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Dr. Malcolm D. Siegel
Division 6431
Sandia National Laboratories
Albuquerque, NM 87185

Dear Dr. Siegel:

SUBJECT: CONTRACT NO. NRC-50-19-03-01/FIN A-1756, "GEOCHEMICAL SENSITIVITY ANALYSIS"

I have reviewed the December, 1985 monthly progress report for the above contract, dated January 15, 1986. Based on my review of this report, progress to date is satisfactory.

Concerning conceptual models for the sites, when do you wish to come to Silver Spring to discuss them with NRC staff? You may wish to talk to the technical leads directly. They are as follows:

Hydrology:	NNWSI	Jeff Pohle	427-4725
	BWIP	Mike Weber/Neil Coleman	427-4746/427-4131
	Salt	Fred Ross	427-4539
Geology-Geophysics:	BWIP	Harold Lefevre	427-4532
	NNWSI	Charlotte Abrams	427-4390
	Salt	John Trapp	427-4545

The geochemistry lead for BWIP and NNWSI are Dave Brooks and John Bradbury, respectively. The above individuals can also explain their contractor support.

I enclose a copy of a letter I received from Dr. Lester Morss, Argonne, on the peer review meeting.

The action taken by this letter is considered to be within the scope of the current contract FIN A-1756. No changes to costs or delivery of contract

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products is authorized. Please notify me immediately if you believe this letter would result in changes to costs or delivery of contracted products.

Sincerely,

Walton R. Kelly
Geochemistry Section
Geotechnical Branch
Division of Waste Management
Office of Nuclear Material Safety
and Safeguards

Enclosure:
As Stated

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January 8, 1986

Dr. Sidney L. Phillips
Computation Department
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

Dear Sid:

Thank you for inviting me to the NRC Chemical Thermodynamics Advisory Committee meeting on December 17. It was a worthwhile experience in several ways: to familiarize me with your and Mal Siegel's work, to benefit from the interesting and competent presentations of Drs. Haas, Plummer, and Goldberg; and to learn about the research interests of NRC divisions.

I was impressed with the scope and depth of your database. Although I'm not in a position to compare it with EQ3/EQ6, PHREEQE, or other similar databases, it is clear you are trying hard to acquire a comprehensive set of assessed experimental data and to use powerful theoretical models to multiply the database's effectiveness.

The following recommendations are directed more to NRC than to you so I'm sending a copy of this letter to Walt Kelly:

1. The establishment of an internally consistent and comprehensive set of thermochemical data is a multi-year, multi-person task. I am not competent intellectually or psychologically to extract, to assess, and to correlate the multitude of property values that you must deal with, but I suspect you need help! (The fact that your dataset is heavy with europium values, but appears to lack other, important fission-product rare earths, and is weak in geochemical elements such as aluminum, probably reflects your inability to take advantage of a collaborator like Vivian Parker, Joe Rard, or Neil Plummer.) It would seem to me that the NRC database should make use of others - DOE, NEA - or should contract for high-caliber assessment help. Trying to remain impartial, I could recommend a distinguished Argonne colleague who is not involved in my program.

2. To achieve "quality control", two suggestions:

   a. involvement of an experienced actinide chemist such as Drs. Ryan or Serne, and a geochemist, to ensure that "ghost species" or missing significant reactions can be avoided, and
   b. selection of some test equilibria for experimental verification by an independent laboratory.

3. Your printout tables, with ionic strength and temperature as variables, would be enhanced by experimental determination of key activity coefficients, osmotic coefficients, and heat capacities of electrolyte components as a function of ionic strength or temperature. These do happen to be areas of research to which I am partial and for which I plan to propose research to NRC. You could help me by identifying crucial species (Pu^{3+}, U^{4+} come to mind) for such studies.

I hope we meet again in the near future, and to hear from you if you have any suggestions for experimental studies

Sincerely,

Lester

Lester R. Morss
Chemistry Divison

LRM:jln

cc: Dr. Walton Kelly
U. S. Nuclear Regulatory Commission
MS623-SS
Washington, DC 20555