

Sandia National Laboratories

Albuquerque, New Mexico 87185

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A-1756  
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WM Project IC-11-16  
Docket No. \_\_\_\_\_  
PDR   
LPDR  (P.W.S.)

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

Distribution:  
Kelly \_\_\_\_\_  
HITTE \_\_\_\_\_  
(Return to WM, 623-SS) \_\_\_\_\_  
JOHN - TICKET \_\_\_\_\_  
\_\_\_\_\_

Dear Mr. Kelly:

Enclosed is the monthly report for FIN A-1756, Geochemical Sensitivity Analysis for July 1984.

Please feel free to contact me if you have any questions or comments.

Sincerely,

Malcolm D. Siegel  
Waste Management Systems  
Division 6431

MDS:6431:jm

Enclosure

Copy to:  
Office of the Director, NMSS  
Attn: Program Support  
Robert Browning, Director  
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6431 R. M. Cranwell  
6431 M. S. Chu  
6431 M. D. Siegel

PROGRAM: Geochemical Sensitivity  
Analysis

FINW: A-1756

CONTRACTOR: Sandia National  
Laboratories

BUDGET PERIOD: 4/20/84 -  
9/30/84

DRA PROGRAM MANAGER: W. R. Kelly

BUDGET AMOUNT: 200K

CONTRACT PROGRAM MANAGER: R. M. Cranwell

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PRINCIPAL INVESTIGATOR: M. D. Siegel  
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#### 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 JULY 1984

##### Task I Uncertainty in Integrated Radionuclide Discharge

###### Subtask 1A. Speciation Effects

A contract with S. Phillips (Lawrence Berkeley Laboratories) was placed to obtain assistance in compilation of a state-of-the-art critically-assessed thermochemical data base. The tentative date for the first data peer review meeting is October 1, 1984. The meeting will be held at Oak Ridge National Laboratories. An agenda and list of invitees will be included in the next monthly report.

###### Subtask 1B. Equilibrium Sorption Effects

A contract was placed with J. O. Leckie (Stanford University) to obtain assistance in theoretical sorption calculations and chemical transport simulation.

Several discussions were held dealing with the problem of non-linear adsorption of radionuclides. The far-field extension of an existing code RBAKFIL which treats non-linear adsorption and transport through a backfill is being

considered. This code might be used to identify conditions under which non-linear adsorption must be included in transport calculations.

The possibility of the use of a sorption data management system in this subtask is still under review. It is the understanding of SNLA that the NRC has not agreed that such a system is required for this project. No activities related to acquisition or creation of such a system have been undertaken. Present activities are confined to obtaining information about alternative data management systems. Toward this goal, SNLA has received a cost estimate of approximately \$14K from Pacific Northwest Labs for the installation, training and upgrading of the ISIRS at Sandia Labs. The existence of another computer-based sorption data system was revealed at the NNWSI/NRC Geochemistry Workshop. DOE staff suggested that this data base for tuff could be accessed by SNLA/NRC personnel. The possibility that this data base could be the nucleus for a NRC sorption data management system will be investigated during August and discussed in the next monthly report. In addition, a detailed discussion of the uses of a computerized sorption data base will be included.

#### Subtask IC. Kinetic Effects

Documentation of previous results continued during July.

#### Subtask ID. Dynamic Effects

Activities related to studies of matrix diffusion and equivalent porous medium approximations for fractured rock (reported under Subtask IB last month) continued during July. Henceforth, these activities will be described under Subtask ID. This work is related to work in the other subtasks in the following way: many expressions that are derived in the other subtasks (e.g. reaction rate and retardation factor sensitivity studies) are derived for porous media. The results of the work described under Subtask ID will allow the extension of these expressions to fractured media when it can be shown that the criteria for equivalent porous media are met.

Much of the basic framework for this approach has been described in Appendix C of NUREG/CR-3235 vol.3. Extensive reference will be made to this report in the current and future monthly reports. The objective of the work in Subtask ID is to assess the uncertainties in calculated integrated discharge which result from three alternative assumptions: 1) chemical equilibrium exists between the bulk rock and the fracture fluid; 2) a quasi-steady state exists which can be described approximately by a linear driving force expression for mass transfer between the fracture fluid and the rock matrix; and 3) the rock matrix behaves as a semi-infinite medium.

During July, it was shown that under certain conditions, the quasi-steady state expression provides a conservative bound for

the discharge calculated by the exact solutions of the diffusion equations. The error in the discharge calculated by this approach is less than the error associated with the porous medium approximation described in NUREG/CR-3235.

### Reference

Siegel, M. D. and Chu, M. S. Y., Technical Assistance for Regulatory Development: Review and Evaluation of the EPA Standard 40CFR191 for Disposal of High-Level Waste, vol. 3. A Simplified Analysis of a Hypothetical Repository in a Tuff Formation, NUREG/CR-3235, SAND82-1557, April 1983.

### Task II Evaluation of Error Due to Organics and Colloids

Subtask IIA Organics

No activity during July

Subtask IIB Colloids

A detailed program plan for short term activities under this subtask is being prepared for submittal to the NRC.

### Task III Representation of Geochemical Processes in Models

No activity in July

### Task IV Short-term Technical Assistance

Four documents were reviewed this month under this task. Written comments have been forwarded to the NRC. A total expenditure of \$5K was authorized and spent for these reviews.

M. Siegel attended the NNWSI/NRC Geochemistry Workshop held at Los Alamos National Laboratory. A trip report summarizing information relevant to FIW A-1756 is being sent to the NRC under a separate cover.

### Future Plans

M. Siegel will participate in a project review meeting with personnel from Oak Ridge National Laboratories and the NRC on August 29 in Oak Ridge, Tennessee.

### Allocation of Resources During July\*

Subtask IA, 1B	- 20%
Subtask IC	- 10%
Subtask ID	- 35%
Subtask IIB	- 5%
Subtask IV	- 30%

\*Amounts are very approximate and should be used for qualitative comparisons only.

Anticipated Problems

None.