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Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Plan for Updating the Microbial Degradation Rates for Performance Assessment

AP-116

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1 INTRODUCTION AND OBJECTIVES

This analysis plan describes a set of excursion calculations which will determine the effects of EPA's decisions regarding the rate and probability of microbial degradation on performance assessment (PA). If the results of this analysis are deemed satisfactory by the EPA, the results could potentially lead to changes to the parameter database for use in future PA.

In January, 2005, during a technical exchange meeting in Dallas, the Environmental Protection Agency (EPA) indicted that they were concerned that the implementation of the microbial degradation and gas generation process used in the CCA, PAVT, and 2004 CRA may not be sufficiently adequate considering new information available since the time of the CCA. They based this assertion on general advances in the field of microbiology made since the CCA as well as long-term (~10 years) results of gas generation experiments done at Brookhaven National Laboratory (BNL). The results of these experiments after 2-3 years duration were used to derive the microbial degradation rates for the CCA. Following this initial period, the gas generation rates (and degradation rates) dropped significantly and remained slow the remaining years until the experiments were terminated

Based on general advances in microbiology, which have found that microbes exist in a wide variety of so called "extreme" environments that were previously considered devoid of life, EPA argued that the probability that microbial degradation will occur in the WIPP should be changed from 50% to 100% of realizations. In addition, they acknowledged that there is a significant probability that microbial activity would slow considerably as microbes cycled through the available electron acceptors and the biochemical environment in the waste rooms changed with time. For this reason and because the experimental evidence suggests that long-term rates are likely much slower than the fast rates derived from the first 2-3 years of data alone, EPA also favored a reduction in the long-term microbial degradation rates used in PA.

A set of excursion BRAGFLO calculations are described that will test the effects of these changes to the probability of microbial action and the decrease in microbial degradation rates on predicted repository conditions that influence performance, such as pressure, saturation, and brine flow.

2 APPROACH

This analysis is separated into two separate but related tasks: (1) calculation of new first-order microbial degradation rates that are based on long-term BNL experimental data, and (2) implementation of new rates and associated uncertainties in BRAGFLO to test the impact of the changes on repository conditions.

2.1 Updated Microbial Degradation Rates

The first task of this analysis is to analyze the 10 years of experimental data from the BNL experiments and develop updated parameter distributions for the parameters describing the rates of microbial degradation under inundated and humid conditions: WAS_AREA: GRATMICH and WAS_AREA: GRATMICI. BRAGFLO simulates the degradation of cellulose, plastic, and rubber materials (CPR) by microbes and the subsequent production of gas. While the BNL experiments measured the accumulation of CO_2 (moles CO_2 per gram cellulose) over time, the BRAGFLO code requires as input the CPR degradation rate in units of moles of CPR consumed per kg of CPR initially present per second. The conversion between these two rates is based on the stoichiometry.

The BNL experimental data (Wang et al., 2002) used to define the gas generation rates is plotted in figures 1 to 3. Figure 1 is a plot of CO_2 generation as a function of time for inundated experiments that were anaerobic, inoculated, and given excess nutrients and nitrate. The figure includes a blue line, which defines the maximum inundated rate that was developed from the early data available at the time of the CCA. The approach used for the CCA rates is described in Appendix I of Wang and Brush (1996). The maximum CCA rate was defined as the slope between two data points (69 and 411 days) (Wang and Brush, 1996).

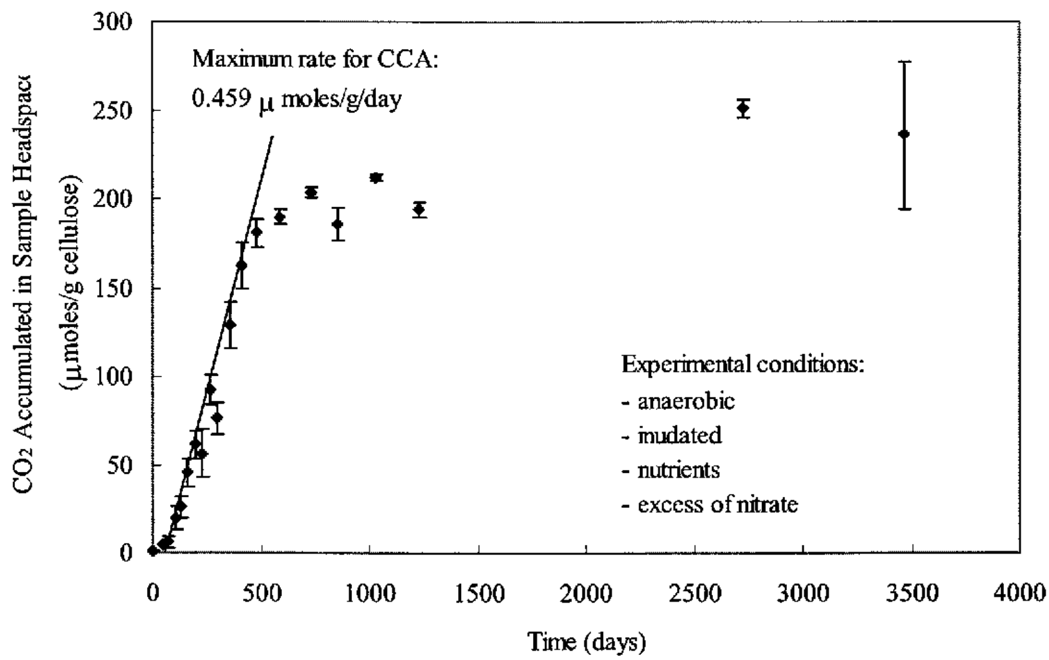

Figure 1. Carbon dioxide produced in experiments that were inundated, inoculated, amended, and with excess nitrate. Points in dark blue were available at the time of the CCA. Points in red were available later. The straight line connects the points used to determine the rate used in the CCA/CRA.

Figure 2 is a plot of CO_2 generation as a function of time for inundated experiments that were anaerobic, inoculated with microbes but unamended with nutrients. These experiments were used to define the minimum inundated rate. As in Figure 1, the minimum inundated rate used for the CCA is shown as a blue line, which is defined as the slope between two data points (0 and 1034 days) (Wang and Brush, 1996).

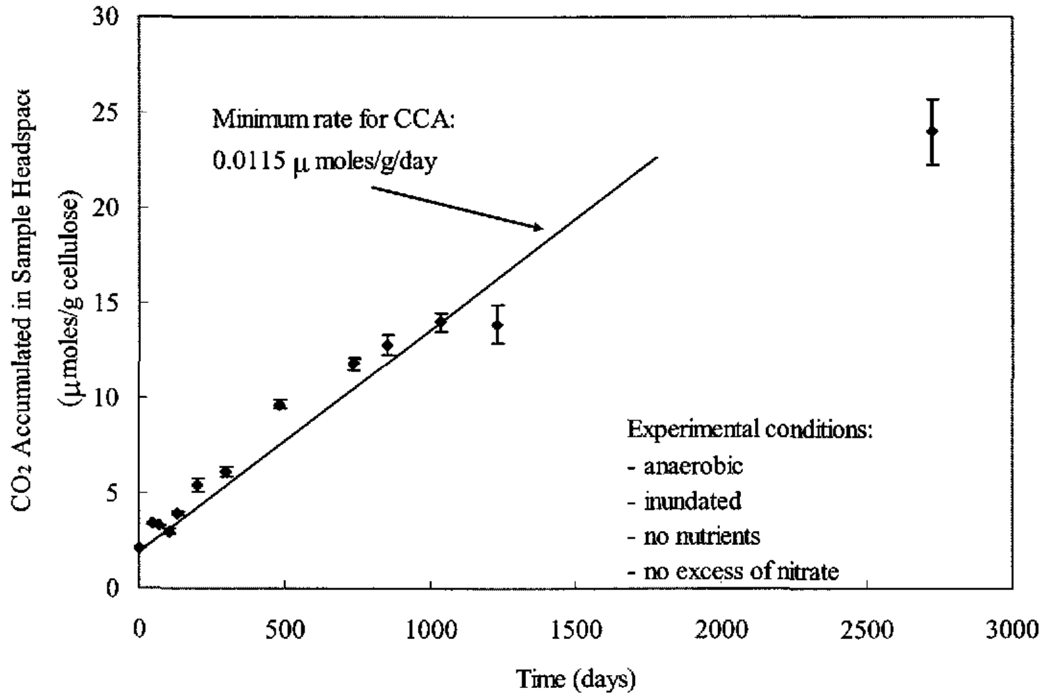

Figure 2. Carbon dioxide produced in experiments that were inundated, but were not inoculated, amended, or provided excess nitrate. Colors and lines are the same as Figure 1.

Figure 3 is a plot of CO_2 generation as a function of time for humid experiments that were anaerobic, inoculated, and unamended with nutrients. These experiments were be used to define the maximum humid rate. As in previous figures, the maximum humid rate used for the CCA is shown as a blue line, which is defined as the slope between two data points (6 and 415 days) (Wang and Brush, 1996).

The long-term BNL experimental data available after the CCA/CRA shown in red in figures 1-3 will be used to define updated gas generation rates. The calculations required to determine these rates will be included in the analysis report for this task.

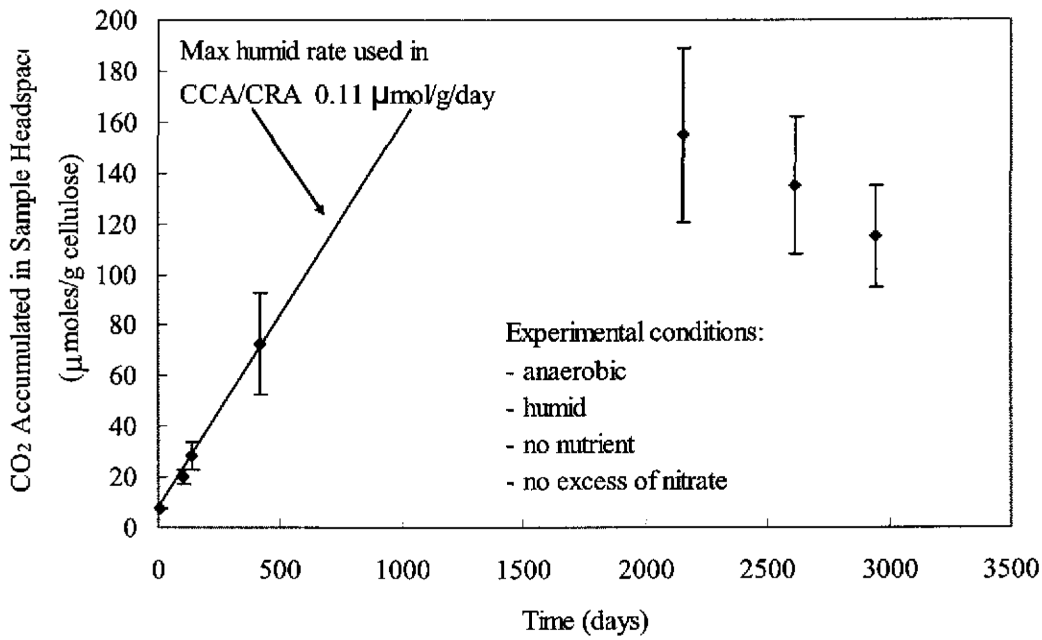

Figure 3. Carbon dioxide produced in experiments that were humid, but were not inoculated, amended, or provided excess nitrate.

2.2 Implementation in BRAGFLO

The second task of this analysis plan is to test the effect of updated microbial gas generation rates on BRAGFLO results. The BRAGFLO code is limited to a single zeroth-order reaction rate that is a function of "effective" brine saturation in each waste cell. The effective brine saturation is calculated as the sum of the predicted brine saturation and a wicking factor (WAS_AREA:SAT_WICK) with an upper limit of the sum equal to one. The wicking factor is sampled randomly from a uniform distribution between 0 and 1. The rate of microbial gas generation, q_{rgm}, used in BRAGFLO is:

$$q_{rgm} = \left(R_{mi}S_{b,eff} + R_{mh}S_g^*\right)D_c y M_{H2} \tag{1}$$

R_{mi} = inundated microbial degradation rate [mol cellulose / kg cellulose /s]
R_{mh} = humid microbial degradation rate [mol cellulose / kg cellulose /s]
$S_{b,eff}$ = effective brine saturation
S_g* = $(1-S_{b,eff})$ if $S_{b,eff} > 0$
= 0 if $S_{b,eff} = 0$
M_{H2} = molecular weight of H_2 [kg/mol]
D_c = initial mass concentration of CPR in the repository [kg/m^3]
y = average stoichiometric factor for microbial degradation of cellulose [moles of H_2 generated per mole of cellulose consumed.

The rates R_{mi} and R_{mh} will be sampled from a distribution determined from the first task of this analysis. The sampled humid rate will be further constrained to always be less than or equal to the sampled inundated rate,

$$R_{mh} = \min(R_{mi}, R_{mh}). \tag{2}$$

This will be implemented in the ALGEBRA1 input file using the following line:

GRATMICH = MIN(GRATMICH,GRATMICI).

2.2.1 Accounting for Early Gas Generation at a High Rate

In this formulation the gas generation rate used by BRAGFLO only changes as a function of brine saturation and not time. Because we intend to use degradation rates derived from long-term data it is necessary to account in some way for the gas that would have been generated in the very early period of time during which rates are observed to be much higher. As part of this task, the amount of gas that would be generated during the period of faster rates will be calculated. This gas will be accounted for by assuming that this gas is generated instantaneously at the time the repository is closed and the BRAGFLO calculations are started. This will be accomplished by precharging the repository pressure to account for the additional gas generated. The calculations that are required to define the duration of the rapid period of gas generation and the equivalent gas pressure in the repository will be included in the analysis report for this task.

2.2.2 Accounting for Additional Uncertainties in Microbial Viability

The conditions inside the WIPP are likely to be quite different from the conditions represented in the experiments, which were designed to promote microbial growth. In the WIPP the following uncertainties may cause microbial action to be reduced from that observed in the experiments:

1. Whether sterilization could prevent microbial activity in certain regions of the repository
2. Whether microbes will survive for a significant fraction of the 10,000-year regulatory period
3. Whether sufficient H_2O will be present
4. Whether sufficient quantities of biodegradable substrates will be present
5. Whether sufficient electron acceptors will be present and available
6. Whether enough nutrients will be present and available

Due to these and other uncertainties the EPA has suggested that it would be appropriate to add an additional uncertain parameter to the calculations to capture this uncertainty, at least in a qualitative sense. This parameter will be added to the definition of the degradation rate such that the final microbial gas generation rate used in BRAGFLO will be the rate defined above in equation 1 multiplied by this factor. The factor will be sampled from a uniform distribution between 0 and 1.

Thus the result will be a possible further reduction in the gas generation rates used in BRAGFLO.

2.2.3 BRAGFLO Runs

We will run two BRAGFLO scenarios (undisturbed and a disturbed scenario S2 (Castile brine pocket intrusion at 350 years) to test the effect of the changes described above. These changes include:

1. Increase probability of microbial action to 100% of realizations. In 25% of these realizations microbial degradation of cellulose, plastic and rubber materials will be allowed, while in the remaining 75% only the degradation of cellulosics will be considered.
2. Humid and inundated microbial degradation rates (WAS_AREA: GRATMICH and WAS_AREA: GRATMICI) will be updated to reflect the results of the long-term gas generation experiments. The gas generation rates needed by BRAGFLO will be multiplied by the uncertain scaling factor. The humid rate will be constrained to be less than or equal to the inundated rate.
3. Initial pressure in the waste areas will be increased to reflect the precharging of gas that may be produced in the fist couple of years at a much higher rate than will be used in the BRAGFLO calculations for 10,000 years.

Results of these calculations will be compared with similar calculations for the 2004 CRA calculations. The same LHS replicate will be used for all variables not being changed so individual vectors can be compared.

3 SOFTWARE LIST

The major codes to be used for these calculations are listed in Table 1. Calculations will be performed on the ES-40 DEC ALPHA running Open VMS Version 7.3-1

Table 1. Codes to be used in this analysis.

Code	Version
ALGEBRACDB	2.35
BLOTCDB	1.37
BRAGFLO	5.00
GENMESH	6.08
ICSET	2.22
LHS	2.41
MATSET	9.10

Code	Version
POSTBRAG	4.00
POSTLHS	4.07
PREBRAG	7.00
PRELHS	2.30
SPLAT	1.02
SUMMARIZE	2.20

4 TASKS

This analysis plan will lead to two separate but related written reports. The first report will describe the methods used to determine the new humid and inundated microbial degradation rate distributions and could be used as the basis for entering these new rates into the WIPP parameter database at a later time. The second report will document the BRAGFLO calculations and results. The schedule, tasks, and responsible individuals are outlined in Table 2.

Table 2. Tasks and responsibilities.

Estimated Date	Task(s)	Responsible
Feb 3, 2005	Prepare input files	Martin Nemer, William Zelinski
Feb 4-Feb 9, 2005	Begin BRAGFLO calculations	Bart Buell
Feb 9, 2005	Begin analysis of BRAGFLO results	Martin Nemer, William Zelinksi
Feb 15, 2005	Final BRAGFLO Analysis Package	Martin Nemer, William Zelinski

5 SPECIAL CONSIDERATIONS

None.

6 APPLICABLE PROCEDURES

Analyses will be conducted in accordance with the quality assurance (QA) procedures listed below.

Training: Training will be performed in accordance with the requirements in Nuclear Waste Management Procedure NP 2-1, Qualification and Training.

Parameter Development and Database Management: Selection and documentation of parameter values will follow Nuclear Waste Management

Procedure NP 9-2. The database will be managed in accordance with relevant technical procedure.

Computer Codes: New or revised computer codes that will be used in the analyses will be qualified in accordance with Nuclear Waste Management Procedure NP 19-1. All other codes unchanged since the PAVT are qualified under multi-use provisions of Nuclear Waste Management Procedure NP 19-1. Codes will be run on the ES-40 DEC ALPHA running Open VMS Version 7.3-1

Analysis and Documentation: Documentation will meet the applicable requirements in Nuclear Waste Management Procedure NP 9-1.

Reviews: Reviews will be conducted and documented in accordance with Nuclear Waste Management Procedures NP 6-1 and NP 9-1, as appropriate.

7 REFERENCES

Wang, Y., and Brush, L. 1996. "Estimates of Gas-Generation Parameters for the Long-Term WIPP Performance Assessment." Memorandum to Martin S. Tierney, January 26. Albuquerque, NM: Sandia National Laboratories. ERMS# 231943.

Wang, Y., Brush, L. H., Gao, H. and Stein, J. S. 2002. "Re-evaluation of Microbial Gas Generation Rates for Long-Term WIPP Performance Assessment." Albuquerque, NM: Sandia National Laboratories. ERMS# 524818