



## Scientific Analysis/Calculation Error Resolution Document

QA: QA  
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*Complete only applicable items.*

### INITIATION

1. Originator: Yifeng Wang	2. Date: 03/07/2008	3. ERD No. <b>ANL-EBS-MD-000038 ERD 1</b>
4. Document Identifier: ANL-EBS-MD-000038 Rev. 01	5. Document Title: Evaluation of Potential Impacts of Microbial Activity on Drift Chemistry	

### 6. Description of and Justification for Change (Identify applicable CRs and TBVs):

The following evaluations/changes/corrections are posted to correct the conditions identified in CR 8783. A justification for no impact to results of ANL-EBS-MD-000038 Rev. 01 or subsequent ACNs is included. See attached for a detailed description of the CR.

### CONCURRENCE

	Printed Name	Signature	Date
7. Checker	Susan LeStrange	<i>Susan LeStrange</i>	3/19/08
8. QCS/QA Reviewer	Sounia Kassabian Darnell	<i>Sounia K. Darnell</i>	03/18/2008

### APPROVAL

9. Originator	<i>for</i> Yifeng Wang	<i>Ernest Hardin</i>	3/18/08
10. Responsible Manager	Kathryn Knowles	<i>For</i> <i>Paul</i>	3-19-08

## CR 8783 Evaluation

### I. Background Information Summary:

Condition Report (CR) 8783 documents a set of issues related to Analysis/Model Report (AMR) *Evaluation of Potential Impacts of Microbial Activity on Drift Chemistry*, ANL-EBS-MD-000038 Rev. 01 (BSC 2004 [DIRS 169991], herein referred to as the AMR) which were found as part of the extent-of-condition review for CR 6334. This document presents the disposition of those issues, identifying changes to the AMR, and evaluating the impact of those changes on the conclusions of the AMR.

### II. Disposition of major issues/ Description of Change:

**Issue 1:** *Source: Pedersen, K. and Karlsson, F. 1995. Investigations of Subterranean Microorganisms: Their Importance for Performance Assessment of Radioactive Waste Disposal. TIC: 221443. 100810*

(1) Table 6.1-1 in AMR does not match Table 2.9 in reference. Second row third column does not match up well. Electron sources in AMR give specific chemical compounds, source (Table 2.9 page 56) does not list these chemical compounds.

(2) Table 6.4-1 last row maxima is 120°C, but that number is not on page 41 of reference. Reference does not give maxima.

#### AMR Changes:

(1) O<sub>2</sub>, NO<sub>3</sub><sup>-</sup>, MnO<sub>2</sub>, Fe(OH)<sub>3</sub>, SO<sub>4</sub><sup>2-</sup> are common electron acceptors, and new citation is added to support this fact. Change the footnote of Table 6.1-1 to read "Sources:" and add Chapelle, F.H. (2001 [DIRS 171162], Sections 4.6.4-4.6.7 and 10.2.2). This reference provides additional support to the argument presented and there is no impact.

(2) Change the maximum temperature for hyperthermophiles in Table 6.4-1 to 110°C. Being a lower temperature, this has no impact on the argument that only a few known isolates can withstand the temperatures predicted for the repository.

**Impact Evaluation:** Tables 6.1-1 and 6.4-1 provide general information on the metabolic constraints on microbial activity in subsurface environments. The suggested changes do not affect the conceptual model originally documented in AMR: *Evaluation of Potential Impacts of Microbial Activity on Drift Chemistry* (BSC 2004 [DIRS 169991]). Changing the maximum temperature from 120 to 110°C actually favors the argument that the high temperature induced by repository heating will inhibit microbial activity in the Yucca Mountain repository.

**Issue 2:** *Source: GS011108312322.006*

(1) Page 6-29 references 1 M ionic strength. That value [is] not found in SEP tables. This value is not listed in Section 4. (2) Page 6-23 says iron is less than 2.34 PPM, however SEP table 001 gives four values higher than this, the highest being 10.6 PPM. The TDMS truncated view has the highest value at 2.34 PPM. This is likely the reason for the error.

*They used the truncated view instead of the full list. Also this value along with the manganese and ammonia values are not listed in Section 4. (3) Page 6-37 says total carbonate concentration (41 to 430 mg/L). Formula says 41 mg bicarbonate / mL. SEP table 001 says 41 to 978 for bicarbonate. 430 is the next highest number. This value is not listed in Section 4.*

**AMR Changes:**

(1) Change the last sentence of Section 6.4.4 in the AMR to:

The current Yucca Mountain pore water is relatively dilute, as shown by a recent compilation of pore waters from the Topopah Spring welded tuff (SNL 2007 [DIRS 177412], Section 6.6; DTN: SN0705PAEBSPCE.015 [DIRS 182269], File: *Tsw\_Porewater\_Data.xls*).

(2) The maximum dissolved iron concentration stated on page 6-23 should be changed to 10.6 ppm (instead of 2.34 ppm) to reflect the full range of the data source (DTN: GS011108312322.006 [DIRS 162911]), but with the added note that iron concentrations measured in saturated zone groundwaters were generally much less than 1 ppm.

(3) The concentration range of bicarbonate in Yucca Mountain groundwater should be changed to 41 to 978 mg/L (instead of 41 to 430 mg/L) to reflect the full range of the data source (DTN: GS011108312322.006 [DIRS 162911]).

(4) The authors consider these data to provide indirect input to the arguments concerning microbial abundance, so they need not be added to Section 4.

Note: Two additional sources (SNL 2007 [DIRS 177412], Section 6.6; and DTN: SN0705PAEBSPCE.015 [DIRS 182269], File: *Tsw\_Porewater\_Data.xls*) have been added to Section 8.1 of the report and to the DIRS report.

**Impact Evaluation:** All these concentration values are used qualitatively and indirectly, to support the analysis conclusions about microbial abundance. The change to the iron concentration range for groundwaters does not impact the statements that oxidizing conditions pervade and that dissolved iron and manganese present in porewaters from the host rock are limited to trace concentrations. The change to the range of bicarbonate concentration in groundwaters does not impact the statement that dissolved inorganic carbon is much more abundant in the environment than organic carbon.

**Issue 3:** *Source: BSC (Bechtel SAIC Company) 2005. IED Waste Package Radiation Characteristics [Sheet 1 of 1]. 800-IED-WIS0-01301-000-00A. ENG.20050406.0012. 173426. Table 2 gives maximum dose rate as 1570 rad/hr for the WP Bottom lid. Not 1160 as stated in AMR. 1160 is for WP outer barrier.*

**AMR Change:** No change. The reference given (nor the superseding drawings) is not included in the AMR

**Impact Evaluation:** N/A.

**Issue 4:** *Source: Wang, Y. and Van Cappellen, P. 1996. "A Multicomponent Reactive Transport Model of Early Diagenesis: Application to Redox Cycling in Coastal Marine Sediments." TIC: 256357. 171057. The TIC source gives 1-30 micro M, but the AMR converts this to .4 to 10% Atmospheric oxygen. This conversion is not shown.*

**AMR Change:** For clarity, the discussion on p. 6-21 should be revised as follows: "Wang and Van Cappellen (1996 [DIRS 171057]) have shown that a typical limiting concentration of O<sub>2</sub> for aquatic sediments is 1 to 30 μM, above which anaerobic microbial reactions are completely inhibited. This concentration range is approximately 0.4 (= 100 x 1/231) to 10 (=100 x 30/231) percent of the value measured at the top of the seawater sediments, which was measured to be 231 μM (Wang and Van Cappellen (1996 [DIRS 171057] Table 3)."

**Impact Evaluation:** This change is for clarity only and does not impact the discussion or conclusions of the AMR.

**Issue 5:** *Section 6.3 page 6-12 second paragraph says  $6 \times 10^4$  cells per gram of dry rock, but source says  $6.9 \times 10^4$ . Also, Table 6.3-1 microbacterium barkeri is 4.5/MS in AMR but 4.55/MS in source. Also, Figure 6.4-4 graph shows data for day Zero as zero for all cases, but source shows data as zero at day 1. DTN also listed as source has no data for day zero but starts at day 1. This is probably a graph drawing error. This is a minor graphing error.*

**AMR Change:** No change. The values in the text and table are truncated instead of rounded, so that they are smaller, which is suitable for comparison to the smaller value of the threshold for genetic difference discussed in the text. Figure 6.4-4 is drawn appropriately, because at time 0 the cell density has to be zero.

**Impact Evaluation:** This issue has no impact on the discussion or conclusions of the AMR.

**Issue 6:** *NIST (National Institute of Standards and Technology) 2004. NIST Critically Selected Stability Constants of Metal Complexes Database, Users' Guide. NIST Standard Reference Database 46. Version 8.0 for Windows. TIC: 256840.[171201]. There are multiple Log K values given in the database for Lactic and Acetic acid. No direction or explanation for choosing one selected. There is no log K value for formic acid in database 46.*

**AMR Change:** Add "Values obtained for low ionic strength are used." to the source of Table 6.5-2. Also delete the row for formic acid from the table.

**Impact Evaluation:** Use of values obtained for low ionic strength is appropriate for repository relevant conditions, e.g., seepage that transports microbes into the emplacement drifts after the thermal period. Deletion of the calculation for formic complexation does not change the conclusion of negligible metabolite contributions to radionuclide mobility.

**Issue 7: Assumption:** *NOTE: Percentages of americium complexed are calculated by assuming the concentrations of intermediate metabolites to be 50  $\mu\text{M}$ . (page 6-40 Table 6.5-2)- Also formula not shown for this calculation.*

**AMR Change:** No change. The use of metabolite concentration of 50  $\mu\text{M}$  is justified on p. 6-39 of the analysis report. The formula used in the calculation is provided as Equation 6-5.

**Impact Evaluation:** N/A

**Issue 8: Calculation:** *(page 6-37 under first paragraph)-Organic Carbon calculation Page 6-37 math checked okay, however the numbers cited are not all referenced nor is the basis for the formula explained.*

**AMR Change:** Change the sentence on page 6-37 to read “Yucca Mountain groundwater contains only a trace concentration of organic carbon (1.1 mg/L) (Table 4.1-1), which is much lower than the total carbonate concentration (41 to 978 mg/L) in the solution (DTN: GS011108312322.006 [DIRS 162911]).” The other numbers used in the calculation are molecular weights.

**Impact Evaluation:** Changing the maximum bicarbonate concentration from 430 mg/L to 978 mg/L does not affect the calculation result only the minimum value is used in the calculation on page 6-37.

**Issue 9: Page 6-37 last paragraph.- Conversion of Diesel fuel.** *Math does get 1.4 grams but formula (particularly the .1/8) and justification for using  $\text{C}_8\text{H}_{18}$  is not given. Also, my source says  $\text{C}_8\text{H}_{18}$  is gasoline (not diesel) and diesel is  $\text{C}_{16}\text{H}_{34}$ .*

**AMR Change:** No change. Both gasoline and diesel fuel are mixtures of hydrocarbon compounds. Use of either  $\text{C}_8\text{H}_{18}$  or  $\text{C}_{16}\text{H}_{34}$  does not make any significant difference for the calculation result.

**Impact Evaluation:** N/A

### III. Disposition of other issues

Fifty-nine issues were raised in CR 8783 regarding indirect inputs that may have been used as direct inputs. Based on careful re-evaluation by the authors, it is decided that there is no need for making any changes in indirect inputs. It is important to note that the purpose of the AMR is to develop screening justifications for microbe-related features, events, and processes. Key input data that directly affect the conclusions of the AMR are called out in Section 4.1. The AMR does not produce output that is used directly in total system performance assessment.

#### Inputs and/or Software:

Two sources used as indirect input are added to the report to support an existing argument. SNL 2007 ([DIRS 177412], Section 6.6) and DTN: SN0705PAEBSPCE.015 [DIRS 182269],

File: *Tsw\_Porewater\_Data.xls*), otherwise, there is no change to the input values or to the software.

**Results and Conclusions:**

All issues raised in CR 8783 have been addressed. The suggested changes made to address this CR have no impact on the conclusions originally documented in the AMR. No other documents are impacted by the changes to the AMR as indicated in this ERD.

**General Note:** The resolutions described herein are for the purpose of mitigating the conditions contained in the identified Condition Reports. They are hereby conveyed by this ERD, as a means to notify all users of ANL-EBS-MD-000027 REV 03 and subsequent ACNs, of additional data or information that augments the report and should be considered, by way of explanation, part of the report.