Sandia National Laboratories
Albuquerque, New Mexico 87185

June 14, 1985

Mr. Walton Kelly
U.S. Nuclear Regulatory Commission
Mail Stop 623-SS
Washington, DC 20555

Dear Mr. Kelly:

Enclosed is the monthly report for FIN A-1756, Geochemical Sensitivity Analysis for May 1985.

A review of the letter report "Geochemical Sensitivity Analysis I. Radioelement Speciation" and a letter report containing recommendations on geochemical modeling were received in early May. We appreciate the comments by the Oak Ridge staff and will clarify those sections that led to any confusion. Although we recognize the limitations associated with calculations of radioelement speciation using available thermochemical data, we do not agree with the recommendations suggested by Jacobs. We do not feel they reflect the needs or methods of performance assessment or sensitivity analyses. Our response to these comments and recommendations will be sent to the NRC under a separate cover to prevent delay of the April progress report.

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

Sincerely,

R M Cranwell

R. M. Cranwell
Supervisor
Waste Management Systems
Division 6431

RMC:6431:jm

Enclosure

Copy to:
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PROGRAM: Geochemical Sensitivity Analysis FIN#: A-1756

CONTRACTOR: Sandia National Laboratories BUDGET PERIOD: 10/01/84 - 9/30/85

DRA PROGRAM MANAGER: W. R. Kelly BUDGET AMOUNT: 235K

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

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

PROJECT OBJECTIVES

The objective of this project is to provide technical assistance to the NRC in determining the sensitivity of far-field performance assessment calculations to uncertainties in geochemical and hydrological input 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, kinetic and sorption 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 under Task III. Short-term technical assistance will be carried out under Task IV.

ACTIVITIES DURING MAY 1985

Task I Uncertainty in Integrated Radionuclide Discharge

Subtask IA. Speciation Effects
(M. Siegel, R. Guzowski, S. Phillips)

A copy of the interactive input file preparation code for the PHREEQE geochemical code was acquired and will be installed on the CDC computer.

Hydrogeological data for drill holes DB-15, RRL-2, DC-16A, DC-14 and DC-15 in the Basalt SCR were digitized and entered into the dBase III system. Several hypothetical flow paths for the basalt site will be chosen for system scoping calculations of integrated discharge. These data will be used to describe the characteristics of transport legs in the calculations.

A letter report discussing the limitations and benefits of performing speciation calculations with available thermochemical data is in preparation. The issue will be examined from viewpoints of both experimental thermochemistry and performance assessment. Dr. S. Phillips (Lawrence Berkeley Laboratory) offered the following comments on the issue:

"The question is raised whether the measurement techniques used for solubility/speciation experimental data are current state-of-the-art. Lack of adequate instrumentation may well account for failure to detect important species such as U(OH)5-. A critical survey of instrumental methods for important waste nuclides such as U++++, Pu++++ and Np++++ is recommended.

The Letter Report to Kelly from ORNL (March 28, 1985) should be revised to include information on PuCO3++ published by Rai and Ryan and by Silva and Nitsche (both 1985). The revision should also include discussion of that portion of Lemire's critical evaluation of Np data bearing on hydroxy-Np complexes in aqueous media.

With reference to Kelly's letter (April 29, 1985): the LBL/BES/NRC thermodynamic database is readily edited to include changes in recommended data. Identifying (flagging) data with explanatory information is readily done."

A copy of a letter by Phillips and supporting documents are being sent to the NRC under a separate cover.

References:

D. Rai; J. L. Ryan "Neptunium (IV) Hydrous Oxide Solubility under Reducing and Carbonate Conditions" Inorg. Chem. 1985, v. 24, 247. R. J. Silva; H. Nitsche "Carbonate Complexation of Pu(IV) in Aqueous Solution" 189th ACS National Meeting, Miami, FL, April 29-May 3, 1985.

R. J. Lemire "An Assessment of the Thermodynamic Behaviour of Neptunium in Water and Model Groundwaters from 25 to 150 C" AECL-7817, Atomic Energy of Canada Limited, Whiteshell Nuclear Research Establishment, Pinawa, Manitoba ROE 1LO, Canada (March 1984).

Subtask IB. Sorption Effects
(M. Siegel, A. Trujillo, J.O. Leckie, D. Kent)

The compilation of sorption data from NNWSI publications dealing with tuff has been completed. The data have been installed onto the dBase III management system. Programs to calculate descriptive statistics (mean, standard deviation, kurtosis, skewnese, frequency distributions, transformations) for any subset of the data have been incorporated into the data management system.

Subtasks IC, ID Kinetic and Dynamic Effects
(M. Siegel, K. Erickson, J. O. Leckie)

A paper entitled "Approximate Methods to Calculate Radionuclide Discharges for Performance Assessment of HLW Repositories in Fractured Rock" is in preparation. This paper is to be presented and published in the proceedings of the 1985 MRS Symposium for the Scientific Bases for Nuclear Waste Management.

Task II. Evaluation of Error Due to Organics and Colloids

Subtask 2A Effects of Colloids
(M. Siegel, E. Bonano, H. E. Nuttall, J. Catasca)

A preliminary draft of a report describing calculations to estimate an upper bound for the effect of the transport of radionuclides by colloids is in preparation.

Task IV Short Term Technical Assistance

No activity in May 1985.

Conferences

M. D. Siegel and K. L. Erickson attended the Symposium on Groundwater Flow and Transport Modeling for Performance Assessment of Deep Geologic Disposal of Radioactive Waste, held in Albuquerque, May 20-21, 1985. Results from Sandia's Geochemical Sensitivity Analysis Program were presented by Siegel and Erickson. A significant point made during the meeting was that comprehensive models will help provide fundamental understanding of flow and transport mechanisms, but to engineer a facility, more attention should be given to developing methodologies for reliably predicting upper bounds to radionuclide discharges. This point was encouraging since part of the work presented by Siegel and Erickson involved developing methods for bounding radionuclide discharges when multiple chemical species of the nuclide exist.

Funding Breakdown for May

Task I - 95%
Task II - 5%

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1646.010
May 1985

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)	1.4	10.6
II.	Direct Loaded Labor Costs	14.0	105.0
	Materials and Services	0.0	3.0
	ADP Support (computer)	0.0	2.0
	Subcontracts	20.0	105.0
	Travel	1.0	5.0
	Other	1.0	0.0
	TOTAL COSTS	36.0	220.0

Other = rounding approximation by computer

III. Funding Status

Prior FY Carryover	FY85 Projected Funding Level	FY85 Funds Received to Date	FY85 Funding Balance Needed
67.6K	302.60K	235K	None