A-1756 LPDR-(6)
WM-10 (2); WM-11 (2)
WM-16 (2)
PDR-(1)

January 15, 1987

JAN 15 A11 34

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 December 1986. 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,

Robert M. Cranwell

Robert M. Cranwell, Supervisor
Waste Management Systems
Division 6431

RMC:6431

Enclosure

Copy to:
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1512 J. C. Cummings
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WM-RES
WM Record File
A1756
SNL

WM Project 10,11,16
Docket No.
PDR ✓
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Distribution:
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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 DECEMBER 1986

Task I. Uncertainty in Integrated Radionuclide Discharge

Subtask 1A. Conceptual Models for Repository Sites.

Parametric calculations of radionuclide discharge from a repository in a hypothetical basalt site continued during December. The ability of the GENMIX code to account for both radioactive decay and production in a computationally efficient manner are being exploited in these studies. The effect of dispersivity on the radionuclide discharge was examined for ground-water travel times of 1000 and 8400 years for the 30 radionuclides listed in Table 1. The structures of the associated decay/production chains are illustrated in Figure 1; the remaining radionuclides in Table 1 are fission products. Figure 2 shows the calculated radionuclide discharge of 'unretarded' Americium-241 for a ground-water travel time of 8400 years for 4 different longitudinal dispersivities. It can be seen that the peak and integrated discharges are very sensitive to the dispersivity under these conditions. Analysis of the discharge peaks of Cm-245 and Pu-241, the radiogenic parents of Am-241, show that the discharge of Am-241 is dominated by decay of Cm-241 starting 6000 years after the time of repository closure. For the first 4000 years of the simulation, the discharge

curve is more strongly affected by the decay of the original inventory of Am-241 and the Am-241 produced by the short-lived isotope Pu-241. When the dispersivity is 500 m, a significant fraction of the original Am-241 reaches the accessible environment before it decays. The strong sensitivity of discharge on dispersivity was unexpected and illustrates the importance of including radioactive production in transport codes used in geochemical sensitivity analysis.

A draft report describing the geochemical conceptual model that will be used in the simulations of radionuclide discharge from the basalt site has been written. Data for formulation of a conceptual model of a hypothetical salt site is being compiled.

Subtask 1B. Solubility/Speciation Effects.

No activity to report.

Subtask 1C. Sorption Effects.

Theoretical calculations of the sorption of selected radioelements, using the MINEQL code continued during December.
Critical evaluation of the empirical sorption data in the dBase III+ data base continued during December. Procedures that will allow users to subset the data on experimental criteria are being incorporated into the system.

Subtask 1E. Coupled/Dynamic Effects

No activity to report.

Task 4. Short-Term Technical Assistance.

No activity to report.

Other Activities.

The Annual Progress Report for FY86 is being completed and will be sent to the NRC Program Manager by the end of the month.

Trips.

M. Siegel attended the tenth annual Materials Research Society symposium on the Scientific Basis for Nuclear Waste Management. The conference was held in Boston Massachusetts on December 1-4, 1986. The focus of the symposium stressed materials properties of components of the waste packages in European and American high-level waste research programs. Individual sessions dealt with the topics of long-term projections of waste package performance, behavior of waste glass, spent fuel and cannisters and on materials interactions. Additional sessions focused on radiation effects, low-level waste and ground-water chemistry.
Several general observations can be made about the papers presented at the symposium. First, it was generally agreed that extrapolations of the results of short-term tests could be made only if a fundamental

understanding of the processes and mechanisms active at the repository sites could be obtained. However, nearly all of the talks presented at the symposium were descriptions of empirical data without attempts to obtain a mechanistic understanding of the results. In general, the large number of complex interactions that are possible in natural systems has prevented detailed understanding of the dominant processes. Second, attendance and the quality of the work presented at the symposium was lower than in previous years. Thirdly, the work presented at the meeting was dominated by DOE and European researchers; there was little representation of the NRC staff or contractors.

Allocation of Resources

Task 1.....100%

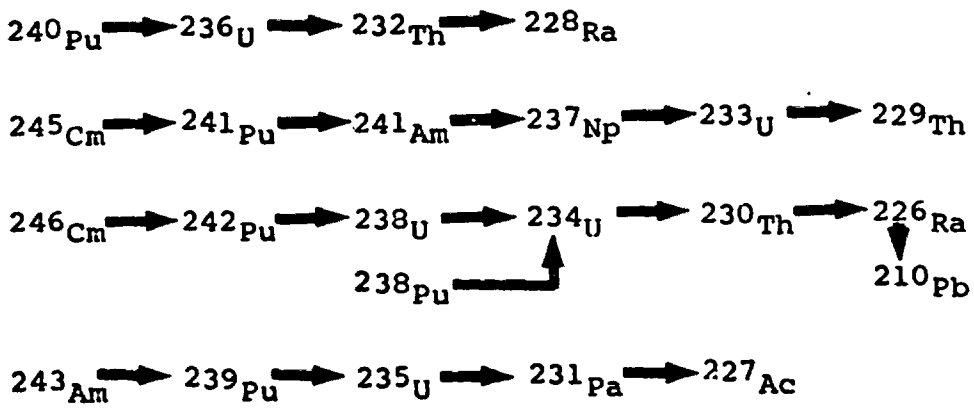

Figure 1. Decay chain representation of radionuclides considered in calculations of radionuclide discharge. Initial inventories and half-lives are listed in Table 1. Fision products are included in a separate chain.

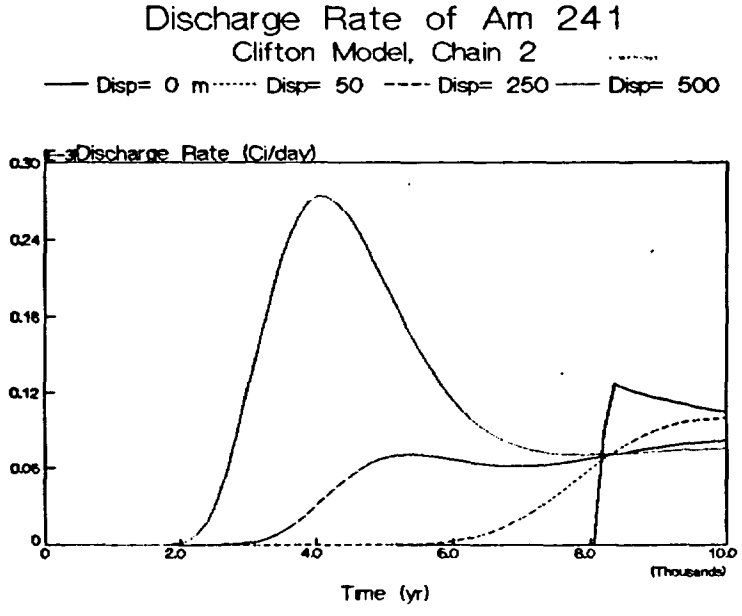

Figure 2. Discharge of Am-241 at distance of 5 km from source at hypothetical basalt repository site. Ground-water travel time is approximately 8200 years; retardation factors are equal to unity for all members of decay chain. Different curves correspond to different values of longitudinal dispersivity. Initial containment period is 300 years; annual fractional release rate is 10 part per million of initial inventory.

Table 1

Inventory of Reference Repository
(Spent fuel from 46,800 MTHM)

Radionuclide	Half Life	Curies (at time=0)
Pu240	6.76E3	2.1E7
U236	2.39E7	1.0E4
Th232	1.41E10	1.7E-5
Ra228	6.7	4.7E-6
Cm245	8.27E3	8.4E3
Pu241	14.6	3.2E9
Am241	433.	7.5E7
Np237	2.14E6	1.5E4
U233	1.62E5	1.8
Th229	7300.	1.3E-3
Cm246	4710.	1.6E3
Pu242	3.79E5	7.5E4
U238	4.51E9	1.5E4
Pu238	89.	9.4E7
U234	2.47E5	3.5E3
Th230	8.E4	0.19
Ra226	1600.	3.5E-4
Pb210	21.	3.3E-5
Am243	7650.	6.6E5
Pu239	2.44E4	1.4E7
U235	7.1E8	7.5E2
Pa231	3.25E4	0.25
Ac227	21.6	5.2E-2
Tc99	2.14E5	6.1E5
I129	1.6E7	1.5E3
Sn126	1.0E5	2.2E4
Sr90	28.9	2.4E9
C14	5730.	3.5E4
Cs135	2.0E6	1.3E4
Cs137	30.	3.5E9

A-1756
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December 1986

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)	0.6	1.5
II. Direct Loaded Labor Costs	5	12
Materials and Services	0	5
ADP Support (computer)	2	4
Subcontracts	11	70
Travel	1	1
Other (computer roundoff)	0	1
TOTAL COSTS	19	93

III. Funding Status

Prior FY Carryover	FY 86 Projected Funding Level	FY 86 Funds Received to Date	FY 86 Funding Balance Needed
32	232K	200K	None

FROM	DATE OF DOCUMENT	DATE RECEIVED	NO
SNL	1/15/87	1/1[illegible]/87	WM-87022

LTR	MEMO	REPORT	OTHER
		XX	

TO	ORIG.	CC	OTHER
WKelly		XX	

ACTION NECESSARY	☒	CONCURRENCE	☐	DATE ANSWERED
NO ACTION NECESSARY	☐	COMMENT	☐	BY 1/30

CLASSIF

POST OFFICE

REG. NO.

FILE CODE: 426.1 (A1756)

DESCRIPTION (Must Be Unclassified)

Dec 86 Report forFFIN A1756

REFERRED TO	DATE	RECEIVED BY	DATE
PJustus	1/16	[illegible]	1/16
WKelly		[illegible]	1/20

ENCLOSURES

Ticket closed out by letter to Dr. Malcolm D. Seigel on 87/01/29.

REMARKS

U. S. NUCLEAR REGULATORY COMMISSION

MAIL CONTROL FORM

FORM NRC 326 (1-75)