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April 15, 1986

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 March 1986.

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

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Mr. Walton Kelly

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April 15, 1986

Copy to:

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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: 365K

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. Computer codes and other sensitivity analysis tools will be transferred to the NRC under Task V.

ACTIVITIES DURING MARCH 1986

Task 1. Uncertainty in Integrated Radionuclide Discharge

Task 1A. Conceptual Models for Sites

Descriptions of the stratigraphy and hydrogeology of conceptual models of basalt and bedded salt sites were revised during March. Sections on mineralogy and geologic setting were added to the reports, sources of data were documented and the simplifications to the stratigraphy that will be used in the sensitivity analysis were justified. The current drafts will be reviewed by SNLA staff members who are currently modeling the hydrology of the BWIP site before they are sent to the NRC for comments.

The review of previous efforts to rank radionuclides according to relative hazard and uncertainty in predicted behavior continued during this month. Reports by Barney and Wood (1980), Kerrisk (1985), Hill (1979), and EPA (1977) have been reviewed.

Task 1B. Solubility/Speciation Effects

Thermochemical data for minerals associated with silicic rocks were recently compiled by the Nuclear Energy Agency (Muller, 1985). These data are being entered into the computer data bank of the Aqueous Solution Database. In addition, the current data in the data base are being reviewed for typographical errors and several new features are being added to the system. These include an index table of the elements whose data are available in the data base, an electronic mail feature to allow users to comment on the contents of the compilation, and a pre-processor for the computer code PHREEQE.

Task 1C. Sorption Effects

The first draft of a report on application of the Stanford General Model for Adsorption to High Level Waste is currently under review. Extensive revision of the document will be required before it can be released as a NUREG report.

Task 1E. Coupled/Dynamic Effects

The paper "Approximate Methods to Calculate Radionuclide Discharges for Performance Assessment of HLW Repositories in Fractured Rock" was delivered at the Waste Management '86 conference, which was held in Tucson, Arizona on March 3-7.

A well-documented version of the TRANQL code and a user's manual were received from Stanford University and installed onto the VAX 11/780 at Sandia. The limitations and potential modifications to the code are currently being assessed.

Task 5. Transfer of Sensitivity Analysis Tools

The computer code RAMBO-1 (Retardation Analysis Model for Broken Overburden), which was written for calculations carried out in support of the Waste Management '86 paper mentioned above, was transferred from the EleXis computer to the VAX 11/780 computer. The code can be used to calculate radionuclide discharge in fractured media as a function of fracture geometry when radioactive production is not important. The current version complies with QA/QC requirements developed at SNLA for the NRC.

Development of an interface between the Aqueous Solution Database and the computer code PHREEQE was initiated this month. The interface will allow the user to update the database of thermochemical data accessed by PHREEQE and to carry out sensitivity and uncertainty analyses.

Trips

Malcolm Siegel completed the second half of the USGS course "Geochemistry of Ground-water Systems" on March 3-7, 1986.

Kenneth Erickson delivered the paper, "Approximate Methods to Calculate Radionuclide Discharges for the Performance Assessment of HLW Repositories in Fractured Rock at the Waste Management '86 conference on March 6, 1986.

References

Barney, G. S., and Wood, B. J., 1980, Identification of key radionuclides in a nuclear waste repository in basalt: RHO, Rept. RHO-BWI-ST-9.

Kerrisk, J. F., 1985, An assessment of the important radionuclides in nuclear waste: LANL, Rept. LA-10410-MS.

Hill, M. D., 1979, Analysis of the effect of variations in parameter values on the predicted radiological consequences of geologic disposal of high-level waste: NRPB, Rept. NRPB-R86.

EPA, 1977, Technical support of standards for high-level radioactive waste management. Volume A - source term characterization: USEPA, Rept. EPA 520/4-79-007A.

Muller, A. B., 1985, NEA compilation of thermodynamic data for minerals associated with granite, Rept. RWM-5, OECD Nuclear Energy Agency, Paris, France.

Allocation of Resources

Task 1. 70%

Task 5. 30%

A-1756
1646.010
March 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)	1.6	6.7
II. Direct Loaded Labor Costs	15.0	69.0
Materials and Services	0.0	1.0
ADP Support (computer)	0.0	1.0
Subcontracts	13.0	36.0
Travel	1.0	5.0
Other	<u>1.0</u>	<u>1.0</u>
TOTAL COSTS	30.0	113.0

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	365K	365K	-0-