

Sandia National Laboratories

Albuquerque, New Mexico 87185

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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 November 1985.

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

Sincerely,

Robert M. Cranwell

R. M. Cranwell
Supervisor
Waste Management Systems
Division 6431

RMC:6431:jm

Enclosure

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PDR WMRES EXISANL
A-1756 PDR

PROGRAM: Geochemical Sensitivity
Analysis

FIN#: A-1756

CONTRACTOR: Sandia National
Laboratories

BUDGET PERIOD: 10/01/85 -
9/30/86

DRA PROGRAM MANAGER: W. R. Kelly BUDGET AMOUNT: 265K

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 NOVEMBER 1985

Task I. Uncertainty in Integrated Radionuclide Discharge

Subtask 1A. Speciation Effects (M. Siegel, S. Phillips, R. Guzowski)

A major part of the work carried out under this subtask was devoted to formulation of conceptual models for repository sites in salt and basalt. Documentation of preliminary NWFT/DVM runs for the conceptual basalt site was completed in preparation for meetings with NRC staff scheduled for December 18, 1985. A preliminary conceptual model for a salt site was formulated. Data for Deaf Smith County was obtained from the DOE Environmental Assessment report DOE/RW-0014. Data from the lithologic log for the J. Friemel No. 1 well, the Repository Site Data Report for the Palo Duro Basin (NUREG/CR-3129) and several other sources of data were consulted to obtain hydrologic properties along potential flow paths.

Efforts to compile the program PHRQINPT on an IBM PC/AT continued this month. Difficulties have been encountered due

to some features of the compiler that has been used (IBM Professional FORTRAN).

Preparations were made for the upcoming meeting of the Thermodynamics Data Base Advisory Committee. A preliminary schedule and list of invitees are appended to this progress report.

A report describing alternative methods to calculate chemical equilibria in saline brines was completed and is under review at SNLA.

Subtask 1B. Equilibrium Sorption Effects
(M. Siegel, J. O. Leckie, and D. Kent)

A preliminary draft of a report on the application of the Stanford Generalized Model for Adsorption (SGMA) was completed during November and is currently under review. The report was received too late to be included or summarized in the progress report for FY85.

Subtask 1C and 1D. Kinetic and Dynamic Effects
(K. Erickson, W. Beyeler, M. Siegel)

A preliminary report describing derivation of approximate methods to calculate radionuclide discharge has been completed and is under review. A computer code is being written to calculate an exact solution for radionuclide discharge in a system of flat plates where matrix diffusion is important. The code will be used to evaluate the error associated with the approximations referred to above. A paper discussing this work has been accepted for the Waste Management "86" conference to be held in Tucson, Arizona on March 6, 1986.

Other Activities

A major portion of activity in FIN-1756 during November was directed toward preparation of the FY85 Annual Report. A draft of the report is under review by the contributors and staff at NRC and SNLA. A final version of the report will be prepared in December.

Breakdown of Funds

Task I - 80%
Task II - 20%



Lawrence Berkeley Laboratory

1 Cyclotron Road Berkeley, California 94720

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TO: Chemical Thermodynamics Advisory Committee
(Distribution)

SUBJECT: Meeting, Tuesday, December 17, 1985
U.S. Nuclear Regulatory Commission
Willste Building
7915 Eastern Avenue
Silver Spring, MD 20555

AGENDA

- 8:30 Welcome
- 9:00 S. Phillips: Chemical Thermodynamic Tables for Geoscientific Research and Advanced Development. Applications to Nuclear Waste Disposal.
- 9:30 Discussion
- 10:30 Coffee break
- 10:45 J. Haas: Thermodynamic Data on Minerals for Nuclear Waste Disposal.
- 11:15 Discussion
- 12:00 Lunch
- 1:00 S. Phillips; L. Silvester: Equilibrium Constants in Saline Brines.
- 1:30 Discussion
- 2:30 Coffee break
- 2:45 M. Siegel: Uncertainty and Error Propagation in Geothermodynamic Equilibrium Calculations
- 3:15 V. Parker: Uncertainty in Thermodynamic Data
- 3:30 M. Siegel: Propagation of Errors
- 3:45 Discussion
- 4:15 Relationship to Other Work (OCED, IAEA, CODATA)
- 5:00 Thanks to Attendees. Adjourn

Sincerely,

Sidney L. Phillips

Malcolm D. Siegel

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A-1756
1646.010
November 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)	0.7	1.4
II. Direct Loaded Labor Costs	7.0	16.0
Materials and Services	0.0	0.0
ADP Support (computer)	0.0	0.0
Subcontracts	-11.0	-5.0
Travel	0.0	1.0
Other	<u>1.0</u>	<u>1.0</u>
TOTAL COSTS	-3.0*	13.0

Other = rounding approximation
by computer

III. Funding Status

Prior FY Carryover	FY86 Projected Funding Level	FY86 Funds Received to Date	FY86 Funding Balance Needed
None	265K	115K	150K

*Negative costs reflect internal transfers at SNLA and are due to
adjustments in subcontract charges described in monthly progress
report for August 1985.