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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 1984.

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

Sincerely,

*Malcolm D. Siegel*

Malcolm D. Siegel  
Waste Management Systems  
Division 6431

MDS:6431:jm

Enclosure

Copy to:  
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A-1756 PDR

PROGRAM: Geochemical Sensitivity  
Analysis

FIN#: 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

FTS PHONE: 844-8368

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 JUNE 1984

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

###### Subtask IA Speciation Effects

A proposal for compilation of a state-of-the-art thermochemical data base for HLW management was received from Dr. S. Phillips of Lawrence Berkeley Labs. This project will also provide assistance in reviews of the methods used to select thermochemical data for a speciation calculation, a study of the uncertainties in solubility calculations and selection of methods used to calculate thermochemical constants in saline brines and in high temperature solutions. The contract is under review and should be placed during July.

###### Subtask IB Equilibrium Sorption Effects

A proposal for compilation of available site binding constants for elements and substrates relevant to HLW disposal was received from Dr. J. Leckie of Stanford University. This project will also include evaluation of the use of the chemical transport simulator TRANQL as a tool in sensitivity analysis. The contract is under review and should be placed by August.

The importance of the assumption of equilibrium sorption to retardation by matrix diffusion in fractured media is currently under investigation. A review of literature describing matrix diffusion is being carried out under this subtask and under Task IV (short-term TA). An objective of this work is to formulate numerical criteria describing physiochemical and hydrological conditions under which the assumptions related to equilibrium sorption are valid. The possibility of acquiring a computerized sorption data base was discussed with NRC and PNL personnel. No decision had been made as of July 1.

#### Subtask IC Kinetic Effects

A paper entitled "Geochemical Sensitivity Analysis for High-level Waste Repository Risk Assessment I. Speciation" was presented at the 1984 annual American Nuclear Society Meeting.

A computer code which plots critical combinations of geochemical and hydrologic parameters was improved during this month to treat the existence of variable absolute and relative amounts of sorbing and non sorbing species.

#### Subtask ID Dynamic Effects

No activity during June.

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

#### Subtask IIA Organics

No activity during June.

#### Subtask IIB Colloids

A presentation describing scoping calculations designed to assess the "worst-case" importance of colloids to HLW repositories was presented at NRC during the project review meeting (June 25-28). A letter report describing these proposed calculations will be sent to NRC for final approval in early August.

A paper entitled "A Population Balance Model for Radiocolloid Transport" was presented at the 1984 annual meeting of the American Nuclear Society.

### Task III Representation of Geochemical Processes in Models

No activity during June.

### Task IV Short-term Technical Assistance

Four documents were received for review. A revised deadline for completion of this task was set at July 27.

M. Siegel was requested to attend the NNWSI/NRC Geochemistry workshop scheduled to be held July 10-12, 1984 at Los Alamos National Laboratory.

M. Siegel participated in a program review meeting at NRC headquarters on June 25-28.

#### Completion of Tasks Started Under FIN A-1158

After discussions with Peter Ornstein and Walton Kelly, it was agreed that no new letter reports would be required to describe the work authorized under FIN A-1158 (Short-term Technical Assistance). The results of this work will be included in the topical reports and letter reports required under FIN A-1756.

#### Changes in Deadlines

Due to the participation of M. Siegel in the program review meeting and in the NNWSI/NRC Geochemistry workshop, the deadlines for tasks scheduled to be completed in July will be extended approximately 3 weeks. These include the program plan for colloid scoping calculations (new date: August 6) and document reviews authorized under Task IV (new date: July 27).

#### Trips During June

##### American Nuclear Society Meeting

Malcolm Siegel and Eric Nuttall (University of New Mexico) presented papers at the 1984 annual meeting of the American Nuclear Society in New Orleans, LA on June 5, 1984. A brief trip report and excerpts from the transactions are being sent to the NRC under a separate cover.

##### NRC Program Review Meeting

M. Siegel participated in a review of SNLA programs at NRC headquarters on June 25-28. An overview of the objectives, methods and preliminary results of FIN A-1756 was presented on June 25. More detailed descriptions of the projects were presented to members of the Geochemistry Section of the Geotechnical Branch/NMSS on June 27-28. Summaries of the topics discussed with the NRC staff are given below.

##### o Funding

The funding for FY84-87 is approved for the duration of the contract. This will enable long term (2-3 yr) subcontracts to be placed with Stanford University and Lawrence Berkeley Labs. The Schedule 189 budget is expressed in terms of constant 1984 dollars. The actual budgeted dollar amounts adjusted for inflation will be authorized by the NRC yearly.

##### o Milestones

It was suggested by the NRC that several topical letter reports listed in the draft milestone chart (Table 1) be consolidated. It was agreed that many of the letter reports would be

submitted to NRC as draft letter reports for review and would appear in revised form as separate chapters in the consolidated NUREG reports.

o Project Scope

It was suggested by several members of the NRC that the scope of A-1756 may be too broad. In response to this comment, it is important to note that although very broad issues are addressed in this contract, the project is designed to focus on very specific, (and significant) aspects of these issues. Furthermore, in responding to the NRC Statement of Work for this project, certain assumptions were made. It was assumed that close coordination between this study and NRC projects at Oak Ridge National Laboratories, Lawrence Berkeley Laboratories and the OECD/NEA-funded ISIRS would be possible. The project deals specifically with integrated radionuclide discharge and stresses far-field geochemical phenomena. Within this framework, it is anticipated that FIN A-1756 will provide the NRC with useful insights concerning the adequacy of available geochemical models currently used in performance assessment studies. It will also aid the NRC in prioritizing research needs designed to assess the compliance.

o Suggested Changes in Project Scope

It was suggested by M. Knapp that FIN A-1756 might address two issues that are outside the original scope of work: 1. the ground-water protection requirements of the proposed EPA Standard 40CFR191 and 2. geochemical conditions in the near-field of the repository. These suggestions are currently under consideration at SNLA. Neither of these two additional tasks could be carried out within the current budget and schedule. Estimation of the additional resources required to address these issues requires a more precise definition of the tasks. For example, the EPA ground-water protection requirements include both a concentration (radioactivity) limit as well as a health effects requirement. The former could be addressed more easily than the latter within the framework of FIN A-1756. Similarly, a more precise identification of the near-field geochemical processes of interest to the NRC is needed before necessary changes to FIN A-1756 can be made.

o Coordination with Oak Ridge National Laboratory

FIN A-1756 examines the importance of geochemical processes as they relate to the overall performance of repository. The emphasis in this project is not on the behavior of individual geochemical phenomena but rather the interactions of different processes and how they affect the integrated radionuclide discharge. Consequently, FIN A-1756 is dependent upon the results of the research of DOE and other NRC contractors which provide state-of-the-art basic data, models and codes to be used in the system-wide studies. This project can provide guidance to other projects by identifying the most important

research issues for HLW disposal and by suggesting criteria for the design of future NRC or DOE experiments. Close cooperation between SNLA and ORNL will be required to ensure that the maximum possible benefit of this project is obtained.

The exact nature of the cooperation between SNLA and ORNL will be decided after discussions between M. Siegel and Oak Ridge personnel. Possible items under consideration are: 1. compilation of a thermochemical data base under FIN A-1756 which can be used by both ORNL and SNL, 2. participation of ORNL in compilation of a sorption data management system, 3. participation of SNLA in the ORNL document review data bank, 4. coordination of modeling calculations to reduce amount of redundancy, 5. possible use of MINTEQ in theoretical sorption calculations described in subtask 1B of FIN A-1756.

#### o Sorption Data Management System

Completion of Subtask 1B of FIN A-1756 requires use of a computerized sorption data management system. Two existing data management systems are under consideration. 1. ISIRS (International Sorption Information Retrieval System) and 2. the earth sciences data base developed by the CorStar Company for the NRC. ISIRS has sophisticated software specifically designed for sorting, retrieving, plotting and correlating sorption data. The data format is very complete but there are relatively few data currently in ISIRS which can be used for HLW repository studies for basalt, tuff and salt sites. Potential perceptions of conflicts of interest and the poor data base are important weaknesses of any plan to use ISIRS by the NRC. The usefulness of the CorStar data base for FIN A-1756 is currently under study. In addition, the feasibility of compiling a new data management system is also under consideration. The July monthly report will address these issues in more detail.

#### Allocation of Resources During May and June 1984\*

##### May

Subtask 1C - 50%  
Other Tasks - 30%

Subtask 1IB - 20%

##### June

Subtask 1B - 20%  
Subtask 1IB - 30%

Subtask 1C - 30%  
Task IV - 20%

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

#### Anticipated Problems

None.

TABLE 1

Preliminary Draft of Milestones Schedule

|  |       |
|--|-------|
| PROGRAM PLAN   | 8/84  |
| REPORT ON STATUS OF THERMOCHEMICAL<br>DATA AND CRITERIA FOR DATA SELECTION | 11/84 |
| SCOPING CALCULATIONS FOR COLLOIDS  | 12/84 |
| SYSTEM CALCULATIONS FOR SPECIATION   | 2/85  |
| LETTER REPORT ON KINETICS/SPECIATION<br>AND EXPERIMENTAL DESIGN            | 3/85  |
| SYSTEM CALCULATIONS FOR NON-LINEAR<br>SORPTION                             | 4/85  |
| REPORT ON CHOICE AND MODIFICATIONS OF<br>CODES FOR MODELING                | 5/85  |
| REPORT ON REACTION PATHWAYS FOR<br>MODELING                                | 9/85  |
| FIRST COMPILATION OF DATA AVAILABLE  | 12/85 |
| REPORT ON UNCERTAINTIES RELATED TO<br>SORPTION (1B)                        | 5/86  |
| SECOND COMPILATION OF DATA AVAILABLE                                       | 7/86  |
| LITERATURE REVIEW OF ORGANICS (2A)   | 8/86  |
| REPORT DESCRIBING TRANSPORT SIMULATOR                                      | 9/86  |
| REVIEW OF KINETICS DATA AND EQUILIBRIUM<br>ASSUMPTIONS CRITERIA            | 9/86  |
| FINAL REPORT ON KINETICS (1C)  | 10/86 |
| FINAL REPORT ON SPECIATION (1A)  | 12/86 |
| FINAL REPORT ON COLLOIDS (2B)  | 2/87  |
| VERIFICATION CALCULATIONS COMPLETED (10)                                   | 4/87  |
| FINAL TOPICAL REPORT (3A)  | 5/87  |
| PEER REVIEW WORKSHOP REPORT (3B)   | 7/87  |
| WORKPLAN SUBMITTED TO NRC (3C)   | 9/87  |