

Sandia National Laboratories

Albuquerque, New Mexico 87185

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February 1, 1985

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LWM-RES
WM Record File
A1756
SNL

WM Project 10, 11, 16
Docket No.

PDR ✓
LPDR ✓ (B, N, S)

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

Distribution:

Kelly
3-1-11
(Return to WM, 623-SS)

Joan - ticket

Dear Mr. Kelly:

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

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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PDR WMRES EXISANL
A-1756 PDR

1867

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: 267.6K

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 JANUARY 1985

Task I Uncertainty in Integrated Radionuclide Discharge

Subtask IA. Speciation Effects
(M. Siegel, A. Trujillo, S. Phillips)

A draft of a thermochemical data base for the elements: Am, Np, Pu, Sr, O, F, P, Si, Al, Cl, Br, C, As, S, Mo, and I was received this month and is currently under review. Several changes to the data base were suggested by the Technical Advisory Committee (see Progress Report First Quarter FY85) at the first meeting of the committee. During January, work was initiated to incorporate these suggestions into the data base. These changes include: clear identification of calculated versus tabulated values, clearer referencing of sources for each datum and addition of a "comments" section to document changes in the data base as new data are added or mistakes are corrected.

Subtask IB. Equilibrium Sorption Effects
(M. Siegel, A. Trujillo)

Additional data were entered onto the dBASE III sorption data base during January. Compilation of site density and surface binding constant data for use in theoretical sorption calculations continued during this month also.

Subtask ID. Dynamic Effects
(M. Siegel, J. Leckie, K. Erickson)

A report describing an evaluation of the applicability of the code TRANQL to problems of interest in HLW management was reviewed. Additional calculations will be carried out at Stanford University with TRANQL to address several concerns that were raised as a result of this review.

Progress was made towards carrying out a bench-marking calculation which will allow comparison of the values of radionuclide discharge computed by TRANQL with those computed by the analytic solutions to the convective-dispersion-reaction equation developed at SNLA. The calculation requires reformulation of expressions for retardation factors in terms of equilibrium constants for sorption reactions. The results of the calculation should allow formulation of more defensible expressions for radionuclide retardation factors in performance assessment calculations and provide a more accurate estimate of uncertainties in model calculations of radionuclide discharges.

Task II Evaluation of Error Due to Organics and Colloids

No activity in January 1985.

Task IV Short Term Technical Assistance

No activity in January 1985.

Other Activities

The progress report for the first quarter of the 1985 fiscal year was completed during January.

Funding Breakdown for January

Task I - 100%

A-1756
1646.010
January 1985

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

	Month	Current Year-to-Date
I. Direct Manpower (man-months of charged effort)	0.9	5.9
II. Direct Loaded Labor Costs	9.0	59.0
Materials and Services	0.0	3.0
ADP Support (computer)	0.0	1.0
Subcontracts	2.0	39.0
Travel	1.0	4.0
Other	<u>0.0</u>	<u>0.0</u>
TOTAL COSTS	12.0	106.0

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*	267.6K	200K	None

*Includes 40K of committed funds (purchases) that have not been
invoiced.