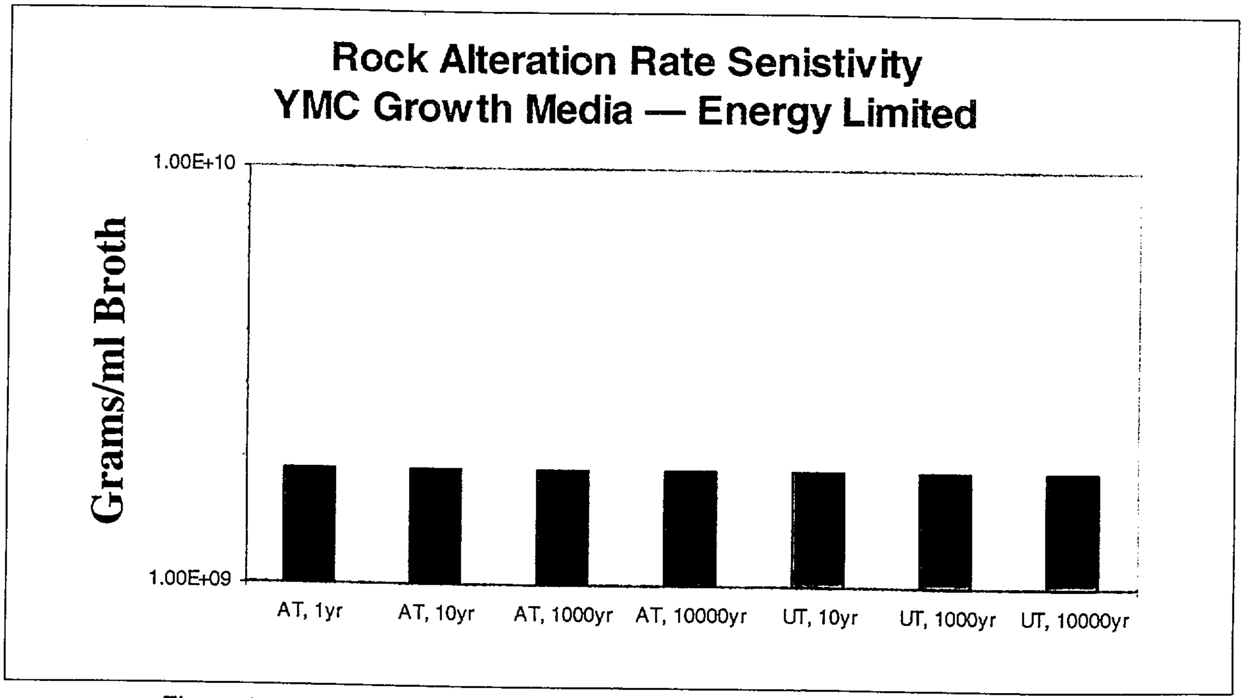


Figure 20. Results of Material Lifetime Sensitivity Calculations for Altered and Unaltered Tuff (Table 13) in an Energy Limited System using the YMC Growth Media.

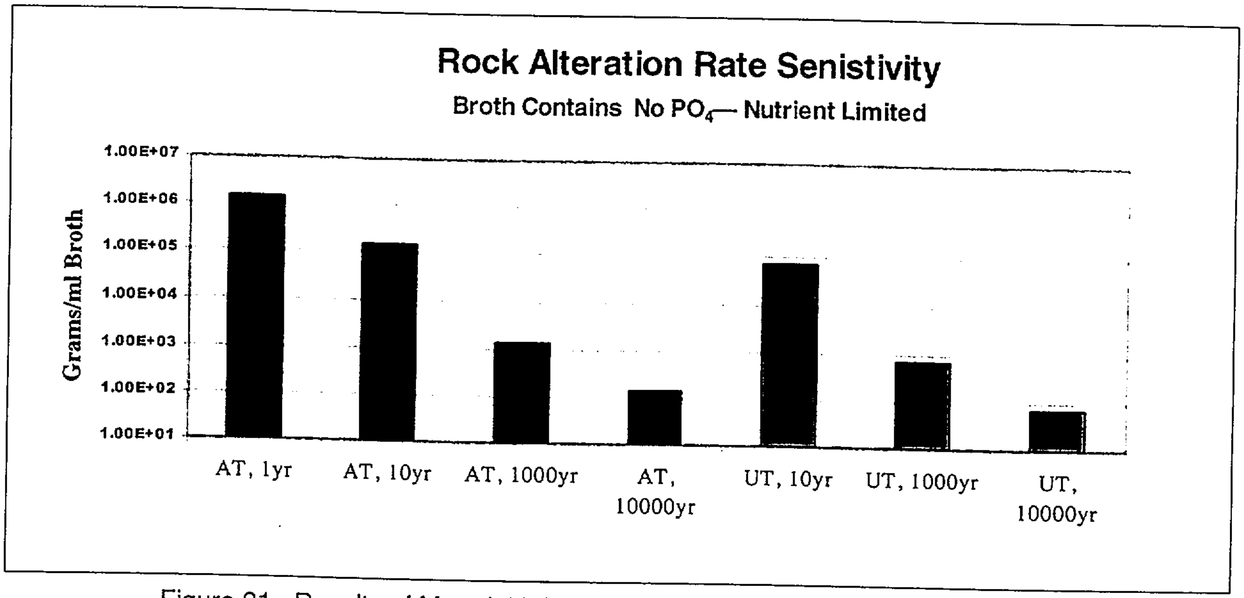


Figure 21. Results of Material Lifetime Sensitivity Calculations for Altered and Unaltered Tuff (Table 13) in a Nutrient Limited System using the PD Growth Media.

6.6.3.4.3 Groundwater Concentration and pH Sensitivity

6.6.3.4.3.1 Test Specific Conditions

This calculation was run in MING using a material lifetime on the altered tuff (Table 13) of 10 years (3650 days) and the gas compositions found on Table I-11. These sensitivity calculations were run in MING using the Yucca Mountain Complete (YMC) media and modifying the concentration by ± 10%. In addition, pH was altered by one pH unit so that the range was between 6.2 and 8.2. Figure 22 below shows the various parametric selections used in each calculation.

The carbon deficient media was also modified by altering the ΣCO_3 values in order to explain the discrepancies in the results (Figure 18). This was done by taking the values for CO_3 on Table 40 and decreasing them by two orders of magnitude during the five time step (day) modeling run. At day 2, the first order of magnitude drop was entered and at day three, the second order of magnitude drop was entered in the input.

6.6.3.4.3.2 Test Results

Nine separate calculations were done in addition to the calculations presented in Section 6.6.3.3.6. Applying equations 8 and 9 to the calculated masses reported on Tables 55 and 56 give the values shown on Figures 22 and 18, respectively.

In all of these calculations, the results indicate that the mass of microbes produced is limited by the available energy. If these runs were nutrient limited, the effects of the pH variation would not appear, although the amount of energy available to the system would vary. The results from Figure 22 show that there is an energy minimum produced at pH of 7.2. This is possible due to the hydrogen ion dependence in most of the half reactions shown on Table 16. Because of this dependence, some of the full reactions that produce the energy above the 15kJ limit at a given pH may not produce the same energy at a different pH. This difference may force the reaction below the 15kJ limit, which will cause the reaction to be discarded by MING.

In these cases, an unmeasured variation in pH for the experimental broth formulas (Tables 39 and 40) of ± 1 pH unit will not force the validation calculations to fall outside the one order of magnitude level. Whether a greater variation on pH would cause larger impacts to an energy-limited system is unknown at this time.

Table 55. Results of YMC Growth Media Concentration and pH Sensitivity Calculations.

Parameters Selected	**Calculated Mass of microbes (g dry)**	**# of Microbes per ml of broth (β)**
pH 6.2, -10%	6.60E-03	2.20E+09
pH 6.2, +10%	8.07E-03	2.69E+09
pH 6.2, YMC	5.86E-03	1.95E+09
pH 7.2, -10%	5.17E-03	1.72E+09
pH 7.2, +10%	6.33E-03	2.11E+09
pH 8.2, -10%	5.92E-03	1.97E+09
pH 8.2, +10%	7.20E-03	2.40E+09
pH 8.2, YMC	5.70E-03	1.90E+09

Table 56. Results of a Sensitivity Study on the Effects to CD Growth Media by Altering ΣCO_3 by Two Orders of Magnitude.

Time step	**Calculated Mass of microbes (g dry)**	**# of Microbes per ml of broth (β)**
1	0.00564818	1.88E+09
2	0.00059503	1.98E+08
3	6.4232E-05	2.14E+07

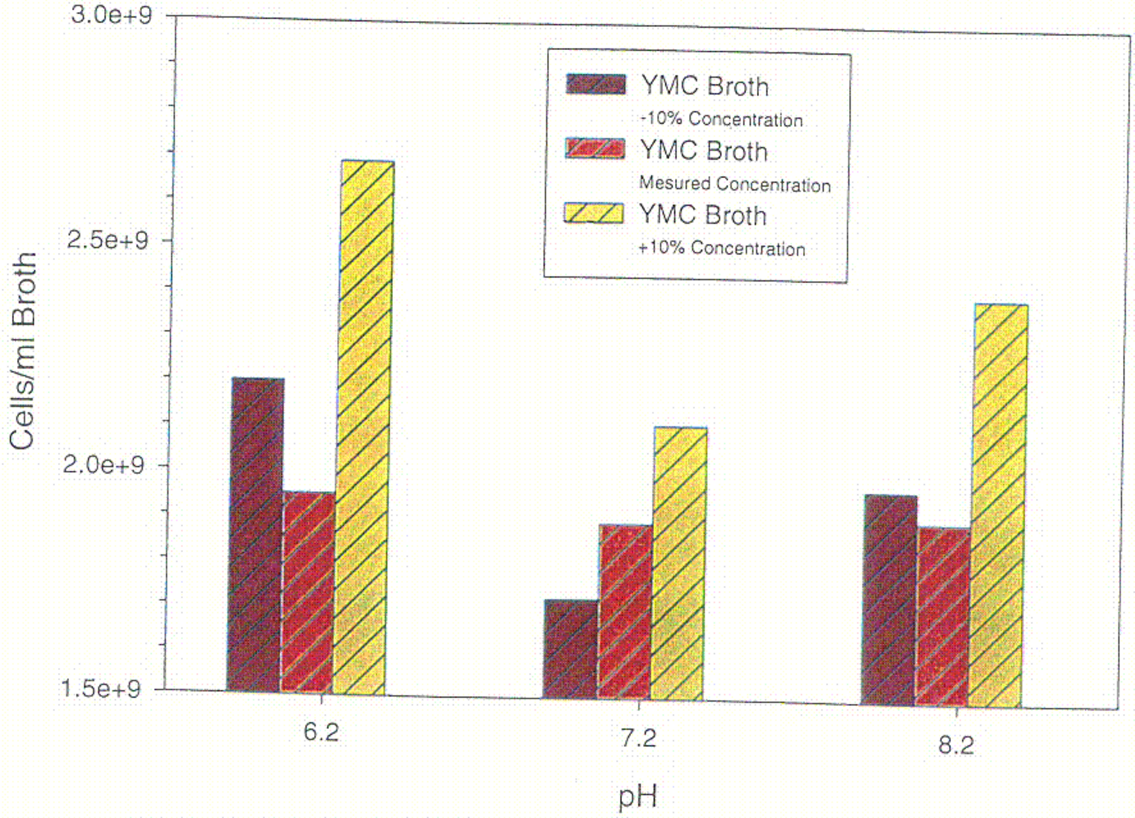


Figure 22. Results of YMC Growth Media Concentration and pH Sensitivity.

6.6.3.5 LLNL Test Case Comparison

For tests shown on Figures 13, 14, 15, and 16, the results show that MING V1.0 adequately replicates the lab tests to within one order of magnitude. For the PD test, the results of MING V1.0 are extremely sensitive to the material lifetime of the tuff (see Figures 17 and 21). The tests reflect the nutrient limiting conditions set up in the lab. By altering the material lifetime of the tuff the MING results of the lab tests can be favorably compared to the actual tests and be found within an order of magnitude. No impact is noted to energy limiting situations as shown on Figure 20.

For the CD test case there are some problematic results. The MING results show a three order of magnitude discrepancy with the values measured in the lab. However, when sensitivity calculations are done on the ΣCO_3 to account for a decrease in ΣCO_3 due to the potential precipitation of calcite or an unknown imposed CO_2 fugacity on the CD growth media, the values approach those measured in the lab experiments (Figure 18).

There does not seem to be sensitivity to gas conditions. There is a slight increase in population when O_2 is accounted for in the redox calculations. Otherwise, there is no impact on results due to sensitivities on gas utilization.

Groundwater and pH sensitivities do not show a large dependence on the minor fluctuations to concentration or a variance of ± 1 unit in pH (Figure 22). These differences are insignificant

C5

when compared to the general order of magnitude of the results shown on Figures 13, 14, 15, and 16.

7. CONCLUSIONS

7.1 CONCEPTUAL MODEL SUMMARY

The reader is referred to Section 6.3.6 for the summary of the conceptual model.

7.2 MODEL SUMMARY

As discussed in Section 6.2 there are three general parts to the model. These three parts are the conceptual model, the software code MING V1.0, and the required parameter inputs. These items are summarized below.

1. The results of the conceptual model were incorporated within the MING V1.0 software during software development or are incorporated directly as parameter inputs.
2. MING V1.0 software was developed using approved QA procedures and has passed its software validation.
3. Either model parameters have been developed within the body of this report, or examples of the necessary parameters are given.

This model is designed to be able to bound the microbial communities that could be present within a given length of repository drift. In general, the model uses the constraints on the supply rates of the nutrients to build an idealized microbial composition, comprised of carbon, nitrogen, sulfur, and potassium in addition to the water components. The rates of supply of these constituents are input as constant release rates for each introduced material in the system by specifying the mass and composition of the material and its degradation lifetime. The other major constraint evaluated is the energy available for microbes to grow based on the pH corrected, standard state free energy released from oxidation/reduction reactions. Other constraints on microbial growth are temperature and RH thresholds in the model that limit the start of microbial activity until the boiling period is over. Although microbes could be sterilized out of the drifts during the highest temperature period, because they are present in the water-rock system they will return as water drips back into potential drifts.

It is important to note that the conceptual model discusses potential repository impacts due to microbial transport and localized colonization (biofilm formation and MIC). However, the model as presented herein does not address the specific effects of the localized impacts such as biofilm development, colloid formation, and the production of inorganic acids, methane, organic byproducts, carbon dioxide, and other chemical species that could change the longevity of materials. The transport of radionuclides from the near field was not investigated.

7.3 MODEL VALIDATION SUMMARY

Three general tests were conducted in Section 6.6 above. The first test duplicated the model that was constructed for the Swiss low level repository (see Figure 9). This test indicates that our model handles the types of calculations that are required on a repository level where natural barrier components are combined with the engineered barrier components to calculate microbial growth.

The second test (see Figure 10) demonstrates that the model is able to replicate the ambient system, not only within the ESF but also with other natural analog measurements in arid volcanic tuff. These values are reasonable when compared to the inputs and fall within an order of magnitude of the measured results.

The second test also confirms the results reported by Kieft et al. (1997) where water availability seemed to be a limiting factor to microbial growth. Calculated results shown on Figure 10 also show a dependence on the availability of redox energy to the system. This is demonstrated by a noticeable increase in energy produced when the material lifetimes are decreased. When these two factors are combined, we are able to match the variability in the natural system.

Finally, the results of the third test (Figures 13 - 22) show that the numbers of organisms reported by MING are within an order of magnitude of measured values. The replication of these tests shows that the model as a whole does a good job at estimating the microbial growth in the system.

From the results, we reach the same conclusions that were reported with the lab experiments (Horn et al. 1998a and 1998b; Davis et al. 1998). Namely, the results indicate that the availability of water (growth media) was the primary factor contributing to microbial growth. In addition, we were able to determine that the primary limiting nutrient in the repository system is phosphorous. This same conclusion was reached by Davis et al. (1998). We also show that in energy limited systems there are limited impacts due to gas availability, slight variations in pH and water chemistry, and material lifetimes. However, in nutrient limited systems, there are larger impacts to cell growth due to large variations in water chemistry and material lifetimes.

Results of all three tests indicate that a) the model will function as intended, and b) the model predictions are accurate to within one order of magnitude of measured values.

7.4 TO BE VERIFIED (TBV) IMPACT

It is important to note that with the exception of the parameter and data inputs to this model, all other aspects of model qualification have been met. As seen on the input tables (Tables 1-5) there are many TBV/TBD (unqualified, unverified, or preliminary) inputs. Many of these inputs will have a large impact on the results of the model. Other inputs may have a rather insignificant impact. Yet again, some input may not have a large impact but their status, as TBV/TBD without any sensitivity analysis, will effect the qualification status of any results.

Because there are multiple TBV/TBD's in this revision of the model documentation and it is difficult to determine which of the TBV/TBD's are the most important, no evaluation of each individual TBV/TBD is included. Three areas of focus that will go a long way toward resolving many of the TBV/TBD's are a) the documentation of a qualified repository design, b) the qualification of the natural system models and data that feed these models, and c) the qualification of the thermochemical data used in the energy calculations.

Because of the numerous TBV inputs, any results of this model should be designated TBV until input qualification status is resolved.

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

7.5 EVALUATION OF NRC IRSR CRITERIA

From Section 4.2.1.1 (Data and Model Justification Acceptance Criteria), Criteria 1, 2, 3, 4, and 5 are addressed in this model. However, in accordance with Criterion 3 much of the data used in this model needs further work both to its abundance and to acquisition. Criteria 6 and 7 are outside the scope of this model.

From Section 4.2.1.2 (Data Uncertainty and Verification Acceptance Criteria), Criteria 1, 2, 3, and 4 are addressed in this model. Criterion 5 is outside the scope of this model.

From Section 4.2.1.3 (Model Uncertainty Acceptance Criteria), Criterion 1 was addressed in this model. Criteria 2 and 3 are outside the scope of this model.

From Section 4.2.1.4 (Model Verification Acceptance Criteria), Criteria 1, 2, and 3, are addressed in this model.

7.6 FEATURE, EVENT OR PROCESS (FEP) EVALUATION

Table 6 above documents the FEP's that this model could potentially address. Each of these numbered FEP's will be discussed below.

1. The reduction and oxidation potential in the waste and EBS can be effected by the presence of microbial communities. However, this model only addresses the conceptual processes. It does list many of the redox half reactions that are used by microbes in their metabolic processes. These are discussed in Sections 6.3.1.1 and 6.3.1.2 above. In addition, it discusses the effects of biofilm development in the alteration of local redox environments (see Section 6.3.1.14). However, specific results are not reported in this document.

2. The production of organics in the waste and EBS would be directly effected by the presence of microbial communities. This is a general result of the effects of biofilm growth (see Section 6.3.1.14). Other sources and information (e.g. production of siderophores) are documented in Section 6.3.5. However, specific results are not reported in this document.

3. The results of this model can be used to generate the abundance of microbes in the drift through time. These microbes can be used as a source of potential colloids in other modeling work. These conceptual concepts are discussed in Section 6.3.5. However, this document does not contain specific results.

4. This model was developed to answer this FEP. This model will be used to address this issue. However, the specific results will be documented in future work.

5. This model was developed to answer this FEP. This model will be used to address this issue. However, the specific results will be documented in future work.

6. The sorption potential in the waste and EBS can be effected by the presence of microbial communities. However, this model only addresses the conceptual processes. It does discuss the sorption onto microbes. These are discussed in Section 6.3.5. However, specific results are not reported in this document.

7.7 RECOMMENDATIONS FOR FUTURE REVISION OR CHANGE

The biggest need for this model is to qualify the input data and parameters. Data qualification directly impacts the results and status of this model. Section 7.4 above discusses the major areas of concern. Another important item is to eventually incorporate the TSPA-SR/LA model results in a future revision or interim change to this document once the TBD input for SR/LA is finalized.

One technical issue may be added in a future revision of the model. Redox half reactions for uranium, along with their temperature dependant parameters, should be incorporated. This is due to two reasons. First, some species of microbes derive their metabolic energy from half reactions involving uranium (see Section 6.3.1.1). Second, there will be a large abundance of uranium in the waste. In general, however this will only impact results during the expected lifetimes of the CSNF and HLW.

A slight modification to the software would be helpful in resolving some of the scaling issues as is discussed in Attachment I. With modification, the documentation for drift (or borehole, flask, etc.) scaling would be more efficient.

Finally, more sensitivity to uncertain parameters should be conducted and evaluated.

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9. ATTACHMENTS

Attachment	Title
I	Model Validation Test Case Input Parameters
II	Repository Subsurface Design Input Parameters
III	Waste Package Design Input Parameters
IV	Waste Form Composition Determinations
V	Reactant Composition Determinations

ATTACHMENT I: MODEL VALIDATION TEST CASE INPUT PARAMETERS

I-1. PURPOSE

The purpose of this attachment is to create the appropriate parameter input for MING 1.0 (CSCI 30018 V1.0, CRWMS M&O 1998d) that will allow the testing of the MING code with both scientific measurements of microbial populations at the site and natural analogs to the site. This is being done for the QA model validation of the in-drift microbial communities model as directed in CRWMS M&O (1999e).

I-2. METHOD

This section has three parts: 1) the determination of the iron bearing minerals in the host rock, 2) to determine the numbers of microbes in one lineal meter of repository drift, 3) the generation of gas inputs for the LLNL lab experiments and for ambient conditions within the repository host rock.

I-2.1 PART 1: DRIFT MINERALS

The following steps were used to calculate the quantity of iron bearing minerals in the host rock.

1. Calculate the volume of rock in one lineal meter of repository drift.
2. Calculate the mass of ambient materials in one lineal meter of repository drift.
3. Determine the mass of iron bearing minerals found in one lineal meter of repository drift.
4. Determine the wt % composition of iron in the iron bearing minerals in one lineal meter of repository drift.

I-2.2 PART 2: MICROBIAL COUNTS

The following steps were used to calculate the number of microbes in the host rock.

1. Convert mass (kg) of rock in 1 lineal meter of repository drift to grams.
2. Multiply number of cells per gram of crushed tuff (from input) times the number of grams of tuff per lineal meter of repository drift.
3. Multiply the cells per lineal meter of repository by the microbial bulk density to obtain the mass of cells per lineal meter of repository.

I-2.3 PART 3: GAS INPUTS

I-2.3.1 Flask to Drift Scaling

The following steps were used to calculate the appropriate MING V1.0 input parameters:

1. Assume a radius of the open end of a flask.
2. Determine the surface area of the flask opening.
3. Determine MING V1.0 input parameter "drift diameter" by calculating the radius of the flask having a given surface area and a volume of 125 ml.
4. Determine MING V1.0 input parameter "tunnel length" by calculating the length of a flask having a given radius and a volume of 125 ml.

I-2.3.2 Lab Gas

MING V1.0 requires gas flux into the drift in units of kg/m^2 year. The following steps are used to calculate the flux of atmospheric gas into a 125 ml flasks.

1. Determine the mass of atmospheric gases in air.
2. Determine the total gas available to enter the flask (kg/m^2)
3. Determine the daily flux into the flask (kg/m^2 day)
4. Determine the total cumulative flux (over 7 days) into the flask (kg/m^2).

I-3. ASSUMPTIONS

1. Because no specific mineral was designated, the composition of mica group mineral reported in DTN LA000000000086.002 is biotite [Used in Section I-5.1].

The rational for this assumption is that this mineral was chosen to maximize the amount of iron in the system. Other mica group minerals reported in Klein and Hurlbut (1977, p. 430-433), a standard reference for mineralogy, have less potential iron in their elemental structures. In addition, biotite is considered the most abundant mafic silicate phenocryst in the tuffs at Yucca Mountain (Vaniman et al. 1989, Section 4.1.3.5).

2. Bulk density of a microbe is equal to the bulk density of water (1 g/cm^3) [Used in Section I-5.1].

The rational for this assumption is because 99% of a microbe's mass is water as reported in DTN MO9909SPAMICRO.001. The remaining mass is not expected to change this value significantly.

3. The minerals sampled within borehole UZ-16 are representative of repository conditions and will serve as an appropriate surrogate for site wide properties. [Used in Section I-5.1].

The rational for this assumption is based on Vaniman et al. (1989). A review of this synthesis report indicates that although there are differences in mineralogy from borehole to borehole, they do not significantly vary. The same sorts of minerals are found in each borehole within the given lithology.

4. The radius of the open end of a flask is 2.5 cm. [Used in Section I-5.1].

The rational for this assumption is that although the radius was not reported in Horn et al. (1998a and 1998b) or Davis et al. (1998), a reasonable guess can be made based on the fact that a 125 ml flask is not a large flask and the changing the radius will not affect the results in any significant way because gas abundance in the flask is primarily dependant on the volume of the flask.

5. The only gas available over seven days time is in the flask [Used in Section I-4.3.2].

The rational for this assumption is that this value bounds the maximum length of experimental days for the experiments conducted at LLNL that were used in the model validation runs (see Figures 11 and 12, Section 6.6.3.1). Although there could be gas entering the flask from the culture samples taken to do microbial counts, gas consumption or generation within the flask over this time should not significantly affect the calculations. This validity of this assumption was demonstrated in Section 6.6.3.4.1 where including gas as a nutrient or energy source did not significantly impact the results.

I-4. INPUTS

I-4.1 PART 1: DRIFT MINERALS

I-4.1.1 Inputs

Chemical formulas for biotite [$K(Mg,Fe)_3(AlSi_3O_{10})(OH)_2$] and hematite ($Fe_2O_3$) were taken from Klein and Hurlbut (1985). Fe^{2+} and Fe^{3+} can both substitute for the Mg in the crystal structure (Klein and Hurlbut 1985). In order to maximize the amount of Fe available in the biotite, Mg is ignored in the formula and the following is used: $KFe_3(AlSi_3O_{10})(OH)_2$.

The Topopah Spring tuff middle nonlithophysal (TMN) and lower lithophysal (TLL) are the rock units where the repository is currently located. DTN GS931208314211.047 shows the depth of the TMN unit to range from 549.0 ft. to 690 ft. and the TLL to go from 690 ft to at least 1054.6 ft. ESF is an abbreviation for the exploratory studies facility.

Table I-1. Input Values, their DTN #'s, and their Qualification Status for Part 1 Calculations.

Iron Mineral Types	Reported maximum mineral % in repository horizon tuff (borehole UZ 16)	Mineral GFW	Fe GFW	Wt. Fraction Fe	Bulk Density in repository horizon tuff (TMN, Flint 1998)
LA000000000086.002	LA000000000086.002 GS931208314211.047 (See Assumption # 3)	(Sargent-Welch 1979)	(Sargent-Welch 1979)	Fe GFW /Mineral GFW	GS960908312231.004 (See Assumption # 3)
Qualified Data	Qualified Data	Accepted Data	Accepted Data	Qualified	Qualified Data
Biotite (Mica; see Assumption # 1 above)	1%	511.885	167.54	0.3273	2.25 g/cm^3
Hematite	1%	159.692	111.694	0.6994	

I-4.1.2 Formulas Used

The following formulas were used to produce the results in Section I-5.1.

1. $\pi r^2 h$ — used to calculate the volume of tuff in 1 lineal meter of repository drift.
2. **Bulk Density * Volume** — used to determine the mass of tuff per lineal meter of drift.
3. **Mass per lineal meter * mineral % in host rock** — used to determine the mass of material available in the repository drift.
4. **Elemental GFW / Mineral GFW** — used to determine the weight % of each element.

I-4.2 PART 2: MICROBIAL COUNTS

I-4.2.1 Inputs

Table I-2. Input Values, their DTN #'s, and their Qualification Status for Part 2 Calculations.

Microbial Modeling Parameters	Microbial Volume and Mass (calculated)	Microbes/Biomass in Crushed Tuff (Cells/g)			
Water Content 99% by weight MO9909SPAMICRO.001	Microbial Volume 1.5E-13 cm^3, MO9909SPAMICRO.001	LALH831342AQ96.002		MO9909SPABMASS.000	
Accepted Data	Accepted Data	Qualified Data		Accepted Data	
Microbial Composition $C_{160}(H_{280}O_{80})N_{30}P_2S$ MO9909SPAMICRO.001	Microbial Mass Average Microbe volume * Bulk Density of H_2O (see Assumption # 2)	ESF Low Count	ESF High Count	Rainier Mesa Low Count	Rainier Mesa High Count
Accepted Data	1.5E-13 g	1.78E+04	1.95E+05	5.25E+04	2.63E+05

I-4.2.2 Formulas Used

The following formulas were used to produce the results in Section I-5.2.

1. **Mass of tuff in one meter of repository drift * # of cells per gram of crushed tuff** — used to get the # of cells per lineal meter of repository.
2. **# of cells per lineal meter of repository * average microbial mass** — used to get the mass of cells per lineal meter of repository.

I-4.3 PART 3: GAS INPUTS

I-4.3.1 Flask to Drift Scaling

Table 39 above reports the specifics of the batch experiments that are required by MING to duplicate the batch tests. MING V1.0 requires that you input a "tunnel length" and a "drift diameter" as inputs to all model calculations. In order to appropriately account for gas flow, the scaling of the 125 ml flasks used in the LLNL microcosm experiments (Table 39) needs to be calculated.

Because in MING the gas flow into the drift is across the cylindrical walls as opposed to axially along the drift, gas flow in an upright flask has to be scaled appropriately. To scale the gas flow, the surface area of the opening on the flask has to be equal to the surface area of the cylinder formed by the drift wall and the dimensions of the tunnel length and drift diameter have to match the given surface area. The scaling is set up so that the flask walls are generally impermeable to gas flow and the only allowable surface area for gas flow is at the flask opening. Therefore, using assumption 4 in Section I-3 above and the formula for area of a circle (πr^2), the area of the flask opening is 19.63 cm^2. The convex surface area of the "tunnel length" as entered into MING V1.0 has to be equal to the surface area of the flask opening (19.63 cm^2). The formula for the area of the convex surface for a right circular cylinder ($2\pi rh$) is used along with the volume of a right circular cylinder ($\pi r^2 h$) to determine the "tunnel length" and "drift diameter" of the MING V1.0 input.

$$19.63\ \text{cm}^2 = 2\pi rh \qquad \text{(Eq. I-1)}$$

$$125\ \text{cm}^3 = \pi r^2 h \qquad \text{(Eq. I-2)}$$

Solving Equation I-1 for h and substituting the results for h in Equation I-2 to solve for r gives:

$$r = 12.73\ \text{cm}$$

Substituting the value of r or a drift diameter of $2r$=25.46 cm or about 0.25m into Equation I-3 and solving for h gives the tunnel length:

$$h = 0.2454\ \text{cm} = 0.002454\ \text{m}$$

I-4.3.2 Lab Gas

MING V1.0 requires gas flux into the drift in units of kg/m^2 year. However, as long as all time units input into MING are the same there are no conversion problems. The actual air that would be generally present in the 125 ml flask over the 7 day time frame of the LLNL experiments is assumed to be the volume of air in the flask (see assumption 6). The following steps are used to calculate the flux of atmospheric gas into a 125 ml flask.

Step 1 is to determine the grams of each gas (O_2, N_2, and CO_2) in a liter of air. This is calculated using Equation I-4 below.

(Volume fraction of gas in air)(Gram Formula Weight)/(22.4 $L_{(gas)}$/1 $mol_{(gas)}$) (Eq. I-4)

Inputs for this calculation are provided in Table I-3. Argon gas is not included, as it is not a constituent for microbial growth. Table I-4 shows results of step 1.

Table I-3. Composition of Air. Accepted Handbook Data Taken from Weast (1979, page F-211) and Sargent-Welch (1979)

Component	% by Volume	GFW, g/mol
N_2	78.084	28
O_2	20.946	32
CO_2	0.033	44

Table I-4. Results of step 1

Gas Component	Mass in Air g/l
N_2	9.76E-01
O_2	2.99E-01
CO_2	6.48E-04

Step 2: This mass of gas that resides in the flask is assumed to flux into the fluid in the flask over the a surface area corresponding to the diameter of the flask (see assumption 4 above) or 1.96 x 10^{-3} m^2. The flask is filled with ~25 ml of fluid and crushed tuff, thus leaving ~0.1 L of gas in the flask. Thus, Table I-5 is calculated using the following formula

[(mass of gas) (volume of gas in flask)]/(Surface Area) (Eq. I-5)

Table I-5. Total Gas Available to Enter a 125 cm^3 Flask.

Component	Total Gas (kg/m^2)
N_2	4.971E-02
O_2	1.524E-02
CO_2	3.301E-05

Step 3: MING V1.0 requires the gas be entered as a cumulative flux over time. Therefore, we convert the total gas entering the flask to a daily flux. This is done by taking the total flux of gas into the flask and dividing by 7 days (approximate duration of the LLNL experiments), as shown on Table I-6

Table I-6. Gas Flux into a 125 cm^3 Flask (kg/m^2 day).

Component	Daily Flux (kg/m^2 day)
N_2	7.101E-03
O_2	2.177E-03
CO_2	4.716E-06

I-5. RESULTS

I-5.1.PART 1: DRIFT MINERALS

The volume of tuff in one lineal meter of repository drift is calculated using the equation for a right circular cylinder ($\pi r^2 h$) and using a drift radius of 2.75 m ($r=D/2$ where D is 5.5 m, see Table 19). Thus, the volume is 23.76 m^3. The mass of one lineal meter of tuff in an area equaling the repository drift is determined, by multiplying the bulk density of Topopah Spring tuff (Table I-1 above) by the volume and converting grams to kilograms. The results give a mass of 53,460 kg.

The mass of biotite and hematite in the drift is determined by multiplying 53,460 by 1% (percent of biotite and hematite in the tuff). Thus, the mass of each mineral per meter of drift is ~535 kg.

Table I-7. Wt Fraction of Elements Comprising the Mineral Biotite and its Mass in Tuff of an Area Equal to one Lineal Meter of Repository Drift.

Biotite	535 kg/m
Fe	0.327
Al	0.053
Si	0.164
O	0.375
H	0.004
K	0.076

Note: K, Al, Si, O and H are not needed in the MING calculations and are only presented for consistency.

Table I-8. Wt Fraction of Elements Comprising the Mineral Hematite and its Mass in Tuff of an Area Equal to One Lineal Meter of Repository Drift.

Hematite	535 kg/m
Fe	0.7
O	0.3

I-5.2 PART 2: MICROBIAL COUNTS

Table I-9. Determination of the Abundance of Microbes in an Area Equaling a One Lineal Meter of Repository Drift.

Microbial Abundance	ESF Low Value	ESF High Value	Rainier Mesa Low Value	Rainier Mesa High Value
# of cells per g of crushed tuff (Table I-2)	1.78E+04	1.95E+05	5.25E+04	2.63E+05
# of cells per linear m of repository	8.18E+11	8.96E+12	2.41E+12	1.21E+13
Average microbial mass (g) (Table I-2)	1.50E-13	1.50E-13	1.50E-13	1.50E-13
Mass (g) of cells per lineal meter of repository	1.23E-01	1.34E+00	3.62E-01	1.81E+00

I-5.3 PART 3: GAS INPUTS

I-5.3.1 Flask to Drift Scaling

The results of the calculations in section I-4.3 are necessary inputs for MING V1.0 in conducting model validation tests using the LLNL microcosm tests experimental data (Horn et al. 1998a, Davis et al. 1998). The results shown on Table I-10 can be considered qualified.

Table I-10. 125 ml Flask Dimensions used in Model Validation Tests Using LLNL Lab Experimental Data.

MING V1.0 Parameter	Value
"Drift Diameter"	0.25 m
"Tunnel Length"	0.0025 m

I-5.3.2 Lab Gas

Table I-6 gives the daily gas flux (kg/m^2). This is the starting value for the gas tables that need to be entered into MING V1.0. To construct the input table for a 7 day modeling run we multiply the daily value by the number of days as shown on Table I-11. These values are considered qualified values.

Table I-11. Cumulative Gas Flux (kg/m^2) in Closed 125 ml Flask under Atmospheric Conditions for 7 days.

Day	N_2	O_2	CO_2
1	7.101E-03	2.177E-03	4.716E-06
2	1.420E-02	4.354E-03	9.432E-06
3	2.130E-02	6.531E-03	1.415E-05
4	2.841E-02	8.708E-03	1.886E-05
5	3.551E-02	1.089E-02	2.358E-05
6	4.261E-02	1.306E-02	2.830E-05
7	4.971E-02	1.524E-02	3.301E-05

ATTACHMENT II: REPOSITORY SUBSURFACE DESIGN INPUT PARAMETERS

II -1. PURPOSE

This attachment reduces the information reported to PA from EBSO (CRWMS M&O 1999g) to useable parameters required as input to MING V1.0 (CSCI 30018 V1.0) for calculation of the effects of potential in-drift microbial communities as part of the microbial communities model as outlined in CRWMS M&O (1999e).

II -2. METHOD

Data that have been delivered to PA may be complete and necessary for other PA 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 the AP-3.14Q Input Transmittals 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 lineal meter of either waste package or repository.

All input information is converted into this format depending on how the Repository Subsurface Design information was reported to Performance Assessment Operations via input transmittal (CRWMS M&O 1999g).

II -3. ASSUMPTIONS

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 II-5.1].

2. Due to lack of information about the specific composition of the steel and copper in the rail fittings, a composition of 75% A572 steel and 25% Cu was assumed [used in Section II-4.7].

3. Due to the lack of information on the composition of the steel fittings that are part of the conductor bar, the fittings were assumed to be A572 steel [used in Section II-4.7].

4. 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 II-4.6].

5. Due to the lack of information, neoprene is assumed the composition of the insulation on the wire conductors [used in Section II-4.6].

The general rational and or basis for all of these assumptions 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, look at the compositions of the various steel alloys reported in Section II-5.1 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 II-26 below).

II-4. INPUTS

II-4.1 QA STATUS OF INPUTS

The source of most information found herein is CRWMS M&O (1999g) and is based on preliminary design information. Of the information provided in CRWMS M&O (1999g) and used in this calculation, the sources from ASTM standards (see Section 4.3.2) are considered to be accepted data. Perhaps data found in CRWMS M&O (1997a) which is used for the composition of silica fume may potentially be qualified or can eventually be classified as accepted data. However, it and all other data used from this reference (CRWMS M&O 1999g) are considered to be unqualified.

Two other sources of information 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 (Morris and Boyd 1992).

II-4.2 TYPE K CEMENT COMPOSITION

Type K cement is part grout formulation used to anchor rock bolts in the repository drift ground support (CRWMS M&O 1999g). Compositions of Type K cement are given in oxide weight percentage. These have to be converted to elemental weight percentage in order to be fed into MING as input. The oxide composition is shown in Table II-1 below.

Step 1: Calculate formula weights for each oxide. This is done by multiplying each elements 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 $1[Si]*28+2[O]*16 = 60$).

Table II-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 II-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		

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 II-20 below.

II-4.3 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 (CRWMS M&O 1999g). The source of the oxide composition of silica fume (Table II-3) was reported in CRWMS M&O (1997a) to be the data found in DTN MO9912DTMKCCOF.000. 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 II-4.2). Data for the formula weights were taken from Sargent-Welch (1979). Results are found on Table II-21 below.

Table II-3. 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

DTN: MO9912DTMKCCOF.000

Table II-4. 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		

II-4.4 SUPERPLASTICIZER COMPOSITION

Superplasticizer is part of the cement admixtures used in the grout formulation to anchor rock bolts in the repository drift ground support (CRWMS M&O 1999g). This section represents the necessary calculations to determine the appropriate elemental wt % to enter into MING V1.0 for the superplasticizer composition. Data for the rockbolt grout chemistry was taken from CRWMS M&O (1999g) and formula weight data was taken from Sargent-Welch Scientific Company (1979).

Step 1: Determine appropriate proportions of mass in one m^3 of cement (i.e. 15 * 0.6 = 9).

Table II-5. Step 1 Results.

Superplasticizer (15 kg) (CRWMS M&O 1999g)	% Composition	mass (kg)
H2O	60	9
Calcium Naphthalene Sulfonate (CNS)	40	6

Step 2: Determine the appropriate elemental mass of H_2O by first determining the fraction of hydrogen and oxygen in the formula (Formula Wt / Total Formula Wt), then calculate the elemental mass by taking the mass (kg) from above and multiplying by the fraction (mass kg * fraction).

Table II-6. Step 2 Results.

	H*2	O	H_2O Total
Formula Wt	2.0158	15.9994	18.0152
Fraction	0.1119	0.8881	1.000
Elemental Mass (kg)	1.007	7.993	9.000

Step 3: Determine the appropriate elemental mass of CNS by multiplying the fraction composition reported in CRWMS M&O (1999g, Item 1, p. III-3) by the masses determined in Step 1.

Table II-7. Step 3 Results.

CNS	C	H	S	O	Ca	Cl	Total
Wt. Fr. (CRWMS M&O 1999g)	0.403	0.033	0.107	0.322	0.134	0.001	1.0
Mass (mass kg * Wt. Fr.)	2.418	0.198	0.642	1.932	0.804	0.006	6.0

Step 4: Develop input for MING V1.0 by adding the mass for each element (from steps 2 and 3 above) then using the formula [Mass (kg)/ Total Mass (kg)] to calculate the weight fraction (Wt fr.).

Table II-8. Step 4 Results.

Element	Mass (kg) [sums of Mass]	Wt fr.
C	2.418	0.1612
H	1.205	0.0803
S	0.642	0.0428
O	9.925	0.6617
Cl	0.006	0.0004
Ca	0.804	0.0536
Totals	15.000	1.0000

These weight fraction values are reported as weight % values in Table II-22 below.

II-4.5 QUANTITY OF TYPE K CEMENT, SILICA FUME, AND SUPERPLASTICIZER

CRWMS M&O (1999g) reports 91 kg per meter of repository of cement grout will be used in portions of the repository drift ground support. CRWMS M&O (1999b, Attachment II) reports the maximum case masses of grout per meter of drift would be 280 kg per meter of repository. Because PA calculations are designed to be bounding and conservative, both values will be reported in this calculation. Table II-9 below shows the composition of the grout in terms of mass per volume.

Step 1: In order to distribute the appropriate mass of grout between the three materials calculate the proportion of the mass of each of the three materials (Type K Cement, Silica Fume, and Superplasticizer) The percentage of each material in terms of total mass needs to be determined.

Table II-9. Composition of Rock Bolt Grout as Reported in CRWMS M&O (1999g)

Component	Mass per volume (kg/m^3)
Type K cement	1420
Water	525
Silica Fume	75
Superplasticizer	15

This is done by finding the total mass of material per unit volume (2035 kg) and dividing this value into the masses of each material and multiplying by 100 as shown on Table II-10.

Table II-10. Grout Components as a Percentage of Total Mass.

Component	% of total mass
Type K cement	69.8
Water	25.8
Silica Fume	3.7
Superplasticizer	0.7

Step 2: The percentages found on Table II-10 are then multiplied by 280 kg/meter and 91 kg/meter to determine the mass of each material per linear meter of drift.

Table II-11. Masses of Grout Components per Meter of Drift.

Component	For 280 kg (kg/m)	For 91 kg (kg/m)
Type K cement	195.44	63.50
Water	72.24	23.48
Silica Fume	10.36	3.35
Superplasticizer	1.96	0.67
Total	280.00	91.00

II-4.6 WIRE AND CABLE COMPOSITION

Wire conductor and commo cables are part of the repository drift ground support design reported in CRWMS M&O (1999g). This attachment represents the calculations to determine the appropriate elemental Wt % of both materials for the wire conductor to enter into MING. Data were taken from CRWMS M&O (1999g, Attachment III). Composition of the functional groups for polyethylene polymer, neoprene polymer and cellulose were taken from Morrison and Boyd (1992). The assumption (see assumption 5 Section II-3) was made to use neoprene as the jacket/insulating material because CRWMS M&O (1999g, Attachment III) did not specify the exact composition of the EPR used in the wire conductor. Formula weights for each element were taken from Sargent-Welch Scientific Company (1979).

Step 1: Determine the appropriate Wt fraction of polyethylene found in the commo cable 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 (CRWMS M&O 1999g, Attachment III).

Table II-12. Results of Step 1.

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

Step 2: Determine the appropriate Wt fraction of neoprene found in the wire conductor by taking the composition reported in Morrison and Boyd (1992, C_4H_5Cl, Page 420), formula weights (FW) found in from Sargent-Welch Scientific Company (1979), and dividing the elemental FW by the total FW. The values are then normalized to 5% based on design input that the wire conductor insulation is 5% (by weight) (CRWMS M&O 1999g, Attachment III).

Table II-13. Results of Step 2.

C_4H_5Cl	4*C	5*H	Cl	Total
FW (from periodic table)	48.04400	5.03950	35.45300	88.53650
Wt fraction (FW/ total FW)	0.54265	0.05692	0.40043	1.00000
Normalized Wt fraction (5%)	0.02713	0.00285	0.02002	0.05000

Step 3: Determine the appropriate Wt fraction of cellulose found in the wire conductor by taking the composition reported in Morrison and Boyd (1992, $C_6H_{10}O_5$, Page 1200), formula weights (FW) found in from Sargent-Welch Scientific Company (1979), and dividing the elemental FW by the total FW. The values are then normalized to 1% based on design input that the wire conductor separator is 1% (by weight) (CRWMS M&O 1999g, Attachment III).

Table II-14. Results of Step 3.

Cellulose	6*C	10*H	O*5	Total
FW (from periodic table)	72.06600	10.07900	79.99700	162.14200
Wt fraction (FW/ total FW)	0.44446	0.06216	0.49338	1.00000
Normalized Wt fraction (1%)	0.00444	0.00062	0.00493	0.01000

Table II-25 below was developed from the values in step 1 above and the commo cable composition assumptions from CRWMS M&O (1999g, Attachment III).

- 50% Cu
- 50% Polyethylene

Table II-24 below was developed from the values in steps 2 and 3 above and the wire conductor composition assumptions from CRWMS M&O (1999g, Attachment III).

- 94% Cu.
- 5% Neoprene.
- 1% Cellulose.

II-4.7 RAIL FITTINGS COMPOSITION

This section calculates the appropriate composition for rail fittings given an unknown steel composition from CRWMS M&O (1999g, Attachment III) and a 75% to 25% steel copper mix. Because the steel composition is unspecified, we have chosen to use an A572 composition (See assumptions 2 and 3 in Section II-3 above).

Step 1: Convert steel values found in Table II-16 below to values at 75% using the following formula (Formula = Wt % (from Table II-16 below) * 0.75).

Table II-15. 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 II-23 below by taking the values above and adding 25% Cu.

II-5. RESULTS

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 CRWMS M&O (1999g).

II-5.1 MATERIAL COMPOSITIONS

The values found on Tables II-16 to II-18 are considered accepted data having been taken from the ASTM standards listed in Section 4.3.2. Note that assumptions 2 and 3 apply to the use of Table II-16.

Table II-16. Composition of ASTM A572 Steel Used in Conductor Bar Fittings, Steel Set Ground Support, Inverts, and Loading Dock.

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

Table II-17. Composition of ASTM-F432-95 Steel used in Rock Bolts. Note: Bolt Component Values used for All Components of the Set.

Element	Wt %
C	0.79
P	0.058
S	0.13
Fe	99.022

Table II-18. 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 II-19 were taken directly from CRWMS M&O (1999g).

Table II-19. Composition of Steel used in WWF

Element	Wt %
C	1.0
P	0.1
S	0.1
Fe	98.8

The values found on Table II-20 below show the elemental composition of Type K Cement. These data are considered unqualified because the source DTN (MO9912SEPMKTDC.000) is unqualified.

Table II-20. Composition of Type K Cement as Calculated in Section II-4.2.

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 II-21 below show the composition of silica fume. These data are considered unqualified because the source DTN (MO9912DTMKCCOF.000) is unqualified.

Table II-21. Elemental Composition of Silica Fume as Calculated in Section II-4.3

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

The values found on Table II-22 are considered unqualified because values for the superplasticizer composition found in CRWMS M&O (1999g) have not been reported as either accepted or qualified data.

Table II-22. Composition of Superplasticizer as Calculated in Section II-4.4

Element	Wt %
C	16.12
H	8.03
S	4.28
O	66.17
Cl	0.04
Ca	5.36

The values found on Table II-23 are considered unqualified because values for the rail fittings composition reported in CRWMS M&O (1999g) have not been reported as either accepted or qualified data. The results found on Table II-23 below are based on assumption 2 reported in Section II-3 above.

Table II-23. Composition of Rail Fittings as Calculated in Section II-4.7.

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

The values found on Table II-24 are considered unqualified because values for the wire conductor composition reported in CRWMS M&O (1999g) have not been reported as either accepted or qualified data. The results found on Table II-24 below are based on assumption 5 reported in Section II-3 above.

Table II-24. Composition of Wire Conductor as Calculated in Section II-4.6.

Element	Wt %
Cu	94.000
C	3.158
H	0.347
Cl	2.002
O	0.493

The values found on Table II-25 are considered unqualified because values for the commo cable composition reported in CRWMS M&O (1999g) have not been reported as either accepted or qualified data. The results found on Table II-25 below are based on assumption 6 reported in Section II-3 above.

Table II-25. Composition of Commo Cable as Calculated in Section II-4.6.

Element	WT %
Cu	50.000
C	42.82
H	7.18

II-5.2 MATERIAL QUANTITIES

The masses reported below are taken and summarized from in CRWMS M&O (1999g). The values found in the following tables are considered unqualified because values for material quantities reported in CRWMS M&O (1999g) have not been reported as either accepted or qualified data. Note that assumptions 1, 3, and 4 apply to the use of the following tables where appropriate.

Table II-26. Quantities of Materials in a One Lineal Meter Segment of Repository Drift for Lithophysal Areas (~70% of Emplacement Drift Length)

Item	Elemental Composition	Quantity kg/m
Steel Set Ground Support	Table II-16	369*
WWF Steel	Table II-19	70
Gantry Rail	Table II-18	133.9
Rail fittings	Table II-23	10.05*
Steel Invert	Table II-16	587*
Conductor Bar Fittings	Table II-16	0.2*
Commo cable	Table II-25	0.79

*Total amount of ASTM A572 for input into MING is 966.25 kg/m

Table II-27. 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
Rock Bolts/Plates	Table II-17	48
WWF Steel	Table II-19	70
Rail fittings	Table II-23	10.05*
Steel Invert	Table II-16	587*
Gantry Rail	Table II-18	133.9
Type K Cement	Table II-20	63.5
Silica Fume	Table II-21	3.35
Superplasticizer	Table II-22	0.67
Conductor Bar Fittings	Table II-16	0.2*
Commo cable	Table II-25	0.79

*Total amount of ASTM A572 for input into MING is 597.25 kg/m

ATTACHMENT III: WASTE PACKAGE DESIGN INPUT PARAMETERS

III-1. PURPOSE

This attachment reduces the information reported to PA from WPO (CRWMS M&O 1999h and 1999i) to useable parameters required as input to MING V1.0 (CSCI 30018 V1.0) for calculation of the effects of potential in-drift microbial communities as part of the microbial communities model as outlined in CRWMS M&O (1999e).

III-2. METHOD

Data that have been delivered to PA may be complete and necessary for other PA 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 the AP-3.14Q Input Transmittals 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 lineal meter of either waste package or repository.

All input info is converted into this format depending on how the Waste Package Design information was reported to Performance Assessment Operations via input transmittal (CRWMS M&O, 1999h and 1999i).

III-3. ASSUMPTIONS

No assumptions were made.

III-4. INPUTS AND RESULTS

III-4.1 MATERIAL QUANTITIES

The source of the information found herein was taken from CRWMS M&O (1999h) and DOE (1992) and is based on preliminary design information. Therefore, the values reported are considered to be unqualified.

CRWMS M&O (1999h) reports 4 major waste package types: 21-PWR, 44-BWR, 5-DHLW and Navel SNF. The tables below report the waste package materials and the masses for each type. In addition, average lengths of the waste packages are reported and are included in the tables below.

Table III-1. Masses and Materials for a 21-PWR Waste Package with Length of 5.335 Meters.

Material	Mass (kg)	Mass per meter of Waste Package (kg/m)
Alloy C-22	6260	1173
316NG	11237	2106
A516	5725	1073
Neutronit A978	2062	387
Aluminum 6061	335	63
CNSF*		

* CNSF values are calculated in Attachment IV

Table III-2. Masses and Materials for a 44-BWR Waste Package with Length of 5.335 Meters.

Material	Mass (kg)	Mass per meter of Waste Package (kg/m)
Alloy C-22	6400	1200
316NG	11520	2159
A516	7242	1358
Neutronit A978	2142	401
Aluminum 6061	340	64
CNSF*		

* CNSF values are calculated in Attachment IV

Typical Hanford, Savanna River, and INEL DHLW pour canisters are reported to weigh 500kg each (DOE 1992, Table 3.1.1). Each DHLW waste package will contain 5 canisters; therefore, the mass of 304L stainless steel for each package would be 2500 kg.

Table III-3. Masses and Materials for a 5-DHLW Waste Package (Including Pour Canisters) with Length of 3.840 Meters.

Material	Mass (kg)	Mass per meter of Waste Package (kg/m)
Alloy C-22	7852	2045
316NG	11286	2939
A516	3802	990
304L	2500	651
DHLW*		

* DHLW values are calculated in Attachment IV

No information has been provided on the Naval SNF waste package internal materials or fuel types; therefore, only the waste package outer and inner barrier materials are presented here.

Table III-4. Masses and Materials for a Naval SNF Waste Package with Length of 6.525 Meters.

Material	Mass (kg)	Mass per meter of Waste Package (kg/m)
Alloy C-22	10791	1654
316NG	17399	2667

In addition to the waste packages, two additional items are included in the waste package design, namely, the titanium drip shield and the waste package pallet. Each of these items has been reported in CRWMS M&O (1999h) and the materials and masses are reported below.

Table III-5. Masses and Materials for the Drip Shield Design using a Waste Package Length of 5.335 Meters.

Material	Mass (kg)	Mass per meter of Waste Package (kg/m)
Alloy C-22	86	16
Titanium Grade 7	3001	563

Table III-6. Masses and Materials for the Waste Package Pallet Design using a Waste Package Length of 5.335 Meters.

Material	Mass (kg)	Mass per meter of Waste Package (kg/m)
Alloy C-22	1426	267
316L	682	128

III-4.2 MATERIAL COMPOSITIONS

Special instructions for compositions of 316NG stainless steel and Neutronit A978 are given in CRWMS M&O (1999i), where the composition of 316NG is the same as 316L with the exception of the carbon and nitrogen content as specified in American Society for Metals (1987) and the boron content is set at 1.6% in the composition of Neutronit A978. With the exception of data for Neutronit A978, the compositions listed in the tables below are based on the appropriate standard as listed in Section 4.3.2 above and can be considered accepted data. The composition of Neutronit A978 is taken from CRWMS M&O (1999j) and is considered unqualified.

Table III-7. Composition of 304L Stainless Steel
(ASTM A240/A 240M-97a).

Element	Percent
C	0.03
Mn	2.00
P	0.045
S	0.03
Si	0.75
Cr	20.00
Ni	12.00
N	0.10
Fe	65.045

Table III-8. Composition of 316L Stainless Steel
(ASTM A276-91a).

Element	Percent
Mn	2.00
Si	1.00
P	0.045
S	0.03
Cr	18.00
N	0.10
Mo	3.00
Fe	61.795
Ni	14.00
C	0.03

Table III-9. Composition of 316NG Stainless Steel
(ASTM A276-91a and ASM 1987).

Element	Percent
C	0.02
Mn	2.00
Si	1.00
P	0.045
S	0.03
Cr	18.00
N	0.10
Mo	3.00
Fe	61.805
Ni	14.00

Table III-10. Composition of Alloy C-22.
(ASME Section II B SB-575).

Element	Percent
Mo	14.50
Cr	22.50
Fe	6.00
W	3.50
Co	2.50
C	0.015
Si	0.08
Mn	0.50
V	0.35
P	0.02
S	0.02
Ni	50.015

Table III-11. Composition of Aluminum 6061
(ASTM B 209M-92a).

Element	Percent
Si	0.80
Fe	0.70
Cu	0.40
Mn	0.15
Mg	1.20
Cr	0.35
Zn	0.25
Ti	0.15
Al	96.00

Table III-12. Composition of A516 Carbon Steel.
(ASTM A516/A516M-90).

Element	Percent
C	0.27
Mn	1.30
P	0.035
S	0.035
Si	0.45
Fe	97.91

Table III-13. Composition of Neutronit A978 (CRWMS M&O 1999j and 1999i).

Element	Percent
C	0.04
Cr	18.50
Ni	13.00
Co	0.20
B	1.60
Fe	66.66

MO9906RIB00049.000

Table III-14. Composition of Titanium Grade 7 (ASME 1995).

Element	Percent
N	0.03
C	0.10
H	0.015
O	0.25
Fe	0.30
Pd	0.25
Ti	99.055

ATTACHMENT IV: WASTE FORM COMPOSITION DETERMINATIONS

IV-1. PURPOSE

This attachment reduces the data from the following DTN's: SN9911T0811199.003 and MO9912SPADWR90.007 to useable parameters required as input to MING V1.0 (CSCI 30018 V1.0) for calculation of the effects of potential in-drift microbial communities as part of the microbial communities model as outlined above. It also points to CRWMS M&O (1998g) and DTN: MO9911SPAAWC68.002 for the source of the remainder of the information in this attachment.

IV -2. METHOD

Data that have been delivered to PA may be complete and necessary for other PA calculations but for use in MING may be overly detailed or in a format that cannot be directly used. The calculation extracts the necessary information from the DTN's or other documents 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 design materials to be reported in two ways.

1- The material compositions (weight percentage) are required as a minimum for the following elements: C, N, P, S, Mn, and Fe.
2- Composition should include U for potential sensitivity studies on U redox reactions.
3- The mass of each material in the design should be in terms of kilograms per lineal meter of waste package.

IV-3. ASSUMPTIONS

No assumptions were used in this attachment.

IV-4. INPUTS

Table IV-1. Composition of HLW Glass.

Element	Wt%
O	44.51858
U	1.866878
Np	0.000947
Pu	0.014798
Ba	0.112037
Al	2.318745
S	0.128728
Ca	0.658172
P	0.01398
Cr	0.082104
Ni	0.730782
Pb	0.060619
Si	21.76507
Ti	0.593414
B	3.192673
Li	1.468034
F	0.031673
Cu	0.151784
Fe	7.349219
K	2.971929
Mg	0.820129
Mn	1.548915
Na	8.579966
Cl	0.115259
Total	99.09444

DTN: SN9911T0811199.003

Table IV-2. Mass of HLW Glass per Pour Canister from Savanna River.

Material	Mass
HLW	1682 kg per canister

DTN: MO9912SPADWR90.007

IV-5. RESULTS

DHLW values can be used directly from Table IV-1, however not all elements are important. Therefore, only the elements that are necessary for MING V1.0 calculations are included in Table IV-3 below.

Table IV-3. Abstracted DHLW Glass Composition for use in MING

Element	Wt%
U	1.87
S	0.13
P	0.014
Fe	7.35
Mn	1.55

DTN: SN9911T0811199.003

PWR values can be used directly from CRWMS M&O (1998g). These values have previously been abstracted for MING calculations. However, these values are not qualified. The values are shown on Table IV-4 below.

Table IV-4 Abstracted CSNF PWR Composition for use in MING

Element	Wt%
S	0.07
P	0.66
Fe	95.73
Mn	2.55
C	0.60
N	0.38

DTN: MO9911SPAAWC68.002

BWR values can be used directly from CRWMS M&O (1998g). These values have previously been abstracted for MING calculations. However, these values are not qualified. The values are shown on Table IV-5 below.

Table IV-5. Abstracted CSNF BWR Composition for use in MING

Element	Wt%
S	0.106
P	0.176
Fe	95.598
Mn	2.974
C	0.675
N	0.472

DTN: MO9911SPAAWC68.002

The mass of DHLW needs to be converted to a per meter of waste package basis. Therefore, the mass per canister (Table IV-2) is multiplied by 5 (5 pour canisters per waste package) to obtain the appropriate mass of glass per waste package. This is equal to 8410 kg of glass. This is then divided by the length of a DHLW package (3.84 m, CRWMS M&O 1999h) resulting in a mass per meter of waste package as shown on Table IV-6. Masses for BWR and PWR wastes are taken from CRWMS M&O (1998g).

Table IV-6. Mass of Each Waste Form per Meter of Package.

Material	Mass (kg) per meter of waste package
PWR	32.56
BWR	34.36
DHLW	2190

DTN: MO9911SPAAWC68.002

ATTACHMENT V: REACTANT COMPOSITION DETERMINATIONS

V-1. PURPOSE

This attachment uses the data developed in attachments II, III and IV along with the inputs below to develop a useable parameter set for reactant compositions required as input to MING V1.0 (CSCI 30018 V1.0) for calculation of the energy limit to growth as part of the microbial communities model as outlined in CRWMS M&O (1999e).

V-2. METHOD

In order for MING V1.0 to conduct its energy calculations, each of the materials needs to be broken down into the associated chemical species termed "reactant compositions". In order to determine which chemical species can be selected and used within MING V1.0, Table V-1 is used to outline the available redox half reactions that can occur. Each material is then assigned the appropriate reactant compositions based on its chemical composition and general redox state. As an example, for steel set ground support which should be in its most reduced state, whose composition is found on Table II-16, a reactant composition would be assigned for each of the elements: Fe, S, C and Mn of Fe, S, CH_2O and Mn^{2+}, respectively. For the organic materials, which are comprised of several available functional groups (e.g. superplasticizer is comprised of Calcium Naphthalene Sulfonate, which has two functional groups that are attached to the naphthalene structure [SO_3Ca and CH_2O, see CRWMS M&O 1998e, Table 1]) the reactant compositions have been previously assigned and are shown on Table 29 above.

Table V-2 shows the reactant compositions for all repository materials.

V-3. ASSUMPTIONS

No assumptions were used.

V-4. INPUTS

Table V-1. Redox Half Reactions Associated with Microbial Catalysis.

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**
$CO_3^{2-} + 10H^+ + 8e^- = CH_4 + 3H_2O$	$S + H^+ + 2e^- = HS^-$
$CO_3^{2-} + 6H^+ + 4e^- = CH_2O + 2H_2O$	$S + 2H^+ + 2e^- = H_2S$
$CO_3^{2-} + 8H^+ + 6e^- = CH_3OH + 2H_2O$	$SO_4^{-2} + 9H^+ + 8e^- = HS^- + 4H_2O$
$CO_3^{2-} + 3H^+ + 2e^- = HCOO^- + H_2O$	$SO_4^{-2} + 10H^+ + 8e^- = H_2S + 4H_2O$
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**
$2NO_2^- + 8H^+ + 6e^- = N_2 + 4H_2O$	$O_2 + 4H^+ + 4e^- = 2H_2O$
$NO_3^- + 9H^+ + 8e^- = NH_3 + 3H_2O$	

MO9909SPAMING1.003

All other inputs are taken from Attachments II, III, and IV.

V-5. RESULTS

Table V-2. Reactant Compositions Used in the Energy Calculations for Each Material in the Repository and Waste Package Designs.

Material Name	Reactant Compositions
Aluminum 6061	Fe, Mn^{2+}
ASTM A572 Steel	Fe, Mn^{2+}, S, CH_2O
ASTM A579-85 Steel	Fe, Mn^{2+}, S, CH_2O
ASTM F432-95 Steel	Fe, S, CH_2O
304L Stainless Steel	CH_2O, Fe, Mn^{2+}, S
316L Stainless Steel	CH_2O, Fe, Mn^{2+}, NO_3^-, S
316NG Stainless Steel	CH_2O, Fe, Mn^{2+}, NO_3^-, S
C Steel ASTM A516	CH_2O, Fe, Mn^{2+}, S
Neutronit A978	CH_2O, Fe,
Wire Conductor	CH_2O, CH_3OH
Alloy C-22	Fe, Mn^{2+}, S, CH_2O
Conductor Bar fittings	CH_2O, Fe
Type K Cement	Fe^{2+}, SO_4^{2-},
Gantry Rail	CH_2O, Fe, S, Mn^{2+}
Rail Fittings	CH_2O, Fe, S
Ti Grade 7	NO_3^-, CH_2O, Fe
Superplasticizer	CH_2O, SO_3^{2-}
Commo Cable	CH_2O
WWF Steel	CH_2O, Fe, S
Silica Fume	Fe^{2+}, SO_4^{2-}, CH_2O
CSNF PWR	Fe, NO_3^-, CO_3^{2-}, S, Mn^{2+}
CSNF BWR	Fe, NO_3^-, CO_3^{2-}, S, Mn^{2+}
DHLW	Fe, SO_4^{2-}, Mn^{2+}