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December 15, 1986 '86 DEC 18 P3:39

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 November 1986. Please feel free to contact me at (FTS) 844-8368 or Malcolm Siegel at (FTS) 846-5448 if you have any questions or comments.

Sincerely,

Robert M. Cranwell

Robert M. Cranwell, Supervisor
Waste Management Systems
Division 6431

RMC:6431

Enclosure

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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 INVESTIGATOR: 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 NOVEMBER 1986

Task I. Uncertainty in Integrated Radionuclide Discharge

Subtask 1A. Conceptual Models for Repository Sites.

Three conceptual models for ground-water flow at the basalt site have been chosen for the calculations of integrated radionuclide discharge using the GENMIX computer code (NUREG/CR-2081). All three models consider transport only in the flow top above the repository horizon. They are: 1. a model using mean values of hydraulic conductivity and gradient and the measured value of effective porosity from the work of Clifton and Arnett (1984, SD-BWI-TA-013), 2. a model using an assumed distribution of ground-water travel times that corresponds to that described in the NRC Technical Position on the ground-water travel time requirement of 10 CFR Part 60 (Coddell, 1986), and 3. a model using combinations of hydrological parameters produced by the Latin hypercube sampling program from distributions based on reviews of the literature. Calculations of radionuclide discharge using the first model with no geochemical retardation have been carried out and are under review. A sample plot of results for Pu241 is shown as Figure 1.

Subtask 1B. Solubility/Speciation Effects.

A NUREG document, Thermodynamic Tables for Use in Sensitivity and Uncertainty Analysis of High-Level Waste Repository Performance, is under preparation. This report will contain the thermochemical data base that has been compiled with partial support from this project and should be completed during the second quarter of FY87.

Subtask 1C. Sorption Effects.

The first iteration of a quality control check of the data in the basalt sorption data base has been completed. Several statistical subroutines and graphics capabilities have been added to the data base management system.
Preliminary calculations describing the variation of Kd for sorption of uranyl, neptunyl, cadmium, selenate and selenite ions onto iron oxyhydroxides in a range of waters that are a reasonable approximation to basaltic ground waters have been completed. An example of the results is included as Figure 2.

Allocation of Resources

Task 1.....100%

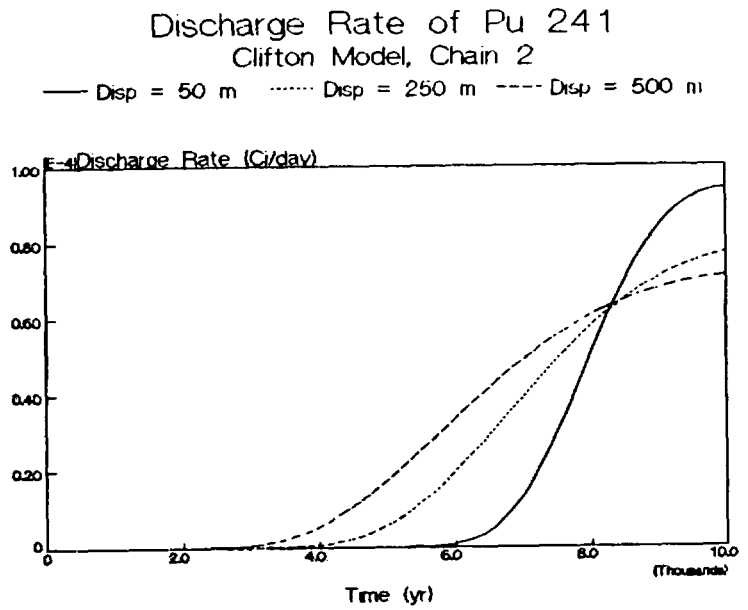

Figure 1. Discharge of Pu241 at distance of 5 km from source for hypothetical basalt site. Ground-water travel time is approximately 8200 years; retardation factor equals 1 for all members of decay chain. Different curves correspond to values of longitudinal dispersivity assumed in 1-D transport calculation.

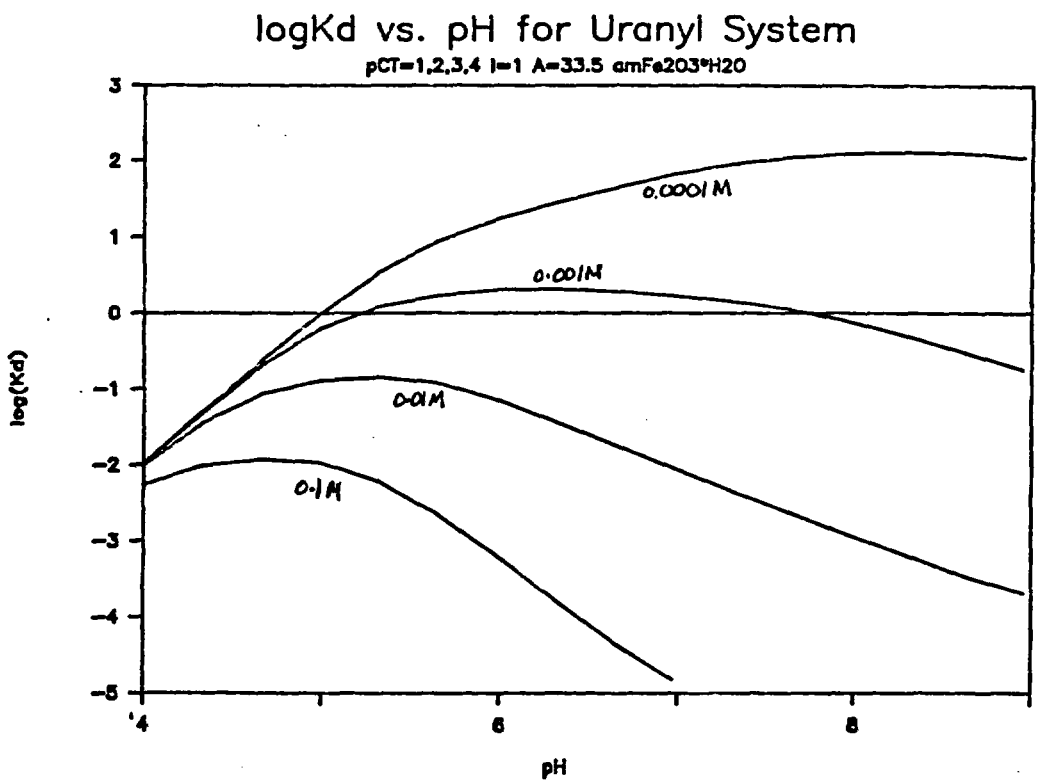

Figure 2. Variation of calculated Kd for sorption of uranium onto amorphous iron oxide as a function of pH under oxic conditions. Surface area of sorbent is 33.5 sq.m/liter; ionic strength is 0.1 molal. The different curves correspond to different concentrations of total carbon in the system.

A-1756
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November 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)	0.3	0.9
II. Direct Loaded Labor Costs	1	7
Materials and Services	5	15
ADP Support (computer)	2	2
Subcontracts	17	49
Travel	0	0
Other (computer roundoff)	1	1
TOTAL COSTS	26	74

III. Funding Status

Prior FY Carryover	FY 87 Projected Funding Level	FY 87 Funds Received to Date	FY 87 Funding Balance Needed
32K	232K	200K	0 K