Sandia National Laboratories
Albuquerque, New Mexico 87185

July 12, 1985

WM-RES
WM Record File A1756 SNL

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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 June 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

2211

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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 JUNE 1985

Task I Uncertainty in Integrated Radionuclide Discharge

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

An assessment of the error in speciation and solubility calculations due to the use of the Davies equation in place of "Pitzer equations" (specific interaction) to calculate activity coefficients in saline brines was initiated. In this study, a comparison of activity coefficients calculated with the two methods will be made for several radionuclides in ionic strengths of up to 3.0 M. The results of this study will provide guidance in the selection of the most appropriate geochemical codes for sensitivity studies for HLW repository sites in salt formations.

Coordination of NRC-sponsored projects which involve compilations of thermochemical data was discussed at recent meetings between NRC staff and M. Siegel. It was suggested that efforts at Pacific Northwest Laboratory (S. Peterson)

should be coordinated with similar efforts at Lawrence Berkeley Laboratory (S. Phillips). As of July 1, no definitive action had been taken by the NRC towards achieving this goal.

It was also suggested that the data in the LBL/NRC/BES data base currently being compiled at Lawrence Berkeley Laboratory should be periodically compared to thermochemical data compiled by DOE for each of the HLW repository sites. The resources for this additional effort will require supplemental funding in FY86 and FY87. This subject is discussed in more detail under the section entitled "Travel-Informal Meetings with NRC staff."

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

Compilation of fundamental thermochemical data and review of experimental studies of sorption of radionuclides by natural and synthetic materials continued during June. The results of this work will be a review of the state-of-the-art of theoretical modeling of radionuclide sorption, an assessment of the error resulting from the assumption of linear sorption isotherms in calculations of integrated discharge, and an evaluation of the feasibility of using phenomenological models of sorption in performance assessment studies.

All of the empirical Kd data published by Los Alamos National Laboratories for tuff has been entered into the dBase III system and have been checked for accuracy and redundancy. Supplemental statistical software for the data base was used to calculate descriptive statistics for sorption ratios of different tuff lithologic types and stratigraphic sorption intervals. These summary tables (see Attachment 1) will be included in the report Repository Site Data Report for Unsaturated Tuff, Yucca Mountain Nevada (funded by FIN A-1158). The data will also be used in setting up conceptual models of a tuff site for system-scoping studies under Subtask IA.

A copy of the dBase III data base was delivered to the NRC for use by staff geochemists. Future efforts under this subtask will include development and documentation of additional supplemental software to create a user-friendly sorption data base for the use of the NRC.

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

Most of the effort under these subtasks during June was directed toward the completion of two papers. The first paper, entitled "Geochemical Sensitivity Analysis for Performance Assessment of HLW Repositories: Effects of Speciation and Matrix Diffusion" was discussed in the May Progress report.

The second paper, entitled "Approximate Methods to Calculate Radionuclide Discharges for Performance Assessment of HLW Repositories in Fractured Rock" is scheduled to be presented at the 1985 MRS symposium on the Scientific Basis for Nuclear Waste Management. Approval for the travel of K. Erickson to the meeting and to meetings with scientists at the Swedish Royal Institute of Technology has been requested from the NRC.

Task II Evaluation of Error Due to Organics and Colloids

No activity during June 1985.

Task IV Short Term Technical Assistance

M. Siegel attended meetings with NRC staff in Washington during the week of June 10-14, 1985.

A letter report discussing the role of radionuclide speciation/solubility calculations in sensitivity analyses is under preparation.

Travel

Informal meetings with NRC staff:

During the week of June 10-June 14, Malcolm Siegel (6431) met with members of the Offices of Nuclear Material Safety and Safeguards (NMSS) and Nuclear Regulatory Research (RES) of the Nuclear Regulatory Commission (NRC). Meetings like these are being requested by the NRC to allow the staff of Division 6431 to obtain a clear understanding of the concerns and constraints of the NRC. Many of the discussions dealt with geochemical aspects of waste management. The NRC staff were particularly interested in the data management systems for thermochemical and experimental sorption data that are being compiled under the Geochemical Sensitivity Analysis Project (FIN A-1756). It was determined that Dr. Siegel will work with NRC geochemists in setting up simple conceptual models of repository sites for sensitivity studies. During the meetings, it became apparent that many NRC staff members were not familiar with the products of the SNLA contracts. This fact is significant because many of the concerns of the NRC could be addressed by ongoing SNLA projects.

Several changes in the structure and schedule of FIN A-1756 were discussed with the NRC Program Manager. A revised milestone schedule is included as Attachment 2 to this progress report. It was agreed that a major focus of the project should be the writing, documentation and transfer to the NRC of a suite of user-friendly computer code data bases for geochemical sensitivity analyses. It was also agreed that the peer review

of the products and approach of the project which is included under Task 3 should be an on-going effort and should not be deferred to the last year of the project as originally planned. The review should include systematic comparisons of the data in the thermochemical data base compiled under Task I with similar data bases being produced by DOE. These changes to the project cannot be acommodated within the current level of funding. In order to support these additional efforts, supplemental funds equivalent to one-half FTE (full-time equivalent) will be requested for the fiscal years 1985, 1986 and 1987. A formal request for the additional funding will be sent to the NRC under a separate cover.

Funding Breakdown for June

Task I	75%
Task IV	25%

Attachment I

Summary of Sorption Data
for Yucca Mountain, Nevada

from Tien, P., Siegel, M. D., Updegraff, C. D., Wahi, K. K., and Guzowski, R. V., Repository Site Data Report for Unsaturated Tuff, Yucca Mountain, Nevada, SAND84-2668, NUREG/CR-4110

Table 5-4. Comparison of sorption ratios for tuff lithologies (mℓ/gm)

Element	Devitrified tuff	Devitrified tuff with clay/glass	Vitric tuff ± clay	Zeolitized tuff
Am	2975 ± 1240 [a] 4, N [c] 1200:4000 [d]	[2.80 ± 0.93] [b] 4, L 130:13000	1430 ± 450 4, N 920:2000	[3.18 ± 0.32] 10, L 490:5500
Ba*	[3.00 ± 0.37] 17, L 340:1400	[2.92 ± 0.44] 29, L 140:10000	1155 ± 766 6, N 420:2100	[4.56 ± 0.60] 33, L 1170:250000
Ce	817 ± 427 13, N 297:1630	332 ± 293 5, N 82:730		[3.52 ± 0.72] 19, L 100: 59000
Cs*	596 ± 237 17, N 290:1100	[2.94 ± 0.45] 29, L 120:13300	[2.64 ± 0.67] 5, L 120:5800	[3.94 ± 0.40] 31, L 1160:42000
Eu*	1154 ± 614 15, N 68:2250	[3.04 ± 0.44] 29, L 90:5600	111 ± 68 4, N 38:190	[3.43 ± 0.45] 29, L 200:15000
Np	5.7 ± 0.8 5, N 4.9:7.0		2.1 ± 0.1 2, N 2.0:2.2	6.5 ± 3.5 6, N 4.0:11
Pu	224 ± 110 7, N 64:420	[2.24 ± 0.56] 4, L 90:1200	325 ± 85 4, N 210:410	[1.66 ± 0.32] 12, L 19:250

Table 5-4. Comparison of sorption ratios for tuff lithologies (mℓ/gm)--continued

Element	Devitrified tuff	Devitrified tuff with clay/glass	Vitric tuff + clay	Zeolitized tuff
Se	10.0 ± 7.1	[0.72 ± 0.46]	3.7 ± 3.1	5.7 ± 4.0
	2, N	5, L	3, N	5, N
	5:15	2:25	1:7	1.8:11
Sr	86 ± 50	111 ± 77	[1.85 ± 0.49]	[3.76 ± 0.68]
	16, N	26, N	5, L	34, L
	30:195	41:280	24:280	148:81000
Tc	0.40 ± 0.32	0	0.02 ± 0.02	0.01 ± 0.01
	7, N	1	6, N	3, N
	0:0.81	-	0:0.04	0:0.02
U	14 ± 26	3.4 ± 4.0	5 ± 10	6.2 ± 3.1
	4, N	8, N	4, N	7, N
	0:54	0:10	0:20	2.5:11

a mean ± standard deviation for assumed normal distribution
b [mean ± standard deviation] in $\log_{10}$ units for assumed lognormal distribution
c number of values, distribution assumed (N = normal; L = lognormal)
d minimum value : maximum value
* data for deionized water and water from well UE25p-1 are included in the means for vitric and zeolitized tuffs for Ba, Cs, and Eu.

Table 5-5. Summary of sorption data for stratigraphic sorption intervals

Sorption Interval	Element			
	Am	Ba, Ra	Cs	Eu
Host Rock	3350±354 2, N 3100:3600	575±332 2, N 340:810	515±163 2, N 400:630	84±23 2, N 68:100
Zeolite 1		3400	855	160000
Basal Vitrophyre	1110±269 2, N 920:1300	1585±690 4, N 640:2100	390±57 2, N 350:430	165±35 2, N 140:190
Vitric Zone	1750±354 2, N 1500:2000	357±250 3, N 82:570	108±58 3, N 45:160	[2.56±1.45] 3, L 38:17000
Zeolite 2	[3.18±0.32] 10, L 490:5500	[4.66±0.43] 23, L 6180:150000	[3.9±0.2] 19, L 3660:17000	[3.74±0.43] 21, L 1340:100000
Central Prow Pass	4700	[2.92±0.64] 11, L 162:1400	[2.81±0.41] 11, L 184:3650	878±598 9, N 110:1900
Zeolite 3	4300	[4.46±0.71] 15, L 1170:250000	[4.02±0.59] 12, L 1160:42000	[3.17±0.27] 12, L 779:5600
Central Bull Frog	372±309 2,N 153:590	[2.70±0.37] 16, L 140:3040	[2.75±0.36] 15, L 120:2020	[2.99±0.43] 12, L 340:5500
Zeolite 4		63000	7700	200
Deep Zone		7427±5685 10, N 1000:15000	[3.52±0.39] 10, L 1080:16000	[3.22±0.54] 9, L 440:15000

Table 5-5. Summary of sorption data for stratigraphic sorption intervals--(continued)

Sorption Interval	Element				
	Np	Pu	Sr	Tc	U
Host Rock	5.1±0.3 4, N 4.9:5.4	287±84 4, N 240:420	46±22 2, N 30:61	0.44±0.38 4, N 0:0.81	5.0±7.1 2, N 0:10
Zeolite 1			260		0 2 0:0
Basal Vitrophyre		365±64 2, N 320:418	121±112 2, N 42:200		0 2 0:0
Vitric Zone	2.1±0.1 4, N 2.0:2.2	285±106 2, N 210:360	22±11 3, N 10:32	0.03±0.02 5, N 0:0.04	10±14 2, N 0:20
Zeolite 2	6.5±3.5 6, N 4:11	[1.66±0.32] 12, L 19:250	[3.86±0.52] 24, L 1760:81000	0.01±0.01 3, N 0:0.02	7.2±3.3 3, N 5.3:11.0
Central Prow Pass	6.4	77	[1.73±0.34] 10, L 22:194		28±36 2, N 2.4:54
Zeolite 3	9	230	[3.50±0.88] 12, L 148:56000	0.18±0.04 2, N 0.15:0.21	6.0±3.8 3, N 2.5:10
Central Bull Frog		85±7 2, N 80:90	[1.94±0.29] 13, L 41:280		1.0±0.9 3,N 0:1.7
Zeolite 4			42000		
Deep Zone			[2.93±1.02] 11, L 68:13200		2.15±2.33 2, N 0.5:2.33

Attachment 2

REVISED MILESTONE SCHEDULE FOR FIN-1756

Report on status of thermochemical data and criteria for data selection Updates: M.P.R.* and A.P.R.*	First report: 1/30/85 included in Q.P.R.* and published in LBID-977
Scoping calculations for colloids:	
Particle migration in fracture	11/16/84 A.P.R. for FY84
Interim report on capacity and formation rates of pseudo- and true colloids	Included in A.P.R. FY85
Final report on colloid calculations (included in interim report on system scoping calculations)	12/85
Letter report on kinetics/speciation and experimental design	11/84 A.P.R. for FY84 revised 10/85
NRC/DOE conference paper due (effects of speciation and matrix diffusion)	7/1/85
MRS paper due (transport in fractured rock)	8/1/85
Draft report on chemical transport simulator (TRANQL)	9/15/85 included in M.P.R. for August 1985
Annual Progress Report for FY 1985	10/30/85
Interim report on system calculations for speciation, non-linear sorption, and colloids	12/85
Progress reports on choice and modifications of codes for modeling	Reported in M.P.R.'s, A.P.R. for FY85 and interim reports
Progress reports on reaction pathways for modeling	Reported in M.P.R.'s and interim reports
First BES/NRC data base available	2/86
Updates to data base	Reported as available in M.P.R.'s
Second BES/NRC data base published	T.B.D.
Interim report on contaminant transport in fractured rock	3/86

Interim report on uncertainties related to speciation and sorption (Tasks 1A and 1B)	8/86
Annual Progress Report for FY 1986	10/30/86
Interim report on uncertainties related to kinetics (Task 1C)	12/86
Interim report related to coupled effects (Task 1D)	3/87
Draft Final Topical Report (Task 3A) 1. Data bases 2. Theory 3. Computer Codes	6/87
Report on Peer Review Workshop and Final Report (Task 3B) included in Annual Report for FY 1987	10/87

*Q.P.R. = Quarterly Progress Report; M.P.R. = Monthly Progress Report; A.P.R. = Annual Progress Report

A-1756
1646.010
June 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	12.0
II.	Direct Loaded Labor Costs	13.0	118.0
	Materials and Services	0.0	3.0
	ADP Support (computer)	0.0	2.0
	Subcontracts	10.0	115.0
	Travel	1.0	6.0
	Other	0.0	0.0
	TOTAL COSTS	24.0	244.0

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