A1756

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March 15, 1987

Mr. Walton Kelly
Geotechnical Branch
Division of Waste Management
U.S. Nuclear Regulatory Commission
7915 Eastern Avenue
Silver Spring, MD 20910

Dear Mr. Kelly:

Enclosed is the monthly report on FIN A-1756, Geochemistry Sensitivity Analysis for February 1987. Please feel free to contact me at (FTS) 844-8368 or Malcolm Siegel at (FTS) 864-5448 if you have any questions or comments.

Sincerely,

Jeffrey S Philbin for
Robert M. Cranwell, Supervisor
Waste Management Systems
Division 6416

RMC:6416

Enclosure

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PROGRAM: Geochemical Sensitivity Analysis FIN#: A-1756

CONTRACTOR: Sandia National Laboratories BUDGET PERIOD: 10/86 - 9/87

NMSS PROGRAM MANAGER: W. Kelly BUDGET AMOUNT: 200K

CONTRACT PROGRAM MANAGER: R. M. Cranwell FTS PHONE: 844-8368

PRINCIPAL INVESTIGATORS: M. D. Siegel FTS PHONE: 846-5448

PROJECT OBJECTIVE

The objective of this project is to provide technical assistance to the NRC in determining the sensitivity of performance assessment calculations to uncertainties in geochemical data and in the representation of geochemical processes in transport models. In Task I, the error in model calculations of integrated radionuclide discharge due to speciation, sorption and kinetic effects will be evaluated. In Task II, the potential importance of organic molecules and colloids will be examined. SNLA will assist the NRC in determining how geochemical processes should be represented in transport models in Task III. Short-term technical assistance will be carried out under Task IV and the codes and data bases developed under this project will be transfered to the NRC under Task V.

ACTIVITIES DURING FEBRUARY 1987

Task I. Uncertainty in Integrated Radionuclide Discharge

Subtask 1A. Conceptual Models for Repository Sites.

During February, calculations of integrated radionuclide discharge using the NEFTRAN and EPACDF codes were initiated on the VAX computer system.

Subtask 1B. Solubility/Speciation Effects.

The second draft of "Thermodynamic Tables for Use in Performance Assessment of High-Level Waste Repositories. Volume 1. Aqueous Solutions Data Base," NUREG/CR-4864, SAND87-0323 was prepared during February. A description of the report is included as Attachment 1 to this monthly progress report.

Subtask 1C. Sorption Effects.

Critical evaluation of the empirical sorption data in the dBase III+ data base continued during this month. The first draft of the users'

manual for the data management system was completed and is under revision.

Subtask 1E. Coupled/Dynamic Effects

No activity to report.

Task IV. Short-Term Technical Assistance.

No activity to report.

Allocation of Resources

Task 1.....100%

Attachment 1

NUREG/CR-4864
SAND87-0323
LBL-22860

Thermodynamic Tables for Analysis of High-Level Waste Repository Performance

Vol. 1 Aqueous Solution Database

Sidney L. Phillips, Frank V. Hale, *Malcolm D. Siegel, Lenard F. Silvester
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Prepared for
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U.S. Nuclear Regulatory Commission
Washington, DC 20555

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Office of Basic Energy Sciences, Division
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April 1987

Attachment 1 (continued)

Table of Contents

ABSTRACT

A consistent and critically evaluated thermodynamic data base for nuclear waste disposal is tabulated. The computerized data base consists of values for Gibbs energy of formation, enthalpy of formation, entropy and heat capacity for minerals, simple solids, elements, aqueous ions, ion pairs and higher complex ions of actinides and fission decay products at 25°C and zero ionic strength. Standard deviations are given for Gibbs energy data, and usually for the other properties. Integrity constraints for the tabulation center on consistency with theoretical expectation and correlation; self-consistency with $\Delta_r G^\circ = \Delta_r H^\circ - (298.15)\Delta_r S^\circ$ for each species ; internal consistency of chemical and electrode reaction processes; consistency in reproductibility of critically assessed experimental measurements; and documentation of references to sources of data tabulated. These tables provide a well-documented set of thermodynamic property values and associated uncertainties for use in geochemical speciation codes. The scope and quality of the data and the structure of the computerized data management system are designed to facilitate the use of the data base in analyses of the sensitivity of calculated radionuclide speciation and release to uncertainties in available thermodynamic data. The potential use of the Aqueous Solutions Database in geochemical sensitivity analysis is described. Recommendations for additional research are given.

APPENDIX

I. Table of Auxiliary Data

II. Thermodynamic Tables for Waste Repository Assessment

- Aluminum
- Americium
- Calcium
- Carbon
- Europium
- Iodine
- Neptunium
- Palladium
- Plutonium
- Protactinium
- Radium
- Ruthenium
- Selenium
- Silicon
- Strontium
- Technectium
- Thorium
- Tin
- Uranium

III. Thermodynamic Data for Geologic Materials
Primary Oxides and Silicates
Secondary Minerals; clays and zeolites
Evaporite Minerals.

A-1756
1646.010
February 1987

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

	Current Month	Year -to- Date
I. Direct Manpower (man-months) of charged effort)	0.5	2.5
II. Direct Loaded Labor Costs	3	20
Materials and Services	1	7
ADP Support (computer)	1	5
Subcontracts	18	77
Travel	0	1
G & A	2	14
Other (computer roundoff)	-1	0
TOTAL COSTS	24	124

III. Funding Status

Prior FY Carryover	FY 87 Projected Funding Level	FY 87 Funds Received to Date	FY 87 Funding Balance Needed
29K	229K	200K	None