OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
CALCULATION COVER SHEET

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In-Drift Microbial Communities Model Validation Calculations

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9. Remarks
This calculation supercedes the calculations presented in Section 6.7.2 and 6.7.3 of the In-Drift Microbial Communities AMR ANL-EBS-MD-000038 Rev 00 ICN 01. It also replaces Attachment I of that document. This is due to the supersession of the following DTN MO9909SPAMING1.003 with DTN MO0106SPAIDM01.034 as documented in CAL-EBS-PA-000001 Rev 00

Revision History

10. Revision No.	11. Description of Revision
00/01	ICN to address programatic review comments from DOE prior to public release of information, changes include changing wording of repository to proposed repository throughout the document.
00/01	This ICN also addressed a minor technical comment from the DOE programatic review in Section 6.2.7.3 that did not change the results of the calculation.

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1. PURPOSE

The objective and scope of this calculation is to create the appropriate parameter input for MING 1.0 (CSCI 30018 V1.0, CRWMS M&O 1998b) that will allow the testing of the results from the MING software code with both scientific measurements of microbial populations at the site and laboratory and with natural analogs to the site. This set of calculations provides results that will be used in model validation for the *In-Drift Microbial Communities* model (CRWMS M&O 2000) which is part of the Engineered Barrier System Department (EBS) process modeling effort that eventually will feed future Total System Performance Assessment (TSPA) models.

This calculation is being produced to replace MING model validation output that is effected by the supersession of DTN MO9909SPAMING1.003 using its replacement DTN MO0106SPAIDM01.034 so that the calculations currently found in the *In-Drift Microbial Communities* AMR (CRWMS M&O 2000) will be brought up to date. This set of calculations replaces the calculations contained in sections 6.7.2, 6.7.3 and Attachment I of CRWMS M&O (2000) As all of these calculations are created explicitly for model validation, the data qualification status of all inputs can be considered corroborative in accordance with AP-3.15Q.

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

2. METHOD

In general, the method used in this calculation is to use the inputs described in Section 5 in MING V1.0 (software discussed in Section 4 below) to produce the resulting outputs that are discussed in Section 6. However, some of the subsections below have specific instructions to create the parameter input. These are as follows: 1) the determination of the iron bearing minerals in the host rock, 2) to determine the numbers of microbes in one linear meter of potential repository drift, 3) the generation of gas inputs for the LLNL lab experiments and for ambient conditions within the potential repository host rock.

2.1 MICROBIAL COUNTS

The following steps were used in Section 5.2.2 below to calculate the number of microbes in the host rock.

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

2.2 DRIFT MINERALS

The following steps were used in Section 5.2.3 below to calculate the quantity of iron bearing minerals in the host rock.

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

2.3 GAS INPUTS

2.3.1 Flask to Drift Scaling

The following steps were used in Section 5.3.2.5 below 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.

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 in Section 5.3.2.5 below to calculate the flux of atmospheric gas into a 125 ml flasks.

Determine the mass of atmospheric gases in air.

Determine the total gas available to enter the flask (kg/m^2)

Determine the daily flux into the flask (kg/m^2 day)

Determine the total cumulative flux (over 7 days) into the flask (kg/m^2).

3. ASSUMPTIONS

3.1 COMPOSITION OF MICA GROUP MINERALS

Because no specific mineral was designated, the composition of mica group mineral reported in DTN LA000000000086.002 is biotite [used in Section 5.2.3].

The rationale 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 (1985, 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. 1996, Section 4.1.3.5).

3.2 BULK DENSITY OF A MICROBE

Bulk density of a microbe is equal to the bulk density of water (1 g/cm^3) [used in Section 5.2.2].

The rationale for this assumption is because 99% of a microbe's mass is water as reported in DTN MO9909SPAMICRO.001. Any impact to the results of this calculation from not including the remaining mass would be insignificant.

3.3 BOREHOLE UZ-16 MINEROLOGY

The minerals sampled within borehole UZ-16 are representative of potential repository conditions and will serve as an appropriate surrogate for site wide properties. [used in Section 5.2.3].

The rationale for this assumption is based on Vaniman et al. (1996). 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.

3.4 FLASK RADIUS

The radius of the open end of a typical flask is 2.5 cm. [used in Section 5.3.2.5].

The flask radius was not reported in Horn et al. (1998a and 1998b) or Davis et al. (1998). A reasonable deduction can be based on the fact that a 125 ml flask is not a large flask and that 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.

3.5 GAS IN FLASK

The only gas available over seven days time is in the flask [used in Section 5.3.2.5].

The rationale 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 1 and 2). 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 6.2.7.1 where including gas as a nutrient or energy source did not significantly impact the results

3.6 RELATIVE HUMIDITY APPROXIMATION

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 5.2.1 and 5.2.4).

This will not cause any inconsistencies, 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% (CRWMS M&O 2000, Figures 6 and 7).

3.7 BIOTITE LIFETIME

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. 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. 1996, Section 4.1.3.2) and that all hematite is thought to be an alteration product of biotite [used in Section 5.2.1 and 5.2.4].

This assumption 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.

3.8 RAINIER MESA WATER AND ROCK VALUES

J-13 water and TSw tuff serve as surrogates for the tuff and water at Rainier Mesa. [used in Sections 5.2.2, 5.2.1 and 6.1.4]

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 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.

3.9 DISSOLVED ORGANIC CARBON

A value of 1 ppm dissolved organic carbon (DOC) is used to represent the organic carbon available in the groundwater entering the drift [used in Section 5.2.1].

The rationale for this assumption is that values similar to this are present in the groundwater at Yucca Mountain (Harrar et al. 1990 and CRWMS M&O 1997). *Performance Implications to the Potential Yucca Mountain Repository by the Addition of Organics to the Site Surface: The Relations Between Soil Organic Carbon, CO2 from Soil Respiration and Their Interactions with Groundwater* (CRWMS M&O 1997, page 10) presents a discussion on the DOC content of groundwater where the mean and distribution of DOC in well J-13 compares to the mean and distribution in wells in the Death Valley region and other locations within the United States. The values for J-13 water reported in CRWMS M&O (1997, page 10) report an average value for DOC of 0.96 ± 0.52 mg/l. This is equivalent to ~ 1 ppm DOC.

3.10 IDEAL GAS

Equation 3 below is based on the assumption of an ideal gas [used in Section 5.3.2.5].

The rationale for this assumption is that most real gases are nearly ideal under conditions of temperature and pressure normally encountered in the laboratory so the ideal gas law can be used quite accurately to describe their behavior.

4. USE OF COMPUTER SOFTWARE AND MODELS

The following non-exempt software package as defined in AP-SI.1Q is used in this model:

- MING V1.0 (MING V1.0 CSCI 30018 V1.0 MI 30018-M04-001, CRWMS M&O 1998c) 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 1998b and 1998d) and is appropriate for use in this calculation as a tool for conducting model validation calculations for the In-Drift Microbial Communities Model. MING V1.0 was run on a Dell Power Edge personal computer (CRWMS M&O tag # 112370 located in the EBS Department, Las Vegas, NV) using Windows NT 4.0 (build 1381, service pack 4) and Microsoft Access 97 (SR-2).

The following two commercial off the shelf software packages were used to derive and plot results reported in this calculation. They are used in an exempt manner as defined by AP-SI.1Q:

- Microsoft Excel 97: this software was used to apply equations 5 and 6 below and to tabulate and chart results (includes creation of Figures 10-12).

- SigmaPlot for Windows, Version 4.00: this software was used to chart results (includes creation of all other figures besides those listed in the bullet above)

5. CALCULATION

5.1 GENERAL INPUTS

The following inputs (Table 1) are applicable to all MING calculations and are generally included in all calculations below. Any exceptions or additions to these general inputs are noted in the discussion of each specific calculation.

Table 1. General inputs used in all MING calculations.

Input	Source
Temperature Dependent Gibbs Free Energies and Associated Half Reactions	DTN: MO0106SPAIDM01.034
Atomic Masses for Each Element	CRWMS M&O (2000), Table 19
Reactant Compositions	CRWMS M&O (2000), Attachment V Table V-2
Standard Default Input Parameters	CRWMS M&O (2000), Table 23

For each calculation case presented below, the MING output file in parenthesis (e.g. AT 1.mdb, $AT10_PD.mdb, etc.) associated with each case is listed. The files are in Microsoft Access 97 database format. The output file also includes copies of the all inputs used. These files are stored in a model warehouse data tracking number (DTN: MO0108MWDMVC01.036)

5.2 AMBIENT ESF AND NATURAL ANALOG TEST CASES

As discussed in CRWMS M&O (2000, Section 6.3.2), 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 dry wt. per gram of tuff and for the heterotrophs between 3.2×10^4 to 2×10^5 cells dry wt. 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.

Eighteen ambient calculations based on the above findings are presented below 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 build confidence in the Microbial Communities Model as implemented by MING V1.0. If reasonable estimates are obtained the model should predict microbial abundance in the drift within an order of magnitude. These predictions form the starting point for evaluating potential microbial-driven chemistry and its influence on 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. The inputs that are documented in this section for each of these three sets were entered into MING with the results being presented in Section 6.1

5.2.1 Water, Rock, Gas, Temperature and RH Inputs

In all ambient case calculations the following input parameters were utilized: the average composition of J-13 water (Table 2); an average cumulative influx of O_2, N_2 and CO_2 (Table 4) ; a potential repository temperature of 25°C; and a RH of 0.99 (see assumption 3.6). The average J-13 water chemistry values were taken from Harrar et al. (1990). These values are found on Table 33. 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 formaldehyde (CH_2O) in our simplified redox model; see CRWMS M&O 2000, Table V-2) which is the approximate value for DOC in the groundwater at Yucca Mountain (CRWMS M&O 1997). The composition of DOC is comprised of many different compounds including humic substances (CRWMS M&O 1997, Section 2.1). These compounds are too complex for the simplified redox model. Formaldyhyde was chosen to represent DOC so that this important carbon source was included in the model. The composition of rock used in the calculations are found on Table 3 and are taken from DTN: LL981209705924.059.

Table 2. J-13 Water Compositions Used in MING Calculations.

Groundwater Constituent	Concentration (kmol/m^3)
HCO_3^-	2.12E-03
O_2	1.75E-04
NO_3^-	1.42E-04
SO_4^{2-}	1.92E-04
Mn^{2+}	8.00E-07
Fe^{2+}	5.80E-07
PO_4^{3-}	3.80E-06
*DOC	3.30E-05
pH	7.4

* Data derived from Assumption 3.9.

DTN: MO9909SPA00J13.006

Table 3. 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

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 4 below.

Table 4. 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

5.2.2 Microbial Counts Input

To compare the modeled results of the ambient system in MING with the measurements presented in Section 6.3.2, the ambient microbial populations have to be converted to the equivalent unit of measurement reported by MING. Using the methodology described in Section 2.1 and the inputs listed on Table 5 below, the mass of microbes can be determined.

Table 5. Input Values for Microbial Counts Parameter Calculation.

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	
Microbial Composition MO9909SPAMICRO.001	Microbial Mass Average Microbe volume * Bulk Density of H_2O (see Assumption 3.2)	ESF Low Count	ESF High Count	Rainier Mesa Low Count	Rainier Mesa High Count
$C_{160}(H_{280}O_{80})N_{30}P_2S$	1.5E-13 g	1.78E+04	1.95E+05	5.25E+04	2.63E+05

The following formulas were used to produce the results.

1. **Mass of tuff in one meter of potential repository drift * # of cells per gram of crushed tuff** — used to get the # of cells per linear meter of potential repository.

2. **# of cells per linear meter of potential repository * average microbial mass** — used to get the mass of cells per linear meter of potential repository.

Table 6 reports the grams (dry wt) of microbes in a one-meter length segment of TSw2 tuff having a potential repository drift radius of 2.55 m. Therefore, based on the ESF measurements, the mass of microbes in one linear meter of potential repository drift ranges between 0.12 to 1.34 grams (dry). If an equivalent calculation for low and high values for the Rainier Mesa natural analog site (see assumption 3.8) was preformed, the values would fall between 0.36 and 1.81 grams (dry) per linear meter of potential repository drift.

Table 6. Determination of the Abundance of Microbes in an Area Equaling a One Linear Meter of Potential 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 5)	1.78E+04	1.95E+05	5.25E+04	2.63E+05
# of cells per linear m of potential repository	8.18E+11	8.96E+12	2.41E+12	1.21E+13
Average microbial mass (g) (Table 5)	1.50E-13	1.50E-13	1.50E-13	1.50E-13
Mass (g) of cells per linear meter of potential repository	1.23E-01	1.34E+00	3.62E-01	1.81E+00

5.2.3 Rock Mass and Biotite Mineral Inputs

To determine the mass of rock in a potential repository drift and the masses and compositions of iron in the host rock, 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 potential 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. GFW is an abbreviation for gram formula weight.

Table 7. Input Values for Rock Mass and Mineral Inputs.

Iron Mineral Types	Reported maximum mineral % in potential repository horizon tuff (borehole UZ 16)	Mineral GFW	Fe GFW	Wt. Fraction Fe	Bulk Density in potential repository horizon tuff (TMN, Flint 1998)
LA000000000086.002	LA000000000086.002 GS931208314211.047 (See Assumption 3.3)	(Sargent-Welch 1979)	(Sargent-Welch 1979)	Fe GFW /Mineral GFW	GS960908312231.004 (See Assumption 3.3)
Biotite (Mica; see Assumption 3.1)	1%	511.885	167.54	0.3273	2.25 g/cm^3
Hematite	1%	159.692	111.694	0.6994	

The following formulas were used and the methodology in Section 2.2 is used to produce the results below.

1. $\boldsymbol{pr^2h}$ — used to calculate the volume of tuff in 1 linear meter of potential repository drift.

2. **Bulk Density * Volume** — used to determine the mass of tuff per linear meter of drift.

3. **Mass per linear meter * mineral % in host rock** — used to determine the mass of material available in the potential repository drift.

4. **Elemental GFW / Mineral GFW** — used to determine the weight % of each element.

The volume of tuff in one linear meter of potential repository drift is calculated using the equation for a right circular cylinder (pr^2h) 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 linear meter of tuff in an area equaling the potential repository drift is determined, by multiplying the bulk density of Topopah Spring tuff (Table 7 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 8. Wt Fraction of Elements Comprising the Mineral Biotite and its Mass in Tuff of an Area Equal to one Linear Meter of Potential 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 9. Wt Fraction of Elements Comprising the Mineral Hematite and its Mass in Tuff of an Area Equal to One Linear Meter of Potential Repository Drift.

Hematite	**535 kg/m**
Fe	0.7
O	0.3

5.2.4 Sensitivity Test Inputs

Each of the three test case sets differed by altering two inputs that were thought to be the biggest factors to natural microbial variability, water infiltration rate and 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 10.

In addition to the infiltration rate, the material lifetime for the alteration of the potential 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 test cases below were run using the matrix of infiltration rates and material lifetimes as shown on Table 10.

Table 10. Infiltration Rates and Material Lifetimes used in TSPA-VA Ambient Test Cases (see Assumption 3.7).

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

5.2.5 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 3.7). The determination of the maximum mass of biotite that could be potentially found within a 1-meter potential 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 reported on Table 8 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 11 need to be entered into MING. These parameters (see Table 11) are based on the same premise used to develop the layer designators and reactant compositions found in CRWMS M&O (2000; Table 34 and Table V-2 respectively, as discussed in Sections 6.5.2.5 and Attachment V).

Table 11. Reactant Compositions and Layer Designator for Biotite (Table 8), Altered, and Unaltered Tuff (Table 3).

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

Case 1 (Biotite 1.mdb): This calculation was run in MING using a material lifetime on the biotite (Table 8) of 10,000,000 years and an infiltration rate of 7.8 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 2 (Biotite 2.mdb): This calculation was run in MING using a material lifetime on the biotite (Table 8) of 1,000,000 years and an infiltration rate of 7.8 mm from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 3 (Biotite 3.mdb): This calculation was run in MING using a material lifetime on the biotite (Table 8) of 100,000 years and an infiltration rate of 7.8 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 4 (Biotite 4.mdb): This calculation was run in MING using a material lifetime on the biotite (Table 8) of 10,000,000 years and an infiltration rate of 42.06 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 5 (Biotite 5.mdb): This calculation was run in MING using a material lifetime on the biotite (Table 8) of 1,000,000 years and an infiltration rate of 42.06 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 6 (Biotite 6.mdb): This calculation was run in MING using a material lifetime on the biotite (Table 8) of 100,000 years and an infiltration rate of 42.06 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

5.2.6 Altered Tuff Test Cases

Case 1 (AT 1.mdb): This calculation was run in MING using a altered tuff material lifetime (Table 3) of 10,000,000 years and an infiltration rate of 7.8 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 2 (AT 2.mdb): This calculation was run in MING using an altered tuff material lifetime (Table 3) of 1,000,000 years and an infiltration rate of 7.8 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 3 (AT 3.mdb): This calculation was run in MING using an altered tuff material lifetime (Table 3) of 100,000 years and an infiltration rate of 7.8 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 4 (AT 4.mdb): This calculation was run in MING using an altered tuff material lifetime (Table 3) of 10,000,000 years and an infiltration rate of 42.06 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 5 (AT 5.mdb): This calculation was run in MING using an altered tuff material lifetime (Table 3) of 1,000,000 years and an infiltration rate of 42.06 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 6 (AT 6.mdb): This calculation was run in MING using an altered tuff material lifetime (Table 3) of 100,000 years and an infiltration rate of 42.06 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

5.2.7 Unaltered Tuff Test Cases

Case 1 (UT 1.mdb): This calculation was run in MING using an unaltered tuff material lifetime (Table 3) of 10,000,000 years and an infiltration rate of 7.8 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 2 (UT 2.mdb): This calculation was run in MING using an unaltered tuff material lifetime (Table 3) of 1,000,000 years and an infiltration rate of 7.8 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 3 (UT 3.mdb): This calculation was run in MING using an unaltered tuff material lifetime (Table 3) of 100,000 years and an infiltration rate of 7.8 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 4 (UT 4.mdb): This calculation was run in MING using an unaltered tuff material lifetime (Table 3) of 10,000,000 years and an infiltration rate of 42.06 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 5 (UT 5.mdb): This calculation was run in MING using an unaltered tuff material lifetime (Table 3) of 1,000,000 years and an infiltration rate of 42.06 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

Case 6 (UT 6.mdb): This calculation was run in MING using an unaltered tuff material lifetime (Table 3) of 100,000 years and an infiltration rate of 42.06 mm/yr from Table 10, the gas compositions found on Table 4, and J-13 water (Table 2).

5.3 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 experimental 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.

5.3.1 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 12). Each of these media was selected to determine the limiting nutrients in the host rock at YM. Each media shown on Table 13 below was specifically selected to enable the determination of limiting nutrients in the potential 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.

Table 12. 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

Each of these media was placed in a flask in addition to a known quantity of Topopah Spring tuff (see Table 3) 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 12 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 1 and 2 respectively.

Table 13. Growth Media Compositions (kmol/m3) 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

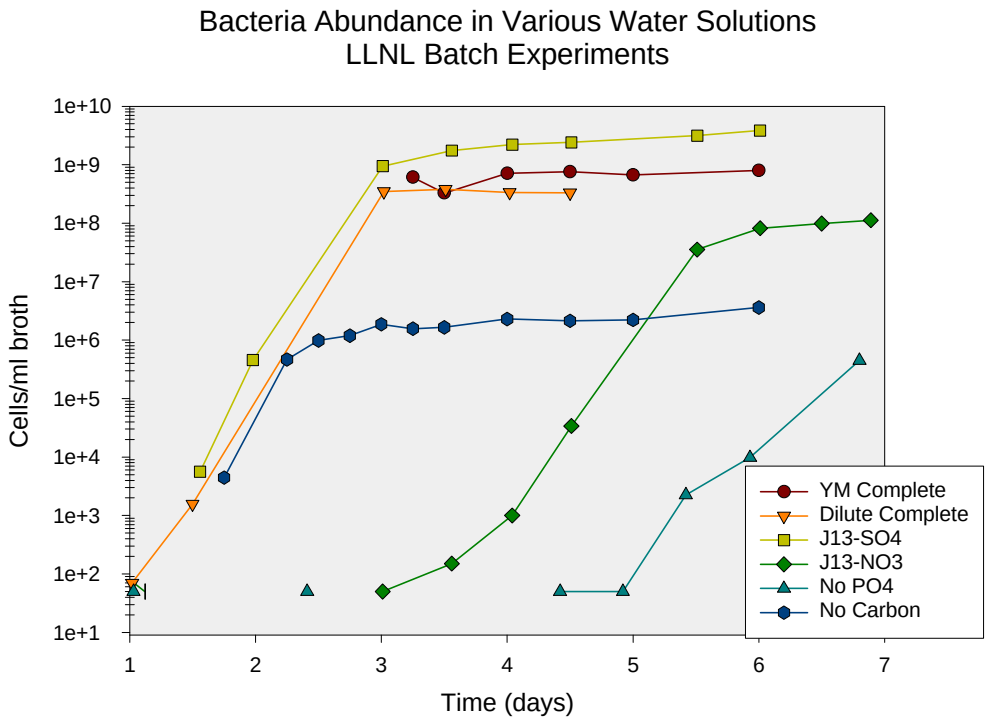

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Figure 1. Results of LLNL *In Situ* Limiting Nutrient Batch Test Growth Experiments.

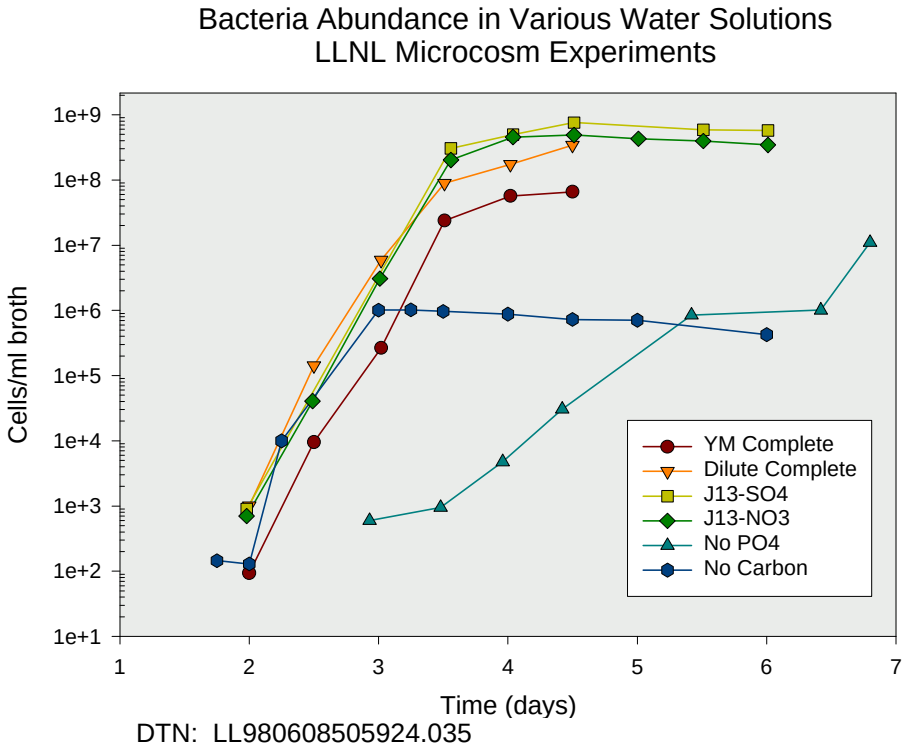

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Figure 2. Results of LLNL *In Situ* Limiting Nutrient Microcosm Test Growth Experiments.

5.3.2 Input Development

5.3.2.1 General MING Inputs

The general inputs found on Table 1 were used in the test calculations with the exception of the values that are substituted on Table 23 of CRWMS M&O (2000) as shown on Table 14 below. 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 3.6 above) and the layer designator parameters for the altered and unaltered tuff (Table 11 above).

5.3.2.2 Lab Values

In addition to the inputs specifically discussed in the sections below the following tables were used as inputs: Table 3 (composition of altered and unaltered tuff), Table 13 (compositions of the various growth media), and Table 12 (various required inputs used to simulate the lab experiments). The same method as discussed in CRWMS M&O (2000; Attachment V) was used to generate the "reactant compositions" for the altered and unaltered tuff. They are shown on Table 11.

Any parameters that were altered for sensitivity cases are presented as part of the discussion in Sections 5.3.3.7, 5.3.3.8 and 5.3.3.9.

5.3.2.3 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.

5.3.2.4 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. The results are provided in Table 12 above, and the calculations are explained below.

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 3.4 and the formula for area of a circle (pr^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 ($2prh$) is used along with the volume of a right circular cylinder (pr^2h) to determine the "tunnel length" and "drift diameter" of the MING V1.0 input.

$$19.63\ cm^2 = 2prh \qquad \text{(Eq. 1)}$$

$$125\ cm^3 = pr^2h \qquad \text{(Eq. 2)}$$

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

$$r = 12.73\ cm$$

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

$$h = 0.2454\ cm = 0.002454\ m$$

The results are shown on Table 14.

Table 14. 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

5.3.2.5 Gas Input

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 3.5). 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 assumption 3.10 and Equation 3 below.

(Volume fraction of gas in air)(Gram Formula Weight)/(22.4 $L_{(gas}$/1 $mol_{(gas)}$) (Eq. 3)

Inputs for this calculation are provided in Table 15. Argon gas is not included, as it is not a constituent for microbial growth (CRWMS M&O 2000, Section 6.3.1.10). Table 16 shows results of step 1.

Table 15. 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 16. 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 3.4 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 17 is calculated using the following formula

$$[(\text{mass of gas})\ (\text{volume of gas in flask})]/(\text{Surface Area}) \qquad \text{(Eq. 4)}$$

Table 17. 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 18.

Table 18. 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

Table 18 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 the daily value is multiplied by the number of days as shown on Table 19. These values are considered qualified values.

Table 19. 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

5.3.3 LLNL *In Situ* Limiting Nutrient Experiment Test Case

5.3.3.1 YM Complete Test ($AT10_YMC.mdb)

This calculation was run in MING using a material lifetime on the altered tuff (Table 3) of 10 years (3650 days), the gas compositions found on Table 19, and the YM-Complete (YMC) growth media composition from Table 13.

5.3.3.2 Dilute Complete Test ($AT10_dilute.mdb)

This calculation was run in MING using a material lifetime on the altered tuff (Table 3) of 10 years (3650 days), the gas compositions found on Table 9, and the Dilute Complete (DC) growth media composition from Table 3.

5.3.3.3 J-13-NO_3 Test ($AT10_NO3.mdb)

This calculation was run in MING using a material lifetime on the altered tuff (Table 3) of 10 years (3650 days), the gas compositions found on Table 19, and the J-13-NO_3 growth media composition from Table 13.

5.3.3.4 J-13-SO_4 Test ($AT10_SO4.mdb)

This calculation was run in MING using a material lifetime on the altered tuff (Table 3) of 10 years (3650 days), the gas compositions found on Table 19, and the J-13-SO_4 growth media composition from Table 13.

5.3.3.5 Phosphate Deficient Test ($AT10_PD.mdb)

This calculation was run in MING using a material lifetime on the altered tuff (Table 3) of 10 years (3650 days), the gas compositions found on Table 19, and the Phosphate Deficient (PD) growth media composition from Table 13.

5.3.3.6 Carbon Deficient Test ($AT10_CD.mdb)

This calculation was run in MING using a material lifetime on the altered tuff (Table 3) of 10 years (3650 days), the gas compositions found on Table 19, and the Carbon Deficient (CD) growth media composition from Table 13.

5.3.3.7 Gas Sensitivity Tests

These sensitivity calculations were run in MING using a material lifetime on the altered tuff (Table 3) of 10 years (3650 days), the gas compositions found on Table 19, and the CD growth media composition from Table 13. 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 10 below shows the various gas switches that were selected for each run.

5.3.3.8 Material Lifetime Sensitivity Tests

These sensitivity calculations were run in MING using a variable material lifetime on altered (AT) and unaltered tuff (UT) (Table 3) ranging from 1 year to 10,000 years, the gas compositions found on Table 19, and the YMC and PD growth media composition from Table 13. Each sensitivity calculation was done using a different material lifetime, growth media composition or rock type. Figures 10 and 11 below (Section 6.2.7.2) 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.

5.3.3.9 Groundwater Concentration and pH Sensitivity

This calculation was run in MING using a material lifetime on the altered tuff (Table 3) of 10 years (3650 days) and the gas compositions found on Table 19. 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 12 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 8). This was done by taking the values for CO_3 on Table 13 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.

5.3.4 Biomass Conversion Equations

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.

$$m/a = f \quad \text{(Eq. 5)}$$

$$f/l = b \quad \text{(Eq. 6)}$$

where:

m = MING result (g) $_{dry}$ per flask
a = Mass of average microbe (g) $_{dry}$ (see value from Table 5)
f = # of microbes in flask
l = Volume of growth media in flask (ml) (See value from Table 11)
b = # of microbes per ml growth media

Equations 5 and 6 are used to create the results tables presented in the sections below. These tables are used in creating Figures 4 through 9 shown below. The calculated results presented on these tables are plotted against both the batch and microcosm results shown in Figures 1 and 2 above.

6. RESULTS

6.1 AMBIENT CASE RESULTS

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.

6.1.1 Results of Biotite as Energy Source Test Cases

Table 20 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. However, if there were more energy available, the system would be limited by phosphorous.

Table 20. 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	0.04938237	0.0007715995	0.0007715995
2	0.3018745	0.4144265	0.006475414	0.006475414
3	0.3018745	4.064868	0.06351356	0.06351356
4	1.6278	0.0881309	0.001377045	0.001377045
5	1.6278	0.453175	0.00708086	0.00708086
6	1.6278	4.103616	0.064119	0.064119

6.1.2 Results of Altered Tuff Test Cases

Table 21 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. However, if there were more energy available, the system would be limited by phosphorous.

Table 21. 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	0.3676371	0.00574433	0.00574433
2	0.8528919	3.603831	0.05630985	0.05630985
3	2.28205	35.96576	0.561965	0.561965
4	1.682902	0.4030394	0.006297491	0.006297491
5	2.178818	3.639233	0.05686301	0.05686301
6	7.137974	36.00116	0.5625182	0.5625182

6.1.3 Results of Unaltered Tuff Test Cases

Table 22 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. However, if there were more energy available, the system would be limited by phosphorous.

Table 22. 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	0.2704675	0.004226055	0.004226055
2	0.5773832	2.632135	0.04112711	0.04112711
3	2.28205	26.24881	0.4101377	0.4101377
4	1.655351	0.3058698	0.004779215	0.004779215
5	1.903309	2.667537	0.04168027	0.04168027
6	4.382887	26.28421	0.4106908	0.4106908

6.1.4 Ambient Case Result Comparison

Figure 3 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 most of the measurements are within an order of magnitude and seem reasonable in comparison to the inputs. Generally those that do not fall within an order of magnitude are those with the ten million year material lifetimes.

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 3.8).

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 microbial growth on groundwater composition and flux, especially since the ESF experiments indicate that water is the limiting nutrient in the ambient system (Kieft et al. 1997). This may indicate that if there is sufficient water and nutrients available, the nutrients and available energy in the tuff will be utilized by microbial activity at a much more rapid rate.

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 6.7.3 below. Therefore, the ambient case allows us to

have increased confidence that MING can produce reasonable modeling results for the potential repository system.

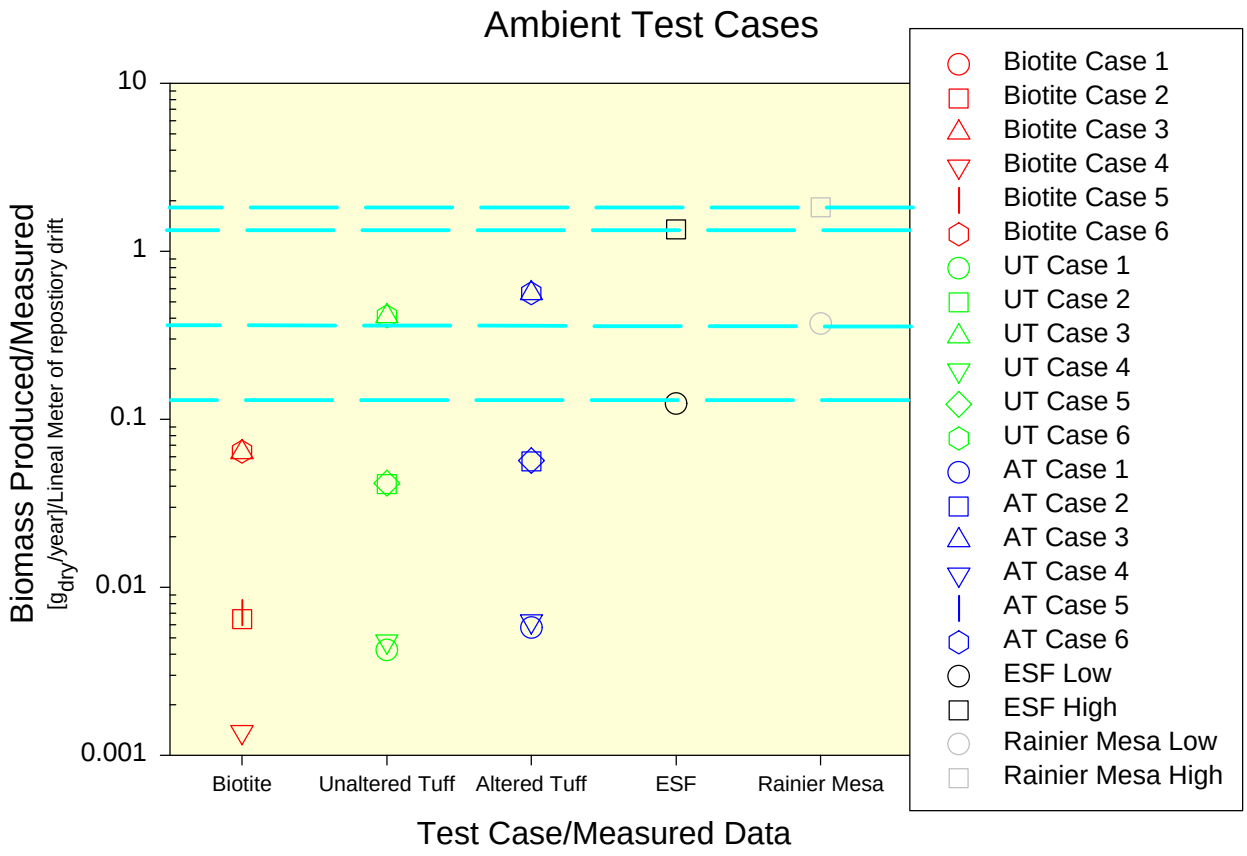

Figure 3. A Comparison of Modeled Results to Ambient Measurements.
ESF and Rainier Mesa Low and High Values are Taken from Table 6. Dashed lines represent the measured values from the ESF and Rainier Mesa.

6.2 LLNL *IN SITU* LIMITING NUTRIENT EXPERIMENT TEST CASE RESULTS

6.2.1 YM Complete Test Results

Table 23 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. Applying equations 5 and 6 (Section 5.3.4) to the calculated mass reported on Table 23 gives the values shown on Table 24. This calculated concentration (1.04E+08 cells/ml) is plotted against the batch and microcosm results and shown on Figure 4.

Table 23. 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	0.02002013	0.0003128145	0.0003128145

Table 24. Calculated Abundance of Microbes per ml of YMC Growth Media using Equations 5 and 6.

Calculated Mass (g dry) (m)	Mass of Average microbe (a)	# of Microbes in Flask (f)	ml of growth media in flask (l)	# of Microbes per ml of broth (b)
3.13E-04	1.50E-13	2.09E+09	20	1.04E+08

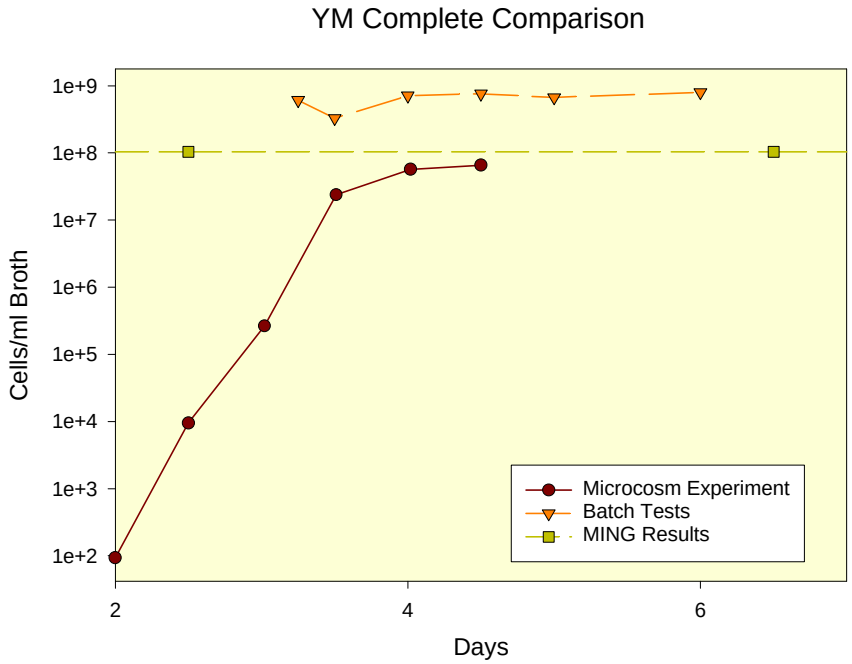

Figure 4. Comparison of Growth Rate Experiments in YMC Growth Media with Calculated Values in MING V1.0.

6.2.2 Dilute Complete Test Results

Table 25 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. Applying equations 5 and 6 to the calculated mass reported on Table 25 gives the values shown on Table 26. This calculated concentration (2.89E+07 cells/ml) is plotted against the batch and microcosm results and shown on Figure 5.

Table 25. 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	0.005551156	8.673681E-05	8.673681E-05

Table 26. Calculated Abundance of Microbes per ml of DC Growth Media using Equations 5 and 6.

Calculated Mass (g dry) (m)	Mass of Average microbe (a)	# of Microbes in Flask (f)	ml of growth media in flask (l)	# of Microbes per ml of broth (b)
8.67E-05	1.50E-13	5.78E+08	20	2.89E+07

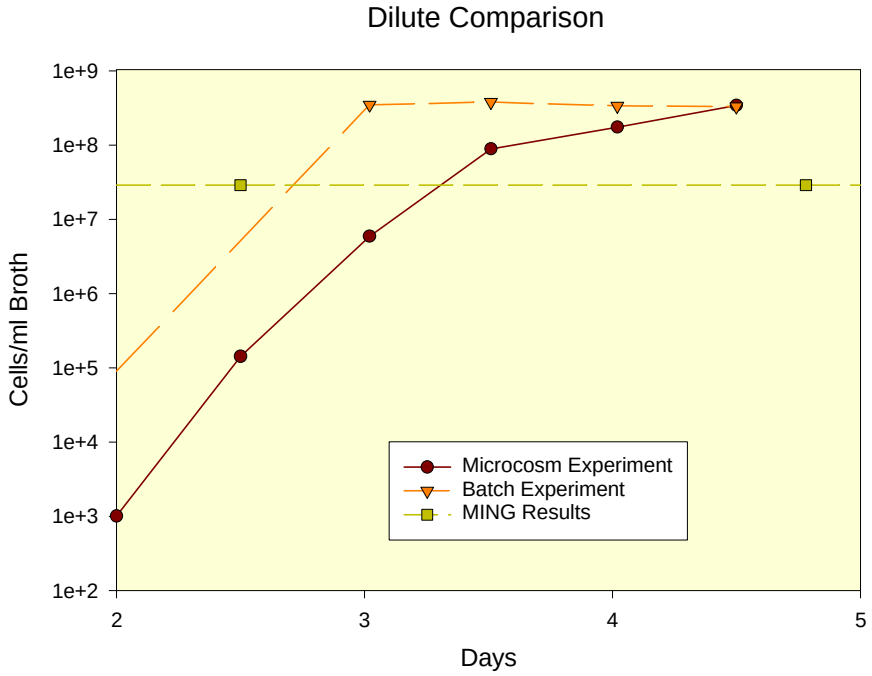

Figure 5. Comparison of Growth Rate Experiments in DC Growth Media with Calculated Values in MING V1.0.

6.2.3 J-13-NO_3 Test Results

Table 27 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. Applying equations 5 and 6 to the calculated mass reported on Table 27 gives the values shown on Table 28. This calculated concentration (2.03E+08 cells/ml) is plotted against the batch and microcosm results and shown on Figure 6.

Table 27. 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	0.0389161	0.0006080641	0.0006080641

Table 28. Calculated Abundance of Microbes per ml of J-13-NO_3 Growth Media using Equations 5 and 6.

Calculated Mass (g dry) (m)	Mass of Average microbe (a)	# of Microbes in Flask (f)	ml of growth media in flask (l)	# of Microbes per ml of broth (b)
6.08E-04	1.50E-13	4.05E+09	20	2.03E+08

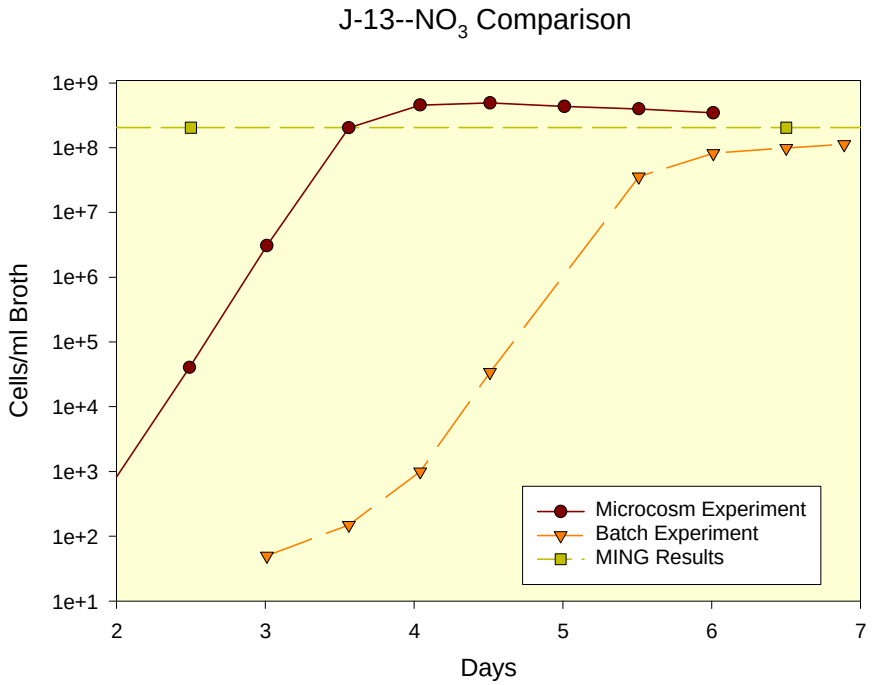

Figure 6. Comparison of Growth Rate Experiments in J-13-NO_3 Growth Media with Calculated Values in MING V1.0.

6.2.4 J-13-SO_4 Test Results

Table 29 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. Applying equations 5 and 6 to the calculated mass reported on Table 29 gives the values shown on Table 30. This calculated concentration (2.03E+08 cells/ml) is plotted against the batch and microcosm results and shown on Figure 7.

Table 29. 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	0.0389161	0.0006080641	0.0006080641

Table 30. Calculated Abundance of Microbes per ml of J-13-SO_4 Growth Media using Equations 5 and 6.

Calculated Mass (g dry) (m)	Mass of Average microbe (a)	# of Microbes in Flask (f)	ml of growth media in flask (l)	# of Microbes per ml of broth (b)
6.08E-04	1.50E-13	4.05E+09	20	2.03E+08

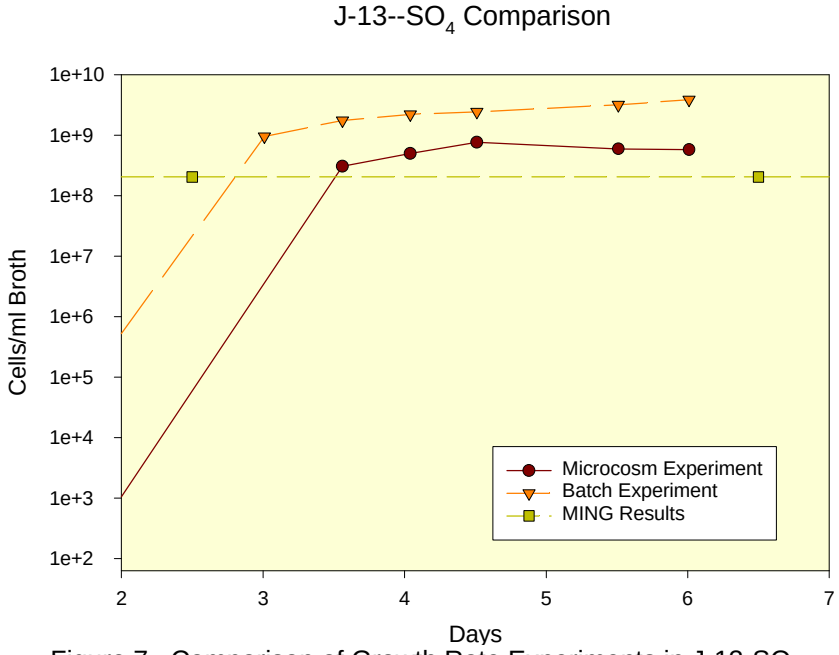

Figure 7. Comparison of Growth Rate Experiments in J-13-SO_4 Growth Media with Calculated Values in MING V1.0.

6.2.5 Phosphate Deficient Test

Table 31 shows that the system is nutrient limited. There is sufficient energy to produce more microbes. Applying equations 5 and 6 to the calculated mass reported on Table 31 gives the values shown on Table 32. This calculated concentration (1.47E+05 cells/ml) is plotted against the batch and microcosm results and shown on Figure 8.

Table 31. 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	0.0763021	0.00119222	4.412285E-07

Table 32. Calculated Abundance of Microbes per ml of PD Growth Media using Equations 5 and 6.

Calculated Mass (g dry) (m)	Mass of Average microbe (a)	# of Microbes in Flask (f)	ml of growth media in flask (l)	# of Microbes per ml of broth (b)
4.41E-07	1.50E-13	2.94E+06	20	1.47E+05

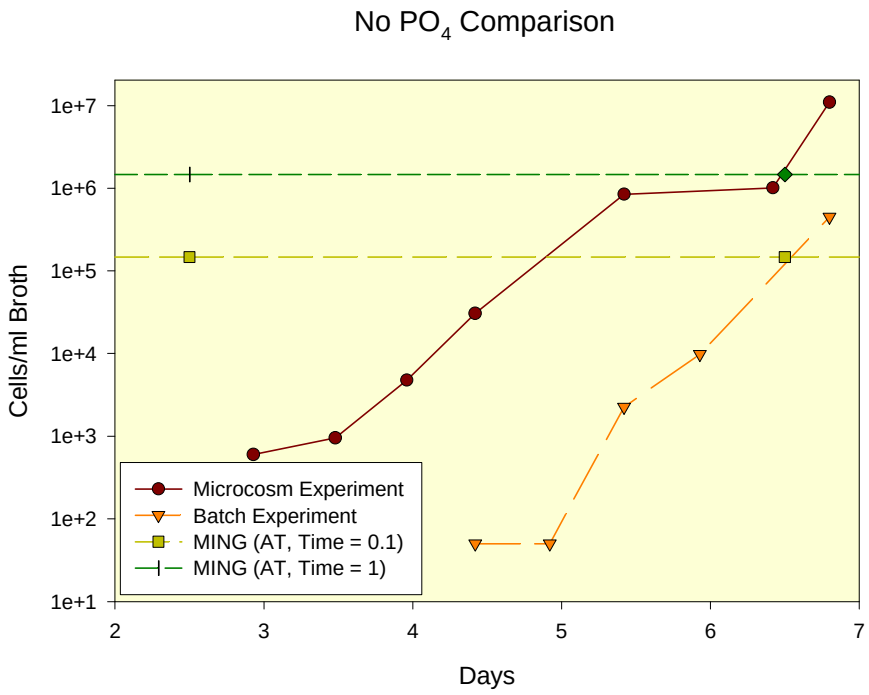

Figure 8. Comparison of Growth Rate Experiments in PD Growth Media with Calculated Values in MING V1.0. A Sensitivity Calculation (see Section 5.3.3.8) using a Modified Material Lifetime for Altered Tuff of One Year (365 Days) is also Shown.

6.2.6 Carbon Deficient Test Results

Table 33 shows that the system is energy limited. There are sufficient nutrients to produce more microbes. Applying equations 5 and 6 to the calculated mass reported on Table 33 gives the values shown on Table 34. This calculated concentration (8.34E+07 cells/ml) is plotted against the batch and microcosm results and shown on Figure 9.

Table 33. 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	0.01601219	0.0002501904	0.0002501904

Table 34. Calculated Abundance of Microbes per ml of CD Growth Media using Equations 5 and 6.

Calculated Mass (g dry) (m)	Mass of Average microbe (a)	# of Microbes in Flask (f)	ml of growth media in flask (l)	# of Microbes per ml of broth (b)
2.50E-04	1.50E-13	1.67E+09	20	8.34E+07

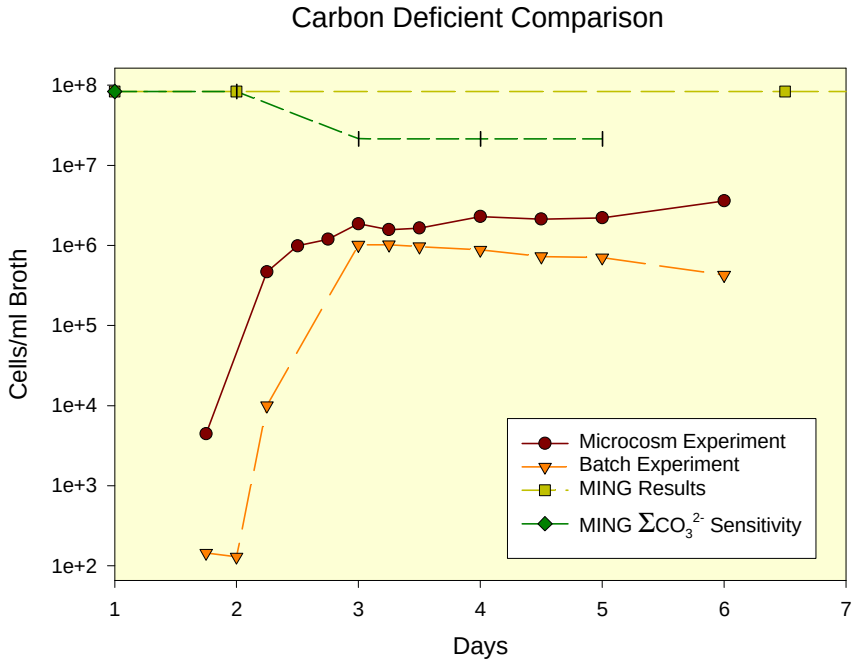

Figure 9. Comparison of Growth Rate Experiments in CD Growth Media with Calculated Values in MING V1.0. A Sensitivity Calculation using Modified Aqueous Carbonate Compositions from Table 12 Spanning Two Orders of Magnitude Decrease is also Shown.

6.2.7 Sensitivity Study Results

6.2.7.1 Gas Sensitivity Tests Results

Seven separate calculations were done in addition to the calculation presented in Section 6.2.6. Applying equations 5 and 6 to the calculated masses reported on Table 35 gives the values shown on Figure 10. Additional gas sensitivity calculation results using the Yucca Mountain complete solution are found in an excel spreadsheet (LLNL MING Compare Rev 01.xls) that can be found in the model warehouse DTN: MO0108MWDMVC01.036.

6.2.7.2 Material Lifetime Sensitivity Tests Results

Twelve separate calculations were done in addition to the calculations presented in Section 6.2.1 and 6.2.5 Applying equations 5 and 6 to the calculated masses reported on Table 36 gives the values shown on Figures 11 and 12.

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. Additional gas sensitivity calculation results are found in an excel spreadsheet (LLNL MING Compare Rev 01.xls) that can be found in the model warehouse DTN: MO0108MWDMVC01.036.

Table 35. Results of Gas Sensitivity Calculations.

Gas Switches on in Sensitivity Test	MING Output File (DTN MO0108MWDMVC01.036)	Calculated Mass of microbes (g dry)
N_2 and O_2	$AT10_CD__N2_O2.mdb	2.50E-04
CO_2 and O_2	$AT10_CD__CO2_O2.mdb	2.50E-04
N_2 and CO_2	$AT10_CD__N2_CO2.mdb	2.26E-04
N_2	$AT10_CD__N2.mdb	2.26E-04
O_2	$AT10_CD__O2.mdb	2.50E-04
CO_2	$AT10_CD_CO2.mdb	2.26E-04
All	$AT10_CD.mdb (see Section 6.2.6)	2.50E-04
None	$AT10_CD__nogas.mdb	2.26E-04

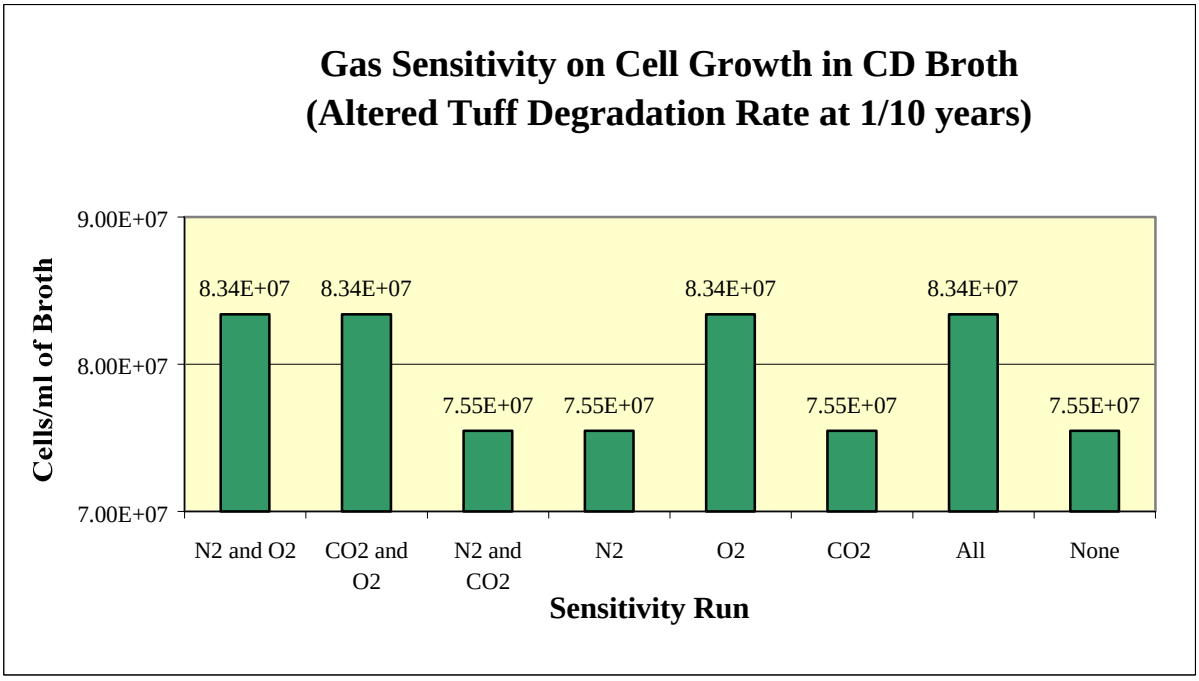

Figure 10. Comparison of Gas Sensitivity on Cell Growth using Modeled Results from the CD Growth Media.

Table 36. Results of Material Lifetime Sensitivity Calculations.

Parameters Selected	MING Output File (DTN: MO0108MWDMVC01.036)	Calculated Mass of microbes (g dry)
YMC, AT, ML=1	$AT1_YMC.mdb	3.13E-04
YMC, AT, ML=10	$AT10_YMC.mdb	3.13E-04
YMC, AT, ML=1,000	$AT1000_YMC.mdb	3.13E-04
YMC, AT, ML=10,000	$AT10000_YMC.mdb	3.13E-04
YMC, UT, ML=10	$UT10_YMC.mdb	3.13E-04
YMC, UT, ML=1,000	$UT1000_YMC.mdb	3.13E-04
YMC, UT, ML=10,000	$UT10000_YMC.mdb	3.13E-04
PD, UT, ML=10	$UT10_PD.mdb	2.21E-07
PD, UT, ML=1,000	$UT1000_PD.mdb	2.21E-09
PD, UT, ML=10,000	$UT10000_PD.mdb	2.21E-10
PD, AT, ML=1	$AT1_PD.mdb	4.41E-06
PD, AT, ML=10	$AT10_PD.mdb	4.41E-07
PD, AT, ML=1,000	$AT1000_PD.mdb	4.41E-09
PD, AT, ML=10,000	$AT10000_PD.mdb	4.41E-10

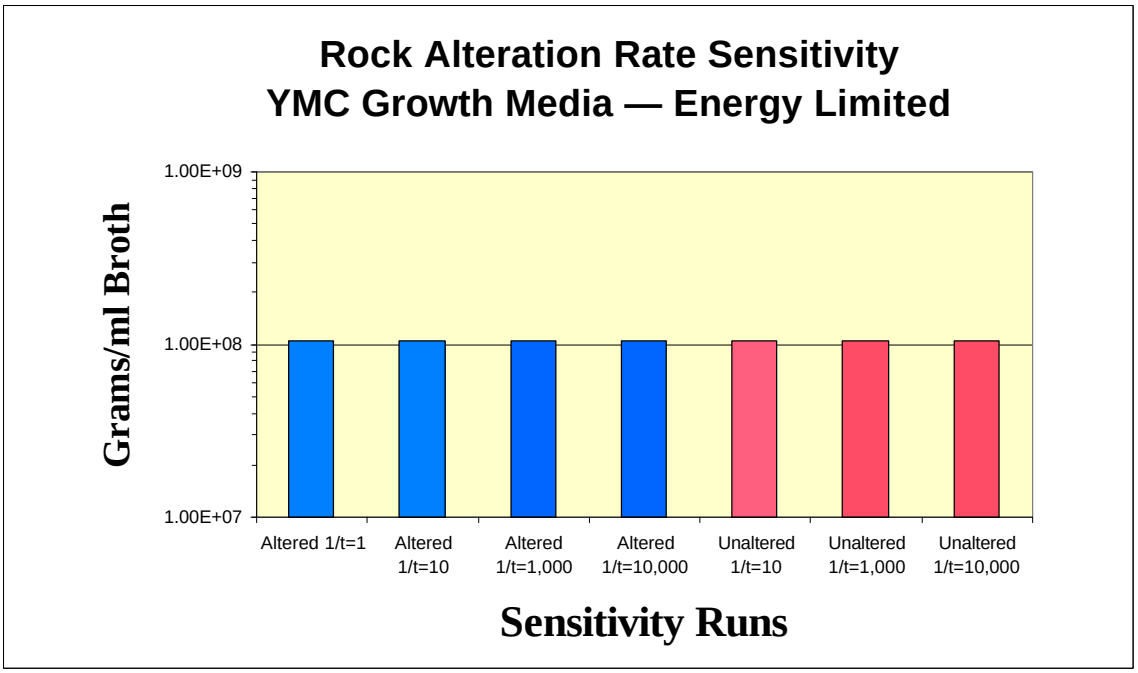

Figure 11. Results of Material Lifetime Sensitivity Calculations for Altered and Unaltered Tuff (Table 14) in an Energy Limited System using the YMC Growth Media.

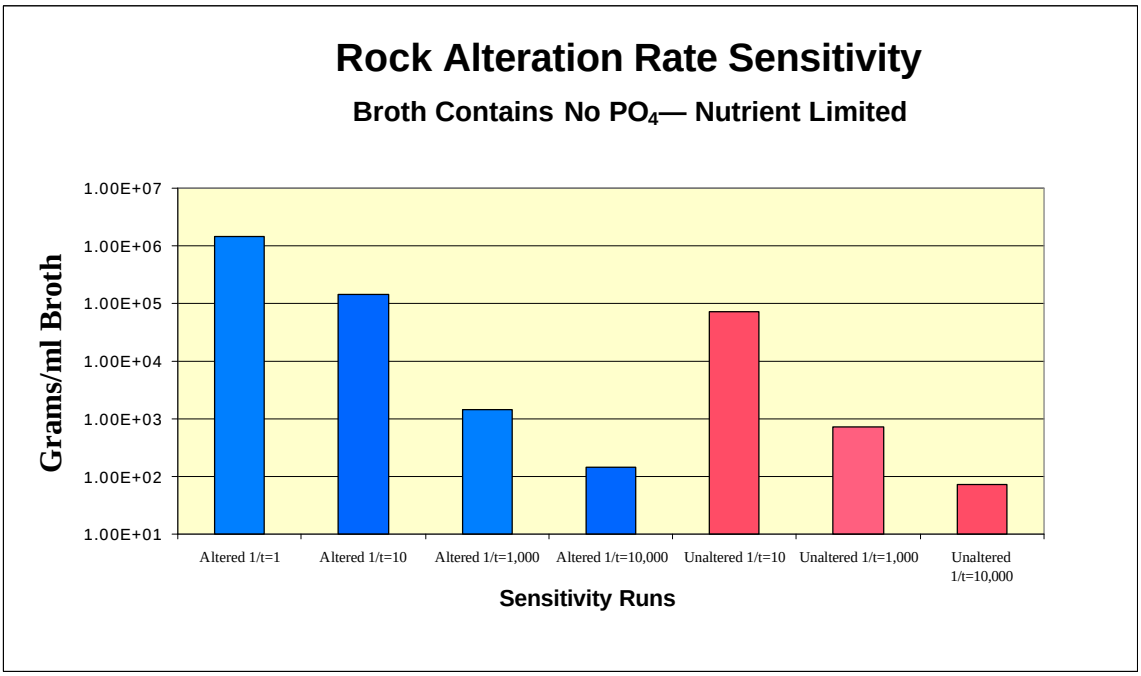

Figure 12. Results of Material Lifetime Sensitivity Calculations for Altered and Unaltered Tuff (Table 14) in a Nutrient Limited System using the PD Growth Media.

6.2.7.3 Groundwater Concentration and pH Sensitivity

Nine separate calculations were done in addition to the calculations presented in Section 6.2.6. Applying equations 5 and 6 to the calculated masses reported on Tables 37 and 38 give the values shown on Figures 13 and 9, 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 13 show that there is limited sensitivity to pH where the biomass decreases slightly with increasing pH. There is a more notable change observed due to concentration differences. The pH difference is possible due to the hydrogen ion dependence in most of the half reactions shown on Table 18. The concentration difference is occurring because some of the full reactions that produce the energy and nutrients will be different. This difference may either force a new subset of reactions above or below the 15kJ limit or some of the limiting nutrients concentrations are modified.

In these cases, an unmeasured variation in pH of ± 1 pH unit or a 10% variation of concentrations for the experimental broth formulas (Tables 11 and 12) will not force the validation calculations to fall outside the one order of magnitude level. Whether a greater variation on pH or concentrations would cause larger impacts to an energy-limited system is unknown at this time.

6.2.8 LLNL Test Case Comparison

For tests shown on Figures 4, 5, 6, and 7, 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 8 and 12). 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 10.

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 8).

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 $\pm$ 1 unit in pH (Figure 13). These differences are insignificant when compared to the general order of magnitude of the results shown on Figures 4, 5, 6, and 7.

Table 37. Results of YMC Growth Media Concentration and pH Sensitivity Calculations.

Parameters Selected	MING Output File (DTN: MO0108MWDMVC01.036)	Calculated Mass of microbes (g dry)	# of Microbes per ml of broth (b)
pH 6.2, -10%	YMC - 1om.mdb	7.85E-04	2.62E+08
pH 6.2, +10%	YMC + 1om.mdb	9.59E-04	3.20E+08
pH 6.2, YMC	$AT10_YMC.mdb	3.13E-04	1.04E+08
pH 7.2, -10%	YMC - 1om.mdb	7.73E-04	2.58E+08
pH 7.2, +10%	YMC + 1om.mdb	9.45E-04	3.15E+08
pH 7.2, YMC	$AT10_YMC.mdb	3.12E-04	1.04E+08
pH 8.2, -10%	YMC - 1om.mdb	7.57E-04	2.52E+08
pH 8.2, +10%	YMC + 1om.mdb	9.25E-04	3.08E+08
pH 8.2, YMC	$AT10_YMC.mdb	3.10E-04	1.03E+08

Table 38. Results of a Sensitivity Study on the Effects to CD Growth Media by Altering ΣCO_3 by Two Orders of Magnitude (MING output file: CD-2 order mag CO3.mdb).

Time step	Calculated Mass of microbes (g dry)	# of Microbes per ml of broth (b)
1	2.50E-04	8.34E+07
2	2.50E-04	8.34E+07
3	6.42E-05	2.14E+07

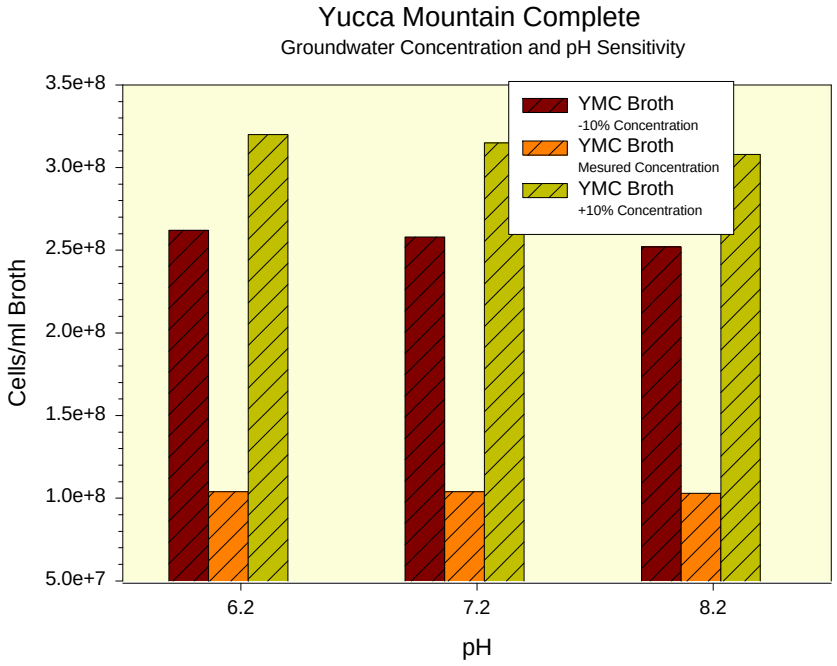

Figure 13. Results of YMC Growth Media Concentration and pH Sensitivity.

6.2.9 Statistical Comparison

For the six growth media shown on Table 39, the results show on average that MING adequately replicates the lab tests to within 17 percent and are generally accurate to within one order of magnitude. Similar calculations are found in the LLNL MING Compare Rev 01.xls file contained in the model warehouse DTN: MO0108MWDMVC01.036 for altered tuff with no gas used and unaltered tuff—both sets using a 10 year material lifetime. The results are similar. The average and standard deviation can be reduced to -0.10 ± 0.86 when considering the phosphate deficient growth media sensitivity results (Table 36) and the carbon deficient growth media sensitivity results (Table 38).

Table 39. Comparison of Calculated Results from MING to Laboratory Experiments for Six Different Growth Media

Growth Media (GM)	MING Output File (DTN: MO0108MWDMVC01.036)	Microbes Calculated in MING (per ml GM)	Maximum Microbes in Batch Tests (per mil of GM)	Maximum Microbes in Microcosm Tests (per mil of GM)	Difference Log10[MING] - Log10[batch])	Difference Log10[MING] - Log10[microcosm])
YM complete	($AT10_YMC.mdb)	1.04E+08	8.00E+08	7.70E+07	-0.88	0.13
Dilute Complete	($AT10_dilute.mdb)	2.89E+07	3.80E+06	3.43E+08	0.88	-1.07
J13-NO3	($AT10_NO3.mdb)	2.03E+08	1.12E+08	4.90E+08	0.26	-0.38
Phosphate Deficient	($AT10_PD.mdb)	1.47E+05	4.50E+05	1.10E+07	-0.49	-1.87
J13-SO4	($AT10_SO4.mdb)	2.03E+08	3.85E+09	7.60E+08	-1.28	-0.57
Carbon Deficient	($AT10_CD.mdb)	8.34E+07	1.02E+06	3.60E+06	1.91	1.36
					Average :	-0.17 ± 1.12

6.3 SUMMARY

Two sets of calculations were conducted above. The first set (see Figure 3) 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 first set 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 3 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, the variability in the natural system can be matched.

Finally, the results of the second test (Figures 4 - 7) 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, the same conclusions can be reached 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, the results demonstrate that the primary limiting nutrient in the potential repository system is phosphorous. This same conclusion was reached by Davis et al. (1998). The results 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.

The output data tracking number containing the electronic files for this calculation is listed in Section 7.4.

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