

Sandia National Laboratories

Albuquerque, New Mexico 87185

June 15, 1986 86 JUN 19 A10:33

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 May 1986. Please feel free to contact me if you have any questions or comments.

Sincerely,

Robert M. Cranwell, Supervisor
Waste Management Systems
Division 6431

RMC:6431

Enclosure

Copy to:

- Office of the Director, NMSS
- Attn: Program Support
- Robert Browning, Director
- Division of Waste Management
- Phillip Justus
- Division of Waste Management
- Malcolm R. Knapp
- Low Level Waste and Uranium Recovery Branch
- Kenneth Jackson
- Division of Waste Management
- Branch Chief
- Health, Siting and Waste Management
- Document Control Center
- 6430 N. R. Ortiz
- 6431 R. M. Cranwell
- 6431 M. D. Siegel
- 6431 R. Rechard
- 1500 W. Herrmann
- 1510 J. W. Nunziato
- 1512 J. C. Cummings
- 1512 K. L. Erickson

WM-RES
WM Record File
A1756
SNL

WM Project 10, 11, 16
Docket No. _____
PDR ✓
LPDR ✓ (B, A, S)

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PROGRAM: Geochemical Sensitivity Analysis FIN#: A-1756

CONTRACTOR: Sandia National Laboratories BUDGET PERIOD: 10/85 - 9/86

NMSS PROGRAM MANAGER: W. Kelly BUDGET AMOUNT: 365K

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

PRINCIPAL INVESTIGATORS: M. D. Siegel FTS PHONE: 846-5448
R. Recharđ FTS PHONE: 844-3194

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 transferred to the NRC under Task V.

ACTIVITIES DURING MAY 1986

Task I. Uncertainty in Integrated Radionuclide Discharge

Subtask 1A. Conceptual Models for Repository Sites.

Preliminary drafts of site descriptions of basalt and bedded salt site hydrogeology have been completed. The description of the bedded salt site has been sent to the NRC under a separate cover. The description of the basalt site will be sent to the NRC in the near future. Efforts to revise the preliminary site descriptions have been initiated. Information from the conceptual model for the Hanford Site as proposed by Williams & Associates and a recent analysis of ground-water travel time by Rockwell-Hanford Operations (BWI-TI-303) will be considered in the revision of the basalt site model. The Level 3 Case 3 HYDROCOIN problem will be examined for the bedded salt site model. Discussions have been held with Adrian Brown of Nuclear Waste Consultants concerning potential collaboration in the definition of conceptual models for the sites and in design of a data base containing sorption, mineralogical and hydrological data.

Efforts to summarise previous geochemical sensitivity analyses and to rank radionuclides by different criteria continued during May. A

preliminary outline of a letter report and draft figures were sent to the NRC during this month.

Subtask 1B. Solubility/Speciation Effects.

Nothing to report for May.

Subtask 1C. Sorption Effects.

Revision of the document 'Surface-Complexation Modeling of Radionuclide Partitioning in Groundwaters' continued; changes in the document that are required for publication as a SAND report are being made. Parametric calculations of the potential dilution of radionuclides during flow through the undisturbed zone of a hypothetical repository in basalt were initiated this month.

Subtask 1E. Coupled/Dynamic Effects

Documentation of completed work concerning matrix diffusion continued during this month.

An evaluation of the TRANQL code is being written; submission of the final draft to the NRC has been delayed until after the NRC/LANL Workshop on Comparative Modeling of Tracer Migration in the Unsaturated Zone. TRANQL was used by LANL staff to model contaminant transport for this workshop. It is felt that observations from the workshop on the use of TRANQL for this study should be included in the report to the NRC.

Task 4. Short-Term Technical Assistance.

M. Siegel and R. Rechard participated in the NRC/ORNL Workshop on Radionuclide Sorption Issues Related to Nuclear Waste Isolation on May 13-15. Work under this subtask included preparation of lists and descriptions of items for discussion at the workshop and review of the Draft Technical Position Paper on Determination of Radionuclide Sorption for High-Level Nuclear Waste Repositories. A copy of comments prepared for the workshop has been sent to the NRC under a separate cover.

M. Siegel has been requested to serve as a panel member at the NRC/LANL Workshop on Comparative Modeling of Tracer Migration in the Unsaturated Zone on June 18-19.

Task 5. Transfer of Sensitivity Analysis Tools.

The design of interfaces between the ASD, the computer code PHREEQE and sensitivity/uncertainty analysis tools developed at SNLA for the NRC continued during May. Graphics post-processors are being written for the 1-D analytical transport code for porous and fractured media described in the March progress report. The RAINBOW code, previously called RAMBO-1, eventually will be expanded to include a variety of simple analytical and numerical routines for use in sensitivity studies.

Trips

M. D. Siegel and R. Rechard attended a 3 day workshop (May 13 - 15, 1986) devoted to discussions of the role of sorption in retarding the migration of radionuclides from HLW repository systems. The meeting was held at the NRC Willste Building, Silver Spring, MD and involved NRC staff and contractors from SNLA, Oak Ridge National Laboratory, Lawrence Berkeley Laboratory, and Pacific Northwest Laboratory. A major topic of discussion was the different roles in repository assessment played by comprehensive geochemical models, like those developed at ORNL and PNL, and performance assessment models developed at SNLA which use simple approximations to represent geochemical processes. Although it was generally agreed that it was important to understand the geochemical processes that may affect radionuclide transport, little consensus was reached on the required level of understanding or the priorities for research activities.

Other Activities

An abstract was submitted for the December meeting of the Materials Research Society and is appended as Attachment 1. An abstract included in the April progress report was accepted for presentation at the September meeting of the American Chemical Society.

Allocation of Resources

Task 1..... 40%
Task 4.....35%
Task 5.....25%

ATTACHMENT 1

DEVELOPMENT OF AN INTEGRATED GEOCHEMICAL DATA BASE FOR MODELING AND SENSITIVITY ANALYSIS IN NUCLEAR WASTE PERFORMANCE ASSESSMENT STUDIES. S. L. Phillips and F. Hale, Lawrence Berkeley Laboratory, Berkeley, CA 94720; and M. D. Siegel, Sandia National Laboratories, Albuquerque, NM 87185. (SAND86-1342A)

The Aqueous Solutions Database is being developed as a national resource of high-quality, documented and critically-evaluated thermodynamic data. In this paper the contents, scope and quality assurance procedures employed in data evaluation will be described. When completed, the data base will contain thermodynamic property and process values for aqueous species, simple oxides and minerals important to understanding the migration of radionuclides in ground waters at HLW and LLW disposal sites. Pre- and post-processors are being written to generate files of stability constants that can be used by the PHREEQE geochemical speciation computer code and to carry out sensitivity/uncertainty analysis with the Latin Hypercube and PRC/SRC programs. The complete integrated data base system will be used to 1) estimate the overall uncertainty in radionuclide concentration and speciation due to the collective uncertainties in thermochemical data and ground water composition at potential sites and 2) identify key variables which dominate the overall uncertainty of the calculated results. Potential uses of the integrated data base system will be illustrated with examples relevant to HLW and LLW disposal.

This work was supported by the United States Nuclear Regulatory Commission and performed at Sandia National Laboratories, operated for the U. S. Department of Energy under contract number DE-AC04-76DP00789, and at Lawrence Berkeley Laboratory.

A-1756
 1646.010
 May 1986

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

| | <u>Current Month</u> | <u>Year -to- Date</u> |
|--|--------------------------|-------------------------------|
| I. Direct Manpower (man-months of charged effort) | 1.7 | 9.4 |
| II. Direct Loaded Labor Costs | 21. | 99. |
| Materials and Services | 0.0 | 2.0 |
| ADP Support (computer) | 0.0 | 1.0 |
| Subcontracts | 11. | 67. |
| Travel | 1.0 | 6.0 |
| Other (computer roundoff) | 0.0 | 1.0 |
| TOTAL COSTS | 33. | 176 |

III. Funding Status

| <u>Prior FY Carryover</u> | <u>FY 86 Projected Funding Level</u> | <u>FY 86 Funds Received to Date</u> | <u>FY 86 Funding Balance Needed</u> |
|-------------------------------|--|---|---|
| None | 365K | 365K | None |