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Analysis Plan AP-028

Analysis of Uranium(VI) Solubility Data for WIPP Performance Assessment

WBS 1.1.10.1.1

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Scope of the Analysis:

Objective

The objective of this work is to provide an analysis of the available data on the solubility of actinide(VI) (applicible only to uranium) expected in a brine-inundated WIPP waste repository room that contains magnesium oxide (MgO) chemical intervention reagent to control the pH and minimize the effect of carbon dioxide gas. Upper limit concentrations (solubility limits) provide the "source term" for potential releases of radionuclides to the accessible environment in future human intrusion scenarios. The development of thermodynamic Pitzer type models for predicting the solubilities of actinide elements in an inundated WIPP repository have been successfully completed by the WIPP Dissolved Concentrations Submodel (DCS) for the trivalent (III as An^{3+}), tetravalent (IV as An^{4+}), and pentavalent (V as AnO_2^{+}) oxidation states. However, the actinide hexavalent (VI as AnO_2^{2+}) model is insufficient at this time. This present analysis will provide a solubility limit for uranium(VI as UO_2^{2+}) based on analysis of a combination of extant published literature data and direct empirical solubility measurements. This value will be utilized as an input to WIPP Performance Assessment calculations and is reported in *WPO#35835 Documentation Package for Solubility Parameters for Actinide Source Term Look Up Tables* (Siegel, 1996)

Assumptions

This analysis will be performed by comparing various sources of solubility data to determine where there is agreement/disagreement in the data and to determine the reasons for the disagreement. Solubility is an intrinsic thermodynamic property of a particular compound and is a scientifically reproducible result no matter what researcher or where the solubility study is performed. Thus all valid solubility data should correlate. When the data does not correlate, often the reason is because the thermodynamic solubility parameter is a function of

specific experimental conditions (e.g., temperature, pressure, hydrogen ion concentration, complexants present,redox potential, ionic strength, identity of the solid phase, etc.). Although data exists that was obtained under varying conditions, this analysis will focus on conditions imposed by MgO chemical controller (pH between 9 to 10 and no carbonate ion present in significant quantities).

It is assumed that this analysis will provide a solubility value for uranium(VI) concentration in brine that will be accurate to approximately the same degree as that determined for the other oxidation states.

Primary Task to Perform the Analysis

Step 1. Assemble Data

To perform the analysis, suitable data must be identified. For this analysis, any reasonable solubility data are potentially useful in the first cut. The literature sources of data are from the German and Japanese Nuclear Waste Programs in collaboration with American researchers. The WIPP-directed empirical data are derived from ongoing experiments at Argonne National Laboratory (ANL), Illlinois, Lawrence Livermore National Laboratory (LLNL), California, and Los Alamos National Laboratory (LANL), New Mexico.

Step 2. Determine Applicability of Data

Because solubility is a thermodynamic property, all valid scientifically determined solubility data on a specific compound should be in reasonable agreement (e.g., order of magnitude). Legitimate reasons for noncorrelation were listed in the Assumptions Section above. It is possible to compare data collected under varying conditions by extrapolation to a limited extent. Any data that does not correlate at all will be excluded from the analysis.

Step 3. Assess Data Correlations/Noncorrelations

The differences between solubility concentration values for uranium(VI) under a diversity conditions may vary by many orders of magnitude. The focus of this analysis is, however, under specific chemical control conditions (MgO backfill) of from pH 9 to 10 and no carbonate ligands present. As such, the data under these conditions should agree within two orders of magnitude or be rejected.

Step 4. Select Value that is Most Probable

The most probable value for U(VI) solubility will be determined by averaging the selected data to result in a single value with error limits that include all of the selected data.

Step 5. Transmittal of Results to PA and SNL WIPP Central Files (SWCF)

Results of this analysis will be documented in the deliverable outlined below with a cover memo. The cover memo will be prepared and reviewed according to applicable requirements of QAP6-3 for Conducting and Documenting Reviews of Documents. The analysis documentation will be prepared according to the requirements of QAP9-1 and submitted to the SWCF.

Individuals to Perform the Analysis

The primary individual who will report the results of this analysis by an ad hoc committee is David E. Hobart, a CTAC-WESTON-RE/SPEC contractor to DOE CAO on assignment at Sandia National Laboratories, (SNL) Albuquerque, Dept. 6748. Members of the Ad Hoc Analysis Panel are listed below in tabular form:

R. Vann Bynum (SAIC/SNL)	C. Crafts (SNL)
R. Moore (SNL)	C. Novak (SNL)
J. Nowak (SNL)	C. Stockman (SNL)
R. Weiner (SNL)	

Task Deliverables

The deliverables from this analysis plan are a memo to Malcolm Siegel (SNL) with copies to the Analysis Panel members transmitting the document *Analysis of*

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Uranium(VI) Solubility Data for WIPP Performance Assessment, by D. E. Hobart and R. Moore.

Controlling Documents

The controlling documents for this analysis are:

QAP6-3 Conducting and Documenting Reviews of Documents

QAP9-1 Quality Assurance Requirements for Conducting Analyses

QAP17-1 Quality Assurance Records Source Requirements

References

Siegel, M. D. (1996) *Documentation Package for Solubility Parameters for Actinide Source Term Look Up Tables WPO#35835* Sandia National Laboratories, Albuquerque, NM.