579803

Sandia National Laboratories

Operated for the United States Department of Energy
National Nuclear Security Administration
by National Technology and Engineering
Solutions of Sandia, LLC.
Albuquerque, New Mexico 87185-0143
Livermore, California 94551-0969

date: June 27, 2023

to: SNL WIPP Records Center
Defense Waste Management Programs

from: Paul Domski *signature on file*

subject: Memo of Correction: Corrections to Section 3.1.3 of the Analysis Report: *An Update to the WIPP EQ3/6 Database DATA0.FM1 with the Creation of DATA0.FM6*

In the period after the analysis report *"An Update to the WIPP EQ3/6 Database DATA0.FM1 with the Creation of DATA0.FM6"* was submitted into WIPP records three non-quality affecting errors were identified in the report. These errors did NOT affect the glushinskite parameters included in DATA0.FM6 (Domski, 2023a), and therefore, did not impact subsequent actinide solubility calculations or uncertainty analysis using DATA0.FM6. The issue was specific to the report only, and had to do with the mineral phase glushinskite [MgOxalate·2H_2O(s)], the first (1) was a typo in the caption for Figure 11, the second and third errors were the use of the dissociation reaction for the Mg – oxalate aqueous species ($Mg(Oxalate)_2^{2-}$) (2) in the text of the report, and (3) in the calculation of the apparent solubility product (log Ksp,app) for glushinskite. The third issue, calculation of log Ksp,app for glushinskite, affected the values in Table 14 and Figure 12 of the report. The updated text, table, and figure are presented below:

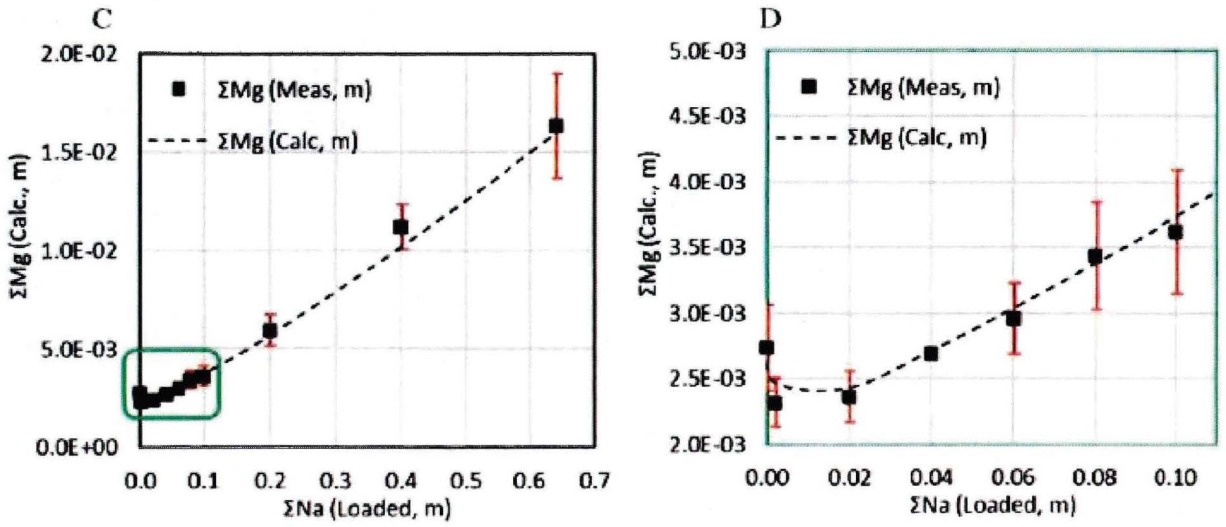

Figure 11. Reproduction of Figure VI.1-10, parts C and D from Jang et al. (2021b). Parametrization of $MgOxalate{\cdot}2H_2O(s) - Na_2Oxalate - H_2O$ system. Fitting of the model using the new recommended glushkinskite log Ksp. D is a zoomed-in view of the green rectangle in C.

To build additional confidence in the glushinskite solubility product its apparent solubility product based on the experimental data (Table VI.1-10, Jang et al., 2021b) and the EQ3NR model response was calculated. The results are plotted in Figure 12, and the method used to calculate the apparent log K is presented below.

The dissolution reaction for glushinskite can be written as:

$MgOxalate{\cdot}2H_2O(s)$ (Glushinskite) $\rightleftharpoons Mg^{2+} + Oxalate^{2-} + 2H_2O$

The apparent solubility product is given by:

$Ksp,app = [Mg^{2+}] \times [Oxalate^{2-}]$

By definition, the activity of a pure solid is equal to 1. The activity of water is purposely set equal to 1 for simplicity of calculation of Ksp,app. Note the square brackets ([-]) indicate concentration in units of molality (m).

The $\log_{10}$ of the apparent solubility product is then given by

$\log Ksp,app = \log [Mg^{2+}] + \log[Oxalate^{2-}]$

Table 14 provides the pmH, Mg, Na, and oxalate molalities used to calculate the log Ksp,app values for glushinskite as a function of sodium concentration for the experimental and simulated values.

Table 1. Apparent Log K values for Glushinskite.

Measured Data from Jang et al. (2021b), Table VI.1-10					**EQ3NR Simulated Data**				
pmH	**Mg (m)**	**Na (m)**	**Oxalate (m)**	**logKsp,app**	**pmH**	**Mg (m)**	**Na (m)**	**Oxalate (m)**	**logKsp,app**
8.34	2.74E-03	5.36E-04	5.33E-03	-4.84	8.34	2.35E-03	5.36E-03	5.03E-03	-4.93
8.31	2.32E-03	4.07E-03	2.56E-03	-5.23	8.31	2.38E-03	4.07E-03	4.41E-03	-4.98
8.13	2.36E-03	1.98E-02	9.27E-03	-4.66	8.13	2.44E-03	1.98E-02	1.23E-02	-4.52
8.19	2.69E-03	6.65E-02	2.15E-02	-4.24	8.19	3.16E-03	6.65E-02	3.64E-02	-3.94
8.26	2.96E-03	8.29E-02	3.19E-02	-4.02	8.26	3.44E-03	8.29E-02	4.49E-02	-3.81
8.27	3.43E-03	1.00E-01	4.21E-02	-3.84	8.27	4.11E-03	1.19E-01	6.36E-02	-3.58
8.29	3.62E-03	1.19E-01	5.21E-02	-3.72	8.29	6.15E-03	2.20E-01	1.16E-01	-3.15
8.37	5.94E-03	2.20E-01	1.04E-01	-3.21	8.37	1.04E-02	4.09E-01	2.15E-01	-2.65
8.49	1.11E-02	4.09E-01	2.27E-01	-2.60	8.49	1.35E-02	5.37E-01	2.82E-01	-2.42
8.59	1.63E-02	5.37E-01	2.61E-01	-2.37	8.59	1.35E-02	5.38E-01	2.82E-01	-2.42

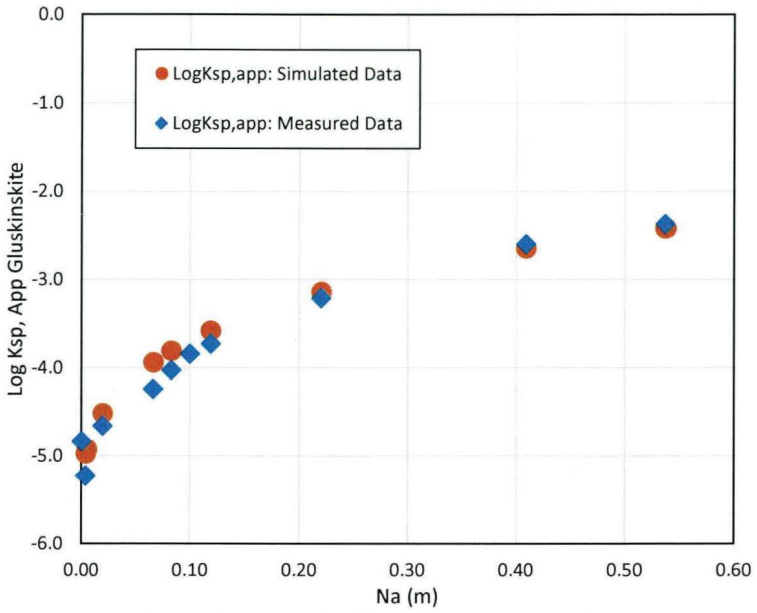

Figure 12. Apparent Log Ksp values for the glushinskite measured data compared to the model predicted apparent Log Ksp values.

The spreadsheet *"Python_LogKsp,app_FM6-Verification.xlsx"* was updated and will replace the version included in the records package. This file is stored at: /data/cvs/CVSLIB/WIPP_EXTERNAL/ap200/Files.

This memo of correction was issued to correct three errors identified in the analysis report *"An Update to the WIPP EQ3/6 Database DATA0.FM1 with the Creation of DATA0.FM6"*. None of the errors identified were quality affecting and had zero impact on the parameter values included in the WIPP thermodynamic database DATA0.FM6 (Domski, 2023a), and subsequently had no impact on the RPPCR baseline solubility calculations (Domski, 2023b), or actinide uncertainty analysis (Domski, 2023c).

References

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

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.

Domski, P.S. 2023c. "Uncertainty Analysis of Actinide Solubilities for the Replacement Panels Planned Change Request (RPPCR) Performance Assessment and the 2024 Compliance Recertification Application (CRA-2024)". Carlsbad, NM: Sandia National Laboratories. ERMS 579525.

WIPP:4.4.2.2.1:TD:QA-L:RECERT:579369