546249

IMPORTANT NOTICE: The current official version of this document is available via the Sandia National Laboratories WIPP Online Documents web site. A printed copy of this document may not be the version currently in effect.

SANDIA NATIONAL LABORATORIES
WASTE ISOLATION PILOT PLANT

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

Task 1.4.2.2

Effective Date: 06/07/07

Authored by:	Yongliang Xiong	*Yongliang Xiong*	June 6, 2007
	Print Name	Signature	Date
Reviewed by:	Shelly Johnsen	*signature*	6-6-07
	Print Name Technical Reviewer	Signature	Date
Reviewed by:	Mario Chavez	*signature*	6/6/07
	Print Name Quality Assurance Reviewer	Signature	Date
Approved by:	Christi Leigh	*signature*	June 6, 2007
	Print Name Department Manager	Signature	Date

Table of Contents

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

Babb, S.C. 1996. "NONLIN, Ver. 2.00, User's Manual." Unpublished report, January 31, 1996. Albuquerque, NM: Sandia National Laboratories. WPO 30740.

Borkowski, M., 2007. "Table 1. The conditional stability constants and protonation constants for CoEDTA complex and log β_{101} 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.

NOTICE: This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness or any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof or any of their contractors.

This document was authored by Sandia Corporation under Contract No. DE-AC04-94AL85000 with the United States Department of Energy's National Nuclear Security Administration. Parties are allowed to download copies at no cost for internal use within your organization only provided that any copies made are true and accurate. Copies must include a statement acknowledging Sandia Corporation's authorship of the subject matter.