

## **Department of Energy**

Carlsbad Field Office P. O. Box 3090 Carlsbad, New Mexico 88221

August 21, 2024

Mr. Tom Peake, Director Center for Waste Management and **Regulations** Radiation Protection Division U.S. Environment Protection Agency 1200 Pennsylvania Avenue NW Washington, D.C. 20460

- Subject: Response 2 to the U.S. Environmental Protection Agency's Questions on the Replacement Panels Planned Change Request dated April 17, 2024, April 24, 2024, and May 10, 2024, from Tom Peake to Michael Gerle
- Reference: 1) EPA letter from Tom Peake to Michael Gerle, dated April 17, 2024; Subject: First set of questions on the Replacement Panels Planned Change Request
	- 2) EPA letter from Tom Peake to Michael Gerle, dated April 24, 2024; Subject: Second set of questions on the Replacement Panels Planned Change Request
	- 3) EPA letter from Tom Peake to Michael Gerle dated May 10, 2024: Subject Third set of questions on the Replacement Panels Planned Change Request

Dear Mr. Peake:

In response to the U.S. Environmental Protection Agency's (EPA) questions on the Replacement Panels Planned Change Request (RPPCR) from the abovereferenced letters dated April 17, 2024, April 24, 2024, and May 10, 2024, the U.S. Department of Energy (DOE) is responding to six of EPA's questions. The DOE will continue to submit phased responses to the EPA until all questions are addressed.

This submittal includes two enclosures:

- Enclosure 1: DOE's responses to six of EPA comments concerning the RPPCR
- Enclosure 2: Status report of DOE responses to EPA questions on the RPPCR. (The report is a table showing the status of all EPA questions received to date)

Mr. Tom Peake -2-



Below are the six responses provided in Enclosure 1.

If you have any questions, please contact Dr. Anderson Ward at (575) 706-5291.

Sincerely,



Michael Gerle, Director Environmental Regulatory Compliance Division Carlsbad Field office

Enclosures (2)

cc: w/enclosures B. Forinash, CBFO \*ED M. Hall, CBFO ED E. Garza, CBFO ED G. Basabilvazo, CBFO ED A. Ward, CBFO ED \*ED denotes electronic distribution **Enclosure 1** 

**Department of Energy Response 2 to EPA's Questions on the RPPCR** 

# **Table of Contents**



# **List of Figures**



## **List of Tables**



## <span id="page-5-0"></span>**RPPCR1-PROPMIC-1: Pu(III) PROPMIC and CAPMIC values**

Please provide a quantitative assessment on how releases are impacted if the recommended Pu(III) values from Swanson and Lucchini (2023) are utilized for PA vectors that showed only Pu(III) releases. Lucchini and Swanson (2023) recommend a PROPMIC and CAPMIC value of 3.52 and 9.00  $\times$  10<sup>-7</sup> M, respectively, for Pu(III). Their recommended values for Pu(IV) are 0.3 and  $1.22 \times 10^{-9}$  M, respectively, and are also the values chosen for all Pu microbial colloids in the RPPCR (Table 4-20 of Brunnell et al. 2023).

The current microbial colloids approach in the PA is that colloid parameter values are element-specific. However, the values that have been recommended in Lucchini and Swanson (2023) also provide oxidation state specific Pu PROPMIC and CAPMIC parameters. Consequently, the RPPCR PA does not utilize a bounding Pu(III) microbial colloids parameter value and could be underestimating releases.

Brunnell, S., Bethune, J., Dochert, P., Kicker, D. Kim, S., King, S. Long, J. Zeitler, T. 2023. Summary Report for the 2023 Replacement Panels Planned Change Request Performance Assessment, Revision 0. Sandia National Laboratories, Carlsbad, NM. ERMS 579729.

<span id="page-5-1"></span>Lucchini, J., Swanson, J. 2023. LANL ACRSP Parameter Recommendations for CRA-2024 Performance Assessment, Revision 0. Los Alamos National Laboratories, Carlsbad, NM. LCO-ACP-34.

## **DOE Response**

The RPPCR PA used the Pu(IV) values for the element-specific Pu microbial colloid parameters as the Pu(IV) state is more likely to be realized in the RPPCR PA calculations. DOE believes these are the most realistic values to use given the element-specific parameter implementation in the PA model. King and Wilgus (2024) performed the quantitative assessment requested for the sensitivity to releases when using the Pu(III) microbial colloid parameter values for vectors that realize the low oxidation state of plutonium. The sensitivity analysis done by King and Wilgus (2024) includes one new PA calculation named PCR\_MIC, based on the RPPCR PA. The only change from the RPPCR in PCR\_MIC is the adjustment of plutonium microbial colloid parameter values for vectors that realize the Pu(III) oxidation state. King and Wilgus (2024) compare results from PCR\_MIC to the RPPCR to demonstrate sensitivity. The results are described in detail in King and Wilgus (2024) and are summarized below.

The PCR\_MIC results for Salado flow and direct release volumes are qualitatively indistinguishable from the RPPCR. Slight differences in distribution and values of mobile concentrations occur between the RPPCR and PCR\_MIC with the most discernable difference being an increase of mean total mobile concentration in PCR\_MIC at times past approximately 4,000 years after repository closure (Figure 1 [Figure 11 of King and Wilgus, recreated below]). Accordingly, differences in releases between PCR\_MIC and the RPPCR are numerically small, demonstrating negligible sensitivity to the oxidation state-specific microbial colloid parameter values (Figure 2 and Table 1 [Figure 22 and Table 8 of King and Wilgus, recreated below]).



**Figure 1. RPPCR1-PROPMIC-1: Mean Total Mobile Concentration Through Time (Figure 11 from King and Wilgus, 2024. Pg 12)** 

<span id="page-6-0"></span>

<span id="page-6-1"></span>**Figure 2. RPPCR1-PROPMIC-1: Total Releases (Three-Replicate Means) (Figure 22 from King and Wilgus, 2024. Pg. 22)**

<span id="page-7-1"></span>

## **Table 1. RPPCR1-PROPMIC-1: Sta�s�cs on the Mean Total Releases (Adapted from King and Wilgus, 2024)**

## <span id="page-7-0"></span>**References RPPCR1-PROPMIC-1**

King, S., and J. Wilgus. 2024. Plutonium Microbial Colloid Sensitivity Analysis. ERMS 581471. Carlsbad, NM: Sandia National Laboratories.

## <span id="page-8-0"></span>**RPPCR2-12PanelAnalyses**

EPA is interested in the possibility of using the individual panel releases shown in Figure 3 of ERMS 580656 Estimation of Releases from a 12-Panel Repository by Hansen et al. (2023) to estimate releases from a 12 panel repository. We have the following two questions:

- 1. Please provide a detailed explanation of how the individual panel releases shown in Figure 3 of ERMS 580656 were calculated, with accompanying conceptual descriptions and justifications.
- 2. Please provide an explanation of how the individual panel releases shown in Figure 3 of ERMS 580656 accumulate to yield the combined releases of all 19 panels shown in Figure 4-43 of ERMS 581044 (the RPPCR PA).

<span id="page-8-1"></span>Hansen, C., Brunell, S., King, S. (2023). Estimation of Releases from a 12-Panel Repository, Revision 0. Sandia National Laboratories, Carlsbad, NM. ERMS 580656.

## **DOE Response**

1. Figure 3 of Hansen et al. (2023a) shows per-panel releases constructed using output from the RPPCR PA (Brunell et al. 2023). When the PA code CCDFGF is simulating intrusions for a random future, it assigns each intrusion to a waste panel based on the waste panel intrusion probabilities (Table 6 of Hansen et al. 2023b). In a standard PA calculation, releases from all future intrusions into all panels are summed together. In Hansen et al. (2023a) individual panel releases are obtained by summing releases from each panel independently. Conceptually the calculation of releases from each intrusion has not been changed for the individual panel releases; only the summing of releases before creation of the CCDFs has been changed.

Mechanically, this calculation is done with CCDFGF's option of writing to a text-based, structured diagnostic output file (Brunell 2022). This text file can be very large; the diagnostic file for Replicate 1 of the RPPCR is approximately 133 GB. The diagnostic file contains information for each intrusion in a future, including the intrusion time, the intruded panel number, intrusion type (i.e., whether a brine pocket was encountered), and releases resulting from each direct release mechanism (e.g., cuttings and cavings, spallings, or direct brine release). Figure 3 below shows an example of the data recorded for three randomly selected intrusions, intrusion numbers 60, 61, and 62, in Replicate 1, Vector 1, Future 1 of the RPPCR.

```
1, FUTURE 1, DRILL INTRUSION 60, TIME(YR)=4.012E+03, PANEL 13 (OTHER )<br>PLUG PATTERN 3, DRILL DIAM(M)=(3.111E-01)<br>NONEXCAVATED, NO BRINE POCKET HAS
OBS
        NO CUTTINGS, SPALLINGS, OR DBR RELEASES
       1, FUTURE 1, DRILL INTRUSION 61, TIME(YR)=4.057E+03, PANEL 1 (UPPER )<br>PLUG PATTERN 3, DRILL DIAM(M)=(3.111E-01)
OBS
                ATED , NO BRINE POCKET HAS<br>CUTTINGS RELEASE
       EXCAVATED
       UIIINGS RELEASE (EPA/M3)=7.604E-02, HT(M)=3.960E+00, VOL(M3)=3.011E-01, VOL FRAC=1.970E-01, FINAL VOL(M3)=5.932E-02<br>WASTE STREAM 211, INTERP TIMES(YR)=(3.000E+03,5.000E+03), RELEASES(EPA/M3)=(7.415E-05,6.797E-05), RELEASE(
       WASTE STREAM(S) AVGD= 3, AVG CONC(EPA/M3)=1.062E-03, RELEASE(EPA)=3.197E-04<br>WASTE STREAM(S) AVGD= 3, AVG CONC(EPA/M3)=1.062E-03, RELEASE(EPA)=3.197E-04
        PREVIOUS E1 INTRUSION IN DIFFERENT(NonAdjacent) PANEL AT TIME(YR)=9.777E+02, DTE1=4.057E+03-9.777E+02=3.079E+03
       FINIERP TIMES(YR)=(2.000E+03-3.500E+02,3.500E+02-1.650E+03)=(3.650E+03,0.000E+00), VOLS(M3)=(0.000E+00,0.000E+00), VOLUME(M3)=<br>INTERP TIMES(YR)=(2.000E+03-3.500E+02,3.500E+02-1.650E+03)=(3.650E+03,0.000E+00), VOLS(M3)=(0.
      0BR RELEASE<br>
PREVIDUS E1 INTRISIVING IN NOMAD (CONSULTION) - 0.777E4-02, DRICLE A 057E4-03, DRICH (N) - 1.12.<br>
NTERP TIMES (YR)=(2.000E+03-3.500E+02, 4.000E+03-3.500E+02)=(1.650E+03, 3.650E+03), VOLS(M3)=(0.000E+00), VOLUM
               DBR RELEASE
       1, FUTURE 1, DRILL INTRUSION 62,<br>PLUG PATTERN 3, DRILL DIAM(M)=(3.111E-01)
                                      DRILL INTRUSION 62, TIME(YR)=4.146E+03, PANEL 18 (OTHER )
       NONEXCAVATED, NO BRINE POCKET HAS<br>NO CUTTINGS, SPALLINGS, OR DBR RELEASES
```
#### <span id="page-9-0"></span>**Figure 3. RPPCR2-12 PanelAnalyses: Example Diagnostic Output for Replicate 1 of the RPPCR**

For the analysis in Hansen et al. (2023a), CCDFGF was run using the same inputs as the official RPPCR analysis and was instructed to output diagnostic data for all futures of all vectors in Replicate 1. To calculate per-panel releases as shown in Figure 3 of Hansen et al. (2023a), the diagnostic file produced by CCDFGF is processed using a Python script created for this purpose. Intrusions are separated by panel, and releases for each panel are summed over intrusions in each future by the release mechanism. For each panel and release mechanism, a CCDF of releases for a vector is constructed from the summed releases of all futures. The mean CCDFs are then found by calculating the average of probabilities, at each release level, for the 100 vectors in Replicate 1. Note that the releases from an individual panel in Figure 3 of Hansen et al. (2023a) represent those releases when the panel is part of the 19-panel repository modeled in the RPPCR.

2. Figure 4 below (Figure 3 of Hansen et al., 2023a) shows the mean CCDFs of total releases attributable to individual panels. Figure 5 below (Figure 4-43 of Brunell et al., 2023) shows CCDFs for each realization of total releases from the repository. A total release from the repository is the sum of releases attributable to each panel, but the CCDFs in Figure 4 below cannot be added in a manner to obtain the mean CCDF in Figure 5 below.

In the PA calculation, random futures are simulated. Each random future comprises a sequence of intrusion events (and possibly a mining event); releases from each intrusion can be attributed to the intruded panel. The releases attributed to one panel can be summed to a total release for that future and panel. The total releases can be sorted in increasing order to form a CCDF and a mean CCDF computed over all realizations. This process produces the mean CCDFs in Figure 4 below.

A total release from the repository is computed by summing, for one future, all releases from intrusions into any panel. At this point, the total release is a sum of releases attributable to individual panels. However, after the panel releases (or the total releases) are sorted to form a CCDF, the identification of a release with a future is lost. As a consequence, at a given probability, the releases from different panels, and the total release, may be from different futures. Thus, the per-panel CCDFs cannot be "added" to obtain the CCDF of total releases.



<span id="page-10-0"></span>**Figure 4. RPPCR2-12PanelAnalyses: Total Mean Releases by Panel for Replicate 1 of the RPPCR (Figure 3 of Hansen et al. 2023a)**



<span id="page-11-1"></span>**Figure 5. RPPCR2-12PanelAnalyses: Total Releases for Replicate 1 of the RPPCR (Figure 4-43 of Brunell et al. 2023)**

#### <span id="page-11-0"></span>**References RPPCR2-12PanelAnalyses**

Brunell, S. 2022. Design Document and User's Manual for CCDFGF Version 8.01. ERMS 577625. Carlsbad, NM: Sandia National Laboratories.

Brunell, S., J. Bethune, P. Docherty, D. Kicker, S. Kim, S. King, J. Long, and T. Zeitler. 2023. Summary Report for the Replacement Panels Planned Change Request Performance Assessment, Rev. 1. ERMS 581044. Carlsbad, NM: Sandia National Laboratories.

Hansen, C., Brunell, S., King, S. 2023a. Estimation of Releases from a 12-Panel Repository, Rev. 0. ERMS 580656. Carlsbad, NM: Sandia National Laboratories.

Hansen, C., S. King, J. Bethune, and S. Brunell. 2023b. Analysis Plan for the Performance Assessment for Replacement Panels Planned Change Request. AP-204, Rev. 1, ERMS 579449. Carlsbad, NM: Sandia National Laboratories.

## <span id="page-12-0"></span>**RPPCR3-CLOSURE-1: Closure of Rooms with New Design**

Please describe the effect of the room closure process with the new design used for RPPCR PA: the abutment pillars (between the waste rooms and the [main] access drifts) are increased from 61.0 m (200 ft) to 122.0 m (400 ft) and the isolation pillars (separating two panels) are increased from 61.0 m (200 ft) to 91.5 m (300 ft).

*EPA would like to know the effect of the new design on the waste-containing areas. Would this affect the timeframe of creep closure? Should this design change have any effect on the room closure, porosity, and gas generation relationship? Would this be reflected in the updated porosity surface?* 

## <span id="page-12-1"></span>**DOE Response**

The proposed widening of the abutment and isolation pillars will decrease the shear stresses in the salt strata surrounding the neighboring access drifts and rooms. By reducing the shear stresses the salt should crack less, such that ground control efforts should be reduced during the operational period (U.S. DOE, 2024, Section 3.0). Reducing the shear stresses will also reduce the rate of salt creep and room closure. The reductions, however, are expected to have a small enough impact on room porosity that they can be ignored in the WIPP Performance Assessment, as discussed in the following three paragraphs.

Cracking is generally thought to have a minor influence on the porosity of waste filled rooms (Vignes et al., 2023, Section 2.1.2). Although the impact of micro- and macro-cracks around waste filled rooms is an active area of research, other factors—such as the lithostatic pressure, the resistance of the room contents, and the viscoplastic behavior of the salt—are considered more important influences on porosity. Accordingly, the effects of cracking are not included in the disposal room porosity model (Vignes et al., 2023, Section 2.1.2), and reducing cracking by widening pillars is not expected to significantly affect room closure/expansion rates.

Previous simulations of room closure by Stone and Argüello (Butcher and Mendenhall, 1993, pg. A-121 to A-134) indicate that salt creep rate reductions related to wider abutment and isolation pillars will be small compared to other variations. Several aspects of the Stone and Argüello model differ from those in the current disposal room porosity model: their model does not include salt creep behavior at low stresses (< 8 MPa), salt transient creep behavior, the anhydrite layers, the clay seams, the waste, or gas trapped within the room. Nevertheless, the trends they found should be similar to the trends that would be predicted by the current disposal room porosity model, presuming the model differences do not strongly interact with the pillar width. As shown in Figure 6 below, one of the Stone and Argüello simulations included the seven rooms that make up a panel, as well as the two neighboring main access drifts. Room 1 was at the far-right end of the panel, adjacent to a practically infinite-width pillar, while Room 7 was to the right of the 61.0 m wide abutment pillar. Another of their simulations considered a single disposal room within an infinite array of parallel rooms. The vertical closure rates from these three cases are compared by averaging the vertical closure rate from time = 0 to the time the roof touches the floor in the fastest case, which is 140 years for the infinite array of parallel rooms. The Stone and Argüello model predicted that Room 1's average vertical closure rate would be 7 % less than that of Room 7. Doubling the width of the abutment pillar should, therefore, reduce the rate of room closure by less than 7 %. To put this 7 % in perspective, Stone and Argüello also predicted that Room 1's average vertical closure rate

would be 22 % less than that of the room in the infinite array (see Figure 7 and Figure 8 below). The legacy and current disposal room porosity models already neglect this 22 % reduction in closure rates by considering an infinite array of parallel disposal rooms (Stone, 1997, pg. 14; Vignes et al., 2023, Section 2.1.4), so a 7 % reduction is small. The Stone and Argüello model did not consider the effects of the isolation pillars between each panel, but it seems reasonable to expect that increasing their width should cause similar reductions in closure rates (< 7%) to the access drifts and parts of rooms close to these isolation pillars.



<span id="page-13-0"></span>**Figure 6. RPPCR3-Closure-1: Schematic of the simulation domain and boundary conditions utilized by Stone and Argüello (Butcher and Mendenhall, 1993, pg. A-130)**



<span id="page-13-1"></span>**Figure 7. RPPCR3-Closure-1 Stone and Argüello's predictions of vertical closure in Rooms 1 and 7 (Butcher and Mendenhall, 1993, pg. A-132)**



<span id="page-14-1"></span>**Figure 8. RPPCR3-Closure-1: Stone and Argüello's predictions of vertical closure in Room 4 and a single room within an infinite array of parallel rooms (Butcher and Mendenhall, 1993, pg. A-134)**

It should be noted that the pillar width does not impact the room's "final" porosity, which is reached once the resistance of the room contents balances the lithostatic pressure. Pillar width is only relevant while the room porosity is evolving. Room porosity evolves quickly if the lithostatic pressure exceeds the room contents' pressure by a large amount. In the Stone and Argüello model simulations of empty rooms and access drifts, the pressure difference was 14.8 MPa and each room reached 100 % vertical closure in 140 to 240 years, which is a small fraction of the 10,000-year regulatory period. Room porosity evolves more slowly, on the other hand, if the room contents supply a back pressure close to the lithostatic pressure, which occurs once the waste is compacted and fluids (gas or brine) cannot easily escape the room. Brown and Weatherby (Butcher and Mendenhall, 1993, pg. A-5 to A-25) included crushed salt, waste, and trapped gas in each room of their infinite array model and they predicted the room would approach its final porosity in the order of thousands of years. Regardless of the time required to reach the final porosity, doubling the pillar widths is still expected to reduce this time by less than 7 %.

#### <span id="page-14-0"></span>**References RPPCR3-CLOSURE-1**

Butcher, B. M. and Mendenhall, F. T. 1993. A Summary of the Models Used for the Mechanical Response of Disposal Rooms in the Waste Isolation Pilot Plant with Regard to Compliance with 40 CFR 191, Subpart B. SAND92–0427. Sandia National Laboratories.

Stone, C. M. 1997. Final Disposal Room Structural Response Calculations. SAND97-0795. Sandia National Laboratories.

U.S. Department of Energy (DOE). 2024. Planned Change Request for the Use of Replacement Panels 11 and 12. United States Department of Energy, Carlsbad Field Office. Carlsbad, NM, USA.

Vignes, C., Bean, J., and Reedlunn, B. 2023. Improved Modeling of Waste Isolation Pilot Plant Disposal Room Porosity. SAND2023-04826. Sandia National Laboratories.

## <span id="page-15-0"></span>**RPPCR1-Inventory-1: Waste Characteristics**

Please provide updated tables that identify and assess waste characteristics for their impact on disposal system performance, with an analysis substantiating all decisions to exclude consideration of a waste characteristic or component.

*DOE is required to identify and assess all waste characteristics for their impact on disposal system performance, and to submit an analysis substantiating decision to exclude consideration of a waste characteristic or component [40 CFR 194.24(b)]. EPA noted during their review of the CRA-2019 that the tables identifying the impacts of waste characteristics have not been updated since CRA-2004 and contained entries inconsistent with the CRA-2019 DPA (see Issue #18). EPA and DOE agreed during an October 2022 Technical Exchange meeting that DOE would provide an updated listing of all waste characteristics and components that are included or excluded from consideration along with substantiating analyses for the RPPCR.*

#### <span id="page-15-1"></span>**DOE Response**

The requirements of 40 CFR 194.24(b) were first met in Appendix WCA of the Compliance Certification Application (U.S. DOE, 1996) and as later amended in the CRA-2004 in Appendix TRUWASTE (U.S. DOE, 2004). The following tables provide updated information on the following:

- A list of the waste characteristics and components expected to have a significant effect on disposal system performance (included in PA),
- a list of the waste characteristics and components expected to have negligible effect on disposal system performance,
- a list of waste characteristics and components that were considered and excluded from performance assessment (PA), and
- references that support the determination of effects on performance.

<span id="page-15-2"></span>

## **Table 2. RPPCR1-Inventory-1: Waste Characteris�cs and Components Used in PA: Characteris�cs Expected to Have a Significant Effect on Disposal System Performance**



(a) Brine Radiolysis was moved from "Not Used in Performance Assessment" to "Expected to have a Significant Effect on Disposal System Performance" based on its inclusion in Performance Assessment discussed in Day (2019) Section 1.1.3.

- (b) Complexation with Actinides by Soil and Humic Material was moved from "Expected to Have a Negligible Effect on Disposal System Performance" to "Expected to have a Significant Effect on Disposal System Performance" based on inclusion in Performance Assessment discussed in Appendix PA 2019 Section 4.4.1.
- (c) Complexation with Actinides by Organic Ligands "Expected to Have a Negligible Effect on Disposal System Performance" to "Expected to have a Significant Effect on Disposal System Performance" based on inclusion in performance assessment discussed in Appendix SOTERM 2019.

## <span id="page-17-0"></span>**Table 3. RPPCR1-Inventory-1: Waste Characteris�cs and Components Used in Performance Assessment:**



## **Characteris�cs Expected to Have a Negligible Effect on Disposal System Performance**

(a) Binding to Organic Ligands by Ferrous Metals was moved from "Not Used in Performance Assessment (Table 4)" to "Expected to Have a Negligible Effect on Disposal System Performance (Table 3)" based on calculations completed for the RPRCR (Domski, 2023) that include iron citrate complexes.



## <span id="page-18-0"></span>**Table 4. RPPCR1-Inventory-1: Waste Characteris�cs and Components Not Used in Performance Assessment**

(a) Waste characteristics and components that influence performance indirectly – by influencing components and characteristics listed in Table 2.

## <span id="page-19-0"></span>**References RPPCR1-Inventory-1**

Brunell, S., J. Bethune, P. Docherty, D. Kicker, S. Kim, S. King, J. Long, and T. Zeitler. 2023. Summary Report for the 2023 Replacement Panels Planned Change Request Performance Assessment. Sandia National Laboratories, Carlsbad, NM. ERMS 579729.

Butcher, B.M. 1997. Waste Isolation Pilot Plant Disposal Room Model. SAND97-0794. Albuquerque, NM: Sandia National Laboratories.

Cotsworth, E. 2005. Letter to I. Triay. Subject: EPA Letter on Conducting the Performance Assessment Baseline Change (PABC) Verification Test. 4 March 2005. U.S. Environmental Protection Agency, Office of Air and Radiation, Washington, DC. ERMS 538858.

Day, B.A. 2019. Reassessment of Need and Parameter Justification for Modeling Gas Generation due to Radiolysis of Brine and Cellulose/Plastic/Rubber in WIPP for CRA-2019. (February 12, 2019). Carlsbad, NM: Sandia National Laboratories. ERMS 570873.

Domski, P.S. 2023. "Prediction of Baseline Actinide Solubilities for the Replacement Panels Planned Change Request (RPPCR) Performance Assessment." Carlsbad, NM: Sandia National Laboratories. ERMS 579503.

Kicker, D. 2023. Radionuclide Inventory Screening Analysis for the Replacement Panels Planned Change Request Performance Assessment (RPPCR PA). Carlsbad, NM: Sandia National Laboratories. ERMS 578878.

Knerr, R. 2020. Response 7 to U.S. Environmental Protection Agency's 2019 Compliance Recertification Application Completeness Comments Letters dated May 6, 2020, June 12, 2020, July 17, 2020, and September 11, 2020, from Tom Peake to Mike Brown. U.S. Department of Energy, Carlsbad Field Office, Carlsbad, New Mexico. Letter to L.B. Veal, U.S. Environmental Protection Agency Radiation Protection Division, Washington, D.C. December 1, 2020.

Lucchini, J. and J. Swanson. 2023. LANL ACRSP Parameter Recommendations for CRA-2024 Performance Assessment. Report LCO-ACP-34. Los Alamos National Laboratory; Carlsbad, NM. LA-UR-23-23839.

Nemer, M.B., and J.S. Stein. 2005. Analysis Package for BRAGFLO, 2004 Compliance Recertification Application Performance Assessment Baseline Calculation (June 28). Carlsbad, NM: Sandia National Laboratories. ERMS 540527.

Nemer, M. and W. Zelinski. 2005. Analysis Report for BRAGFLO Modeling Results with the Removal of Methanogenesis from the Microbial-Gas-Generation Model. February 2005. Carlsbad, NM: Sandia National Laboratories. ERMS 538748.

U.S. Department of Energy (DOE). 2004. Title 40 CFR Part 191 Compliance Recertification Application for the Waste Isolation Pilot Plant (March). 10 vols. Carlsbad, NM: Carlsbad Field Office. DOE/WIPP 2004-3231

U.S. DOE. 2019. Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant. Carlsbad, NM: Carlsbad Field Office. DOE/WIPP-10-3609.

Vaughn, P., Bean, J., Garner, J., Lord, M., MacKinnon, R., McArthur, D., Schreiber, J., and Shinta, A. 1995. FEPs Screening Analysis DR2, DR3, DR6, DR7 and S6. Sandia National Laboratories, Albuquerque, NM. ERMS 238152.

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

#### <span id="page-21-0"></span>**RPPCR1-DATA0.FM6-1: Documentation for Hydromagnesite5424 Solubility**

Please provide a short explanation of the source of the log K value for hydromagnesite5424 in the DATA0.FM6 documentation.

DOE recalculated the DATA0.FM1 hydromagnesite5424 log K value of 32.25 to a value of 31.49 for DATA0.FM4 (Sisk-Scott 2019). EPA (2022, Attachment B, Section 3.4.1) accepted the recalculated hydromagnesite5424 log K value of 31.39 during its review of DATA0.FM4, noting that the recalculated value was more internally consistent with other thermodynamic data in the database.

During development of the DATA0.FM6 database, DOE appropriately revised the hydromagnesite5424 log K value from the DATA0.FM1 value to 31.49, but this change was not included in Table IX.3.1 of Jang et al. (2021) or the discussion of database revisions related to magnesium in Domski (2023, Section 3.1.3). The revised hydromagnesite5424 data block is, however, appropriately included in a summary listing of the database revisions to create DATA0.FM6 (Domski 2023, Appendix A) and in the DATA0.FM6 database. To avoid possible confusion regarding the DATA0.FM6 log K value for hydromagnesite5424, DOE should include a short explanation of its source in the DATA0.FM6 documentation.

Domski, P.S. 2023. An Update to the WIPP EQ3/6 Database DATA0.FM1 with the Creation of DATA0.FM6. ERMS 579370, Sandia National Laboratories, Carlsbad, New Mexico.

EPA (U.S. Environmental Protection Agency). 2022. Technical Support Document for Section 194.24, Evaluation of the Compliance Recertification Application (CRA-2019) Actinide Source Term, Gas Generation, Backfill Efficacy, Water Balance, and Culebra Dolomite Distribution Coefficient Values. EPAHQ-OAR-2019-0534, Office of Radiation and Indoor Air, Washington, DC.

Jang, J., P. Hora, L. Kirkes, C. Miller, and L. Zhang, 2021. Analysis Report Documenting Solubility and Complexation of Iron, Lead, Magnesium, Neodymium, and Boron in the WIPP-Relevant Brines Under TPs 06-03, 08-02, 12-02, 14-03, 14-05, 16-02, 19-01, and 20-01. ERMS 576381, Sandia National Laboratories, Carlsbad, New Mexico.

Sisk-Scott. 2019. Analysis Plan to Update the WIPP Geochemical Thermodynamic Database (DATA0.FM1) to DATA0.FM4 for CRA-2019. AP-183, Revision 1, ERMS 571001, Sandia National Laboratories, Carlsbad, New Mexico

#### <span id="page-21-1"></span>**DOE Response**

The change of the value of log K for hydromagnesite5424 from that in DATA0.FM1 (Xiong, 2011) to the value included DATA0.FM6 (Domski, 2023) was not documented in an appropriate reference for DATA0.FM6 (Domski, 2023). As noted by the EPA in their comment RPPCR1- DATA0.FM6-1 this change was documented in Section 2.1.2 of Sisk-Scott (2019). To summarize from Sisk-Scott (2019):

*"…an error in transcription was discovered when the data from Robie and Hemingway (1973) was compared to that in DATA0.FM1. The error is in the FMT thermodynamic database fmt\_050405.chemdat (Xiong et al. 2005) where the μ<sup>0</sup> /RT value attributed to Robie and Hemingway (1973) does not match what was reported by Robie and Hemingway (1973)."* 

This transcription error was corrected for the DATA0.FM4 database as documented by Sisk-Scott (2019) and was carried over to DATA0.FM6.

To improve the traceability of the log K value presented in Sisk-Scott (2019) the calculation was reproduced and is presented in APPENDIX A.

## <span id="page-22-0"></span>**References RPPCR1-DATA0.FM6-1**

Domski, P.S. 2023. An Update to the WIPP EQ3/6 Database DATA0.FM1 with the Creation of DATA0.FM6. ERMS 579370, Sandia National Laboratories, Carlsbad, New Mexico.

Sisk-Scott. 2019. Analysis Plan to Update the WIPP Geochemical Thermodynamic Database (DATA0.FM1) to DATA0.FM4 for CRA-2019. AP-183, Revision 1, ERMS 571001, Sandia National Laboratories, Carlsbad, New Mexico.

Robie, R. A., and B. S. Hemingway. 1973. The enthalpies of formation of nesquehonite, MgCO<sub>3</sub>·3H<sub>2</sub>O, and hydromagnesite, 5MgO·4CO<sub>2</sub>·5H<sub>2</sub>O. *Journal of Research of the U.S. Geological Survey*, 1: 543-547.

Xiong, Y.-L. 2005. "Release of FMT\_050405.CHEMDAT." E-mail to J.F. Kanney and J.J. Long, April 5, 2005. Carlsbad, NM: Sandia National Laboratories. ERMS 539304.

Xiong, Y.-L. 2011. "Release of EQ3/6 Database DATAO.FM1." E-mail to Jennifer Long, March 9, 2011. Carlsbad, NM: Sandia National Laboratories. ERMS 555152.

## <span id="page-23-0"></span>**APPENDIX A. Calculation of logKsp for Hydromagnesite5424**

The reaction for the dissolution of hydromagnesite5424 is as follows:

 $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O + 6H^+ \rightleftharpoons 5Mg^{2+} + 4HCO_3 + 6H_2O$ 

Robie and Hemmingway (1973) provide the Gibbs free energy of formation for hydromagnesite5424 as -1,401,710 ± 260 cal/mol. Converting to joules (J), 4.184 J/cal, we have ∆Gf = -5864754.64 ± 1087.84 J/mol. Dividing the Gibbs energy by the product of the Ideal Gas Constant (R; 8.3145 J/K·mol) and the absolute temperature (T=298.15K), we get the standard chemical potential for hydromagnesite5424.

Where hydromagnesite5424  $\mu^0/RT$  = -2365.80 ± 0.44

<span id="page-23-1"></span>



The  $log_{10}$  K for hydromagnesite5424 may be calculated via the general expression:

$$
Log_{10} K = \frac{1}{2.303} \sum_{i=1}^{10} v_i \left(\frac{v_i^0}{RT}\right) \sum_{i=1}^{n} v_i \left(\frac{v_i^0}{RT}\right)
$$
 Equation (1)

 $v_i$  = chemical potential of species i

 $Log_{10} K = 1/(2.303) \times ([-2365.8047] + 6 \times [0.0] - 5 \times [-183.4680] - 4 \times [-236.7510] - 6 \times [-95.6635])$ 

 $= 31.4895 \pm 0.19<sup>1</sup>$  $= 31.4895 \pm 0.19<sup>1</sup>$  $= 31.4895 \pm 0.19<sup>1</sup>$ 

This value was rounded up to 31.49 for inclusion in DATA0.FM6.

<span id="page-23-2"></span><sup>&</sup>lt;sup>1</sup> The error values were based on the Gibbs free energy of formation error value ( $\pm$ 260 cal/mol) provided by Robie and Hemmingway (1973).

## <span id="page-24-0"></span>**RPPCR2-DATA0.FM6-4: Omitted Pitzer interaction parameters**

The Pitzer interaction parameters from Moog et al. (2004) listed in the following table were previously included in the DATA0.FM4 database reviewed by EPA (2022). Please explain the reasons for omitting these parameters from DATA0.FM6. Please provide calculations that show whether omission of these parameters would affect predicted dissolved iron concentrations in WIPP brines under repository conditions.



## <span id="page-24-1"></span>**DOE Response**

The iron Pitzer parameters included in DATA0.FM6 are those selected, used, and presented in Table IX.1-2 in GEOC-21-11 (Jang et al., 2021). GEOC-21-11 contained the measurements used to parameterize the Fe-Na-(Cl) and Fe-Mg-(Cl) chemical systems, thus, the Fe parameters of Fe-Na- (Cl) and Fe-Mg-(Cl) in Moog et al. (2004) were used and reported in GEOC-21-11. GEOC-21-11 did not contain measurements regarding Fe-Ca-(Cl) and Fe-K-(Cl), therefore, the Fe Pitzer parameters of Fe-Ca-(Cl) and Fe-K-(Cl) chemical systems in Moog et al. (2004) were not selected in GEOC-21-11. Table IX.1-2 of Jang et al. (2021) provided the Fe Pitzer parameters that were to be added in DATA0.FM1 to create DATA0.FM6. The Pitzer model parameters from Moog et al. (2004) were not included in Data0.FM6 because Data0.FM4 was not used in the creation of Data0.FM6; subsequently, since these parameters were not listed in Jang et al. (2021) they were overlooked during the creation of Data0.FM6.

To test the effect of these parameters on the iron concentration at repository conditions a copy of DATA0.FM6 was made and named DATA0.PCR and the four sets of Pitzer parameters were included. This database was then used to run the RPPCR minimum volume cases of the baseline solubility model for both the GWB and ERDA-6 brine compositions. The results were compared with minimum volume case results using DATA0.FM6. A comparison of the results is tabulated in Table 5 below.

## <span id="page-25-2"></span>**Table 5. Comparison of values at repository condi�ons using DATA0.FM6 (RPPCR) and DATA0.PCR (RPPCR2-DATA0.FM6-4)**



(a) Domski (2023b)

## <span id="page-25-0"></span>**Files**

All files for this comment response are archived at: "/data/cvs/CVSLIB/WIPP\_EXTERNAL/RPPCR\_comments"

## <span id="page-25-1"></span>**References RPPCR2-DATA0.FM6-4**

Domski, P.S. 2023a. An Update to the WIPP EQ3/6 Database DATA0.FM1 with the Creation of DATA0.FM6. ERMS 579370, Sandia National Laboratories, Carlsbad, New Mexico.

Domski, P.S. 2023b. "Prediction of Baseline Actinide Solubilities for the Replacement Panels Planned Change Request (RPPCR) Performance Assessment". Carlsbad, NM: Sandia National Laboratories. ERMS 579503.

Jang, J., P. Hora, L. Kirkes, C. Miller, and L. Zhang, 2021. Analysis Report Documenting Solubility and Complexation of Iron, Lead, Magnesium, Neodymium, and Boron in the WIPP-Relevant Brines Under TPs 06-03, 08-02, 12-02, 14-03, 14-05, 16-02, 19-01, and 20-01. ERMS 576381, Sandia National Laboratories, Carlsbad, New Mexico.

Moog, H. C., Hagemann, S., and Rumyantsev, A. V., 2004. Isopiestic investigation of the systems FeCl<sub>2</sub> - (Na, K, Mg, Ca)Cl<sub>n</sub>-H<sub>2</sub>O at 298.15 K. ZEITSCHRIFT FUR PHYSIKALISCHE CHEMIE-INTERNATIONAL JOURNAL OF RESEARCH IN PHYSICAL CHEMISTRY & CHEMICAL PHYSICS, 218, 1063-1087.

**Enclosure 2** 

**Department of Energy Response 2** 

**Status Report of DOE Responses To EPA Questions on the RPPCR**



