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WM Project 10, 11, 16

July 15, 1987

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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 June 1987. Please feel free to contact me at (FTS) 844-8368 or Malcolm Siegel at (FTS) 846-5874 if you have any questions or comments.

Sincerely,

Robert M. Cranwell

Robert M. Cranwell, Supervisor
Waste Management Systems
Division 6416

RMC:6416

Enclosure

Copy to:
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Malcolm R. Knapp, Director
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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 INVESTIGATORS: M. D. Siegel FTS PHONE: 846-5874

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 transferred to the NRC under Task V.

ACTIVITIES DURING JUNE 1987

Task I. Uncertainty in Integrated Radionuclide Discharge

Subtask IA. Conceptual Models for Repository Sites.

A draft of a letter report describing the conceptual geochemical model for the basalt site was reviewed. A second draft is in preparation.

Subtask IB. Solubility/Speciation Effects.

Preparation of the final draft of "Thermodynamic Tables for Use in Performance Assessment of High-Level Waste Repositories. Volume 1. Aqueous Solutions Data Base," NUREG/CR-4864, SAND87-0323 continued during June.

Sections of the paper 'Development of an Integrated Geochemical Data Base for Modeling and Sensitivity Analysis in Nuclear Waste Repository Performance Assessment Studies' were completed for inclusion in the proceedings of the International Conference on Thermodynamics of Aqueous Systems With Industrial Applications by S. Phillips. Samples of sensitivity calculations of radionuclide speciation are

being carried out by M. Siegel during July and will also be included in the completed paper.

Subtask IC. Sorption Effects.

The final draft of the user's guide for the Sandia Sorption Data Management System was prepared and is now under review.

Subtask IE. Coupled/Dynamic Effects

No activity during June.

Task IV. Short-Term Technical Assistance.

M. Siegel reviewed a preliminary draft of a memo on validation of geochemical models by W. Kelly.

Task V. Technology Transfer

No activity during June.

Trips

A trip report by S. Phillips was received too late to be included in the May monthly report. It is included as Attachment 1 to this report.

Allocation of Resources

Task I.....100%

May 18, 1987

Trip Report: S.L. Phillips

Meeting: International Conference on Thermodynamics of Aqueous Systems with Industrial Applications, Warrenton, Virginia, May 10-14, 1987.

Purpose of Trip: To present a paper on the thermodynamic tables for assessing the performance of nuclear waste repositories to isolate wastes.

This most certainly was a first-class conference which facilitated contact and mutual transfer of information between industrial researchers and the National Laboratories. One area with heavy emphasis was on prediction of chemical reactions using computer codes. For example, Noel Scrivner, Senior Consultant with Du Pont, gave an informative presentation on disposal of industrial wastes through injection into deep wells. Their calculations showed that the wastes became innocuous after a time period which is well within the EPA requirements. An example is an increase in pH of injected acid waste due to reaction of the acid with the native rock. The calculations were done together with a contractor, OLI, Inc., Morristown, New Jersey (Marshall Rafal, President). I talked to both Scrivner and Rafal; they are both interested in receiving data from the Aqueous Solutions Database. Their interest is for the generic geochemical data, e.g., for environmental and geologic work rather than nuclear waste disposal.

Tom Wolery, LLNL, is the central geochemist for the EQ3/EQ6 code which is the virtual if not actual official DOE code for calculations related to nuclear waste disposal. Tom presented a paper highlighting aspects of EQ3/EQ6, and his research related to calculating activity coefficients. There is a substantial amount of quality control involved in his work for DOE. The database for EQ3/EQ6 may not be ready for calculation on actinides for 3-4 year; his data are probably not consistent.

My presentation was on a consistent thermodynamic database for the Nuclear Regulatory Commission for performance assessment studies; this is developed in coordination with Malcolm Siegel (SNLA) and Frank Hale (LBL/ESD). Besides the database, per se, there was interest in our research on developing theoretically based correlations to fill gaps in the data. For example, the linear relationship between both $\Delta_f G^\circ$ and $\Delta_f H^\circ$ and the number of ligands in the complex which we found and reported is apparently new. I was asked the following questions: if I had made use of the thermodynamic data for actinides in the publications by the International Atomic Energy Agency (answer: yes, although only for aqueous ions and solids); are gaseous substances in the database (ans.: yes, selected ones); was the linear plot of $\Delta_f H^\circ$ versus number of F^- theoretical (ans.: this plot on one of my slides was based on my finding that linear plots are obtained when $\Delta_f G^\circ$ or $\Delta_f H^\circ$ is plotted versus ligand

number for about 20 complexes including both actinides and non-actinides); are the correlations empirical (ans.: correlations are based on similar relationships for other aqueous substances published in the research literature); is the database on line and can tapes be obtained (ans.: yes, however, more emphasis now is on actinides, so that coverage of the elements is uneven. Also, tables for each element are given a numerical designation of 1,2 or 3 which defines the status of critical evaluation).

On Thursday I visited Stanley Abramowitz, Chief of the Chemical Thermodynamics Division and Vivian Parker in this Division, at the National Bureau of Standards. Vivian and I exchanged information on thermodynamic data. She is a participant in the new CODATA Key Values which will be published later this year. There are some changes in values, for example the entropy of F^- is changed to -13.8 from -13.18. Stan Abramowitz has an outstanding Division covering research on Biothermodynamics, Biomolecular Structure, Thermodynamic Measurements and Data Centers (which now includes JANAF). I have a copy of his 1986 annual report.

During this trip I telephoned Walt Kelly (NRC) who is program director for the SNLA/LBL performance assessment work. Some NRC research for nuclear waste disposal may be transferred from the National Labs. to a contractor; however, the ASD may continue to receive support.

Sid

Sidney L. Phillips

A-1756
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June 1987

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

	<u>Current Month</u>	<u>Year -to- Date</u>
I. Direct Manpower (man-months of charged effort)	0.6	4.8
II. Direct Loaded Labor Costs	6	42
Materials and Services	0	7
ADP Support (computer)	4	16
Subcontracts	7	154
Travel	0	1
G & A	2	8
Other (computer roundoff)	-1	-1
	<u>18</u>	<u>227</u>
TOTAL COSTS	18	227

III. Funding Status

<u>Prior FY Carryover</u>	<u>FY 87 Projected Funding Level</u>	<u>FY 87 Funds Received to Date</u>	<u>FY 87 Funding Balance Needed</u>
29K	229K	200K	None