Analysis Plan For Derivation of Pitzer Parameters in Support of Experimental Work at LANL-CO

Task 1.4.2.2

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# Table of Contents

1. **Introduction and Objectives** ................................................................. 3  
   1.1 Introduction .................................................................................... 3  
   1.2 Objectives .................................................................................... 3  

2. **Approach** ............................................................................................ 3  
   2.1 Project Resources .......................................................................... 3  
   2.2 Project Tasks and Milestones ....................................................... 3  

3. **Software List** .................................................................................... 3  

4. **Tasks** .................................................................................................. 3  

5. **Special Considerations** ................................................................. 4  

6. **Applicable Procedures** ................................................................. 4  

7. **References** ....................................................................................... 4
1 Introduction and Objectives

1.1 Introduction

Los Alamos National Laboratory-Carlsbad Operation (LANL-CO) has been conducting experimental work concerning the chemistry of actinides and their analogs. In their experiments at high ionic strengths, the Pitzer interaction parameters could be derived. When those Pitzer interaction parameters are derived, they could be employed to refine or enlarge the current database used for predicting the actinide solubility for the WIPP performance assessment. This analysis is a Programmatic Decision analysis per NP 9-1.

1.2 Objectives

The objective of this Analysis Plan (AP) is to derive the Pitzer interaction parameters in support of the experimental work at LANL-CO. The Pitzer interaction parameters between Co$^{2+}$, Ni$^{2+}$ and Gd$^{3+}$-EDTA complexes, and the bulk background electrolyte (i.e., NaCl), will be derived in the Revision 0 of this AP.

2 Approach

2.1 Project Resources

Sandia National Laboratories has a computer program called NONLIN (Babb, 1996). NONLIN fits parameters for the Pitzer's aqueous electrolyte model based on experimental data on stability constants of aqueous complexes, mineral solubility, osmotic coefficients, electromotive force (emf) and solvent extraction. Therefore, this computer program is suitable to achieving the objectives of this AP.

2.2 Project Tasks and Milestones

The project tasks are detailed in Section 4. The tasks identified in the Revision 0 of this AP are planned to be completed by the end of FY07.

3 Software List

The software to be used is NONLIN Version 2.0 (system configuration: DEC Alpha/Open VMS AXP 8.2).

4 Tasks

The tasks for the Revision 0 of this AP include:
(1) Derivation of Pitzer parameters for the interaction between CoHEDTA\(^-\) and the bulk
  electrolyte, NaCl.
(2) Derivation of Pitzer parameters for the interaction between CoEDTA\(^2^-\) and the bulk
  electrolyte, NaCl.
(3) Derivation of Pitzer parameters for the interaction between NiEDTA\(^2^-\) and the bulk
  electrolyte, NaCl.
(4) Derivation of Pitzer parameters for the interaction between GdEDTA\(^-\) and the bulk
  electrolyte, NaCl.

Yongliang Xiong will conduct those tasks, and the completion date is estimated to be by
the end of FY07.

5 Special Considerations

Pitzer interaction parameters will be derived from the conditional equilibrium constants
in Table 1 that Marion Borkowski (2007) at LANL-CO sent to Yongliang Xiong for the Revision
0 of this AP.

6 Applicable Procedures

All applicable WIPP QA procedures will be followed when conducting this AP.
• Training of personnel will be conducted in accordance with the requirements of
  NP 2-1, Qualification and Training.
• Analyses will be conducted and documented in accordance with the requirements
  of NP 9-1, Analyses.
• All software used will meet the requirements laid out in NP 19-1, Software
  Requirements and NP 9-1, as applicable.
• The analyses will be reviewed following NP 6-1, Document Review Process.
• All required records will be submitted to the WIPP Records Center in accordance
  with NP 17-1, Records.

7 References

Albuquerque, NM: Sandia National Laboratories. WPO 30740.
Borkowski, M., 2007. “Table 1. The conditional stability constants and protonation constants for
CoEDTA complex and log \(\beta_{i01}\) values for Co\(^{2+}\), Ni\(^{2+}\) and Gd\(^{3+}\) as a function of NaCl
ionic strength.” Sent to Yongliang Xiong on February 7, 2007 via e-mail. ERMS
#546107.
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