Sac

Sandia National Laboratories
Albuquerque, New Mexico 87185

WM Record File
WM-RES
A-1756
SNL

WM Project 10, 11, 16
Docket No. ____
PDR ✓
LPDR B, N, S

Distribution:
Kelly
STILL
(Return to WM, 623-SS)
Jean Tinkel
23

August 14, 1985

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 July 1985.

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

Sincerely,
Margaret Chu for
R.M. Cranwell

R. M. Cranwell
Supervisor
Waste Management Systems
Division 6431

RMC:6431:jm

Enclosure

Copy to:
Office of the Director, NMSS
Attn: Program Support Staff
Robert Browning, Director
Division of Waste Management
Malcolm R. Knapp
Division of Waste Management
Kenneth Jackson
Division of Waste Management
Office of Research, NRC
Document Control Center,
Division of Waste Management
6400 R. C. Cochrell
6430 N. R. Ortiz
6431 R. M. Cranwell
6431 M. D. Siegel
1500 W. Herrmann
1510 J. W. Nunziato
1512 J. C. Cummings
1512 K. L. Erickson

PROGRAM: Geochemical Sensitivity Analysis FIN#: A-1756

CONTRACTOR: Sandia National Laboratories BUDGET PERIOD: 10/01/84 - 9/30/85

DRA PROGRAM MANAGER: W. R. Kelly BUDGET AMOUNT: 235K

CONTRACT PROGRAM MANAGER: R. M. Cranwell FTS PHONE: 844-8368

PRINCIPAL INVESTIGATOR: M. D. Siegel FTS PHONE: 846-5448

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 1985

Task I Uncertainty in Integrated Radionuclide Discharge

Subtask IA. Speciation Effects
(M. Siegel, R. Guzowski, S. Phillips)

A preliminary draft of a document dealing with the propagation of uncertainties in thermochemical data through speciation/solubility calculations is in preparation.

Several discussions have been held in recent months among NRC, SNLA and LBL personnel concerning peer review of the thermochemical data base being compiled under this subtask. Criteria for data selection have been sent out for peer review. In addition, the initial set of thermochemical data (published as LBL-14996) are being reviewed by recognized experts in the fields of physical chemistry and thermochemical data compilation. Many of the reviewers have responded in writing (see for example Attachment 1). Documentation of the peer review comments and responses from Dr. Phillips and others

can be assembled under subtask 1A and summarized in a future report if requested by the N.R.C. A proposed outline of the report is included as Attachment 3.

Synthesis of a conceptual model for a basalt repository site for use in sensitivity analysis continued during July. Hydrogeological data previously entered onto the dBase III system were manipulated for use with the code NWFT/DVM.

Subtask 1B. Sorption Effects
(M. Siegel, J. O. Leckie, D. Kent)

A comprehensive review of literature pertaining to the Stanford Generalized Model for Adsorption (SGMA) continued at SNLA and Stanford University during July. The purpose of the review is to establish a rigorous conceptual framework within which errors due to assumptions of linear sorption can be evaluated. A report on experimental data available for use in theoretical sorption calculations is nearly complete.

Subtask 1C and 1D. Kinetic and Dynamic Effects

The paper, "Geochemical Sensitivity Analysis ... Speciation and Matric Diffusion," described in the June progress report, was completed and submitted for publication.

A draft of the paper, "Approximate Methods to Calculate Radionuclide Discharge ... Fractured Rock" described in last month's progress report was completed and is under review. The paper was to be presented at the 1985 MRS Symposium on the Scientific Basis for Nuclear Waste Management. However, approval for attendance at the meeting was not received from the N.R.C. and the paper was withdrawn.

Task II. Evaluation of Error Due to Organics and Colloids

No activity in July 1985.

Task IV. Short Term Technical Assistance

Drs. L. Kovach and K. Jackson attended meetings at Sandia Laboratories on July 26. The NRC staff were briefed on the activities of Divisions 6431 (Waste Management Systems) and 1543 (Geochemistry) and given tours of the geoscience laboratories.

ATTACHMENT 2

Lawrence Berkeley Laboratory
1 Cyclotron Road Berkeley, California 94720
(415) 486-4000 • FTS 451-4000

July 24, 1985

Dr. Howard J. White, Jr.
Office of Standard Reference Data
National Bureau of Standards
Gaithersburg, MD 20899

Dear Howard:

Thank you for your letter of June 26, 1985 with the comments about chemical thermodynamic data. I am now preparing a first revision to LBL-14996 which tabulates values of thermodynamic properties for selected substances important to geochemical and related basic energy research. The revision has data for $\Delta_f G^\circ$, $\Delta_f H^\circ$, S° and C_p° as in the initial publication; added emphasis is documentation of publications and other references to sources of recommended values. I am also adding new substances such as solid and ionic forms of Se, Fe, Pb, Cm and Ra. The central idea remains to publish critically evaluated internally consistent data for basic energy research, for example nuclear power production, waste management, corrosion, hydrogen gas production and for lamp applications.

As in the report LBL-14996, this revision develops the data in a way consistent with the CODATA Key Values in Bulletin 28. Needed values absent from Bulletin 28 are obtained from NBS Tables, and from our or other critical evaluation. Examples of the last are data for Fe^{++}, Fe^{+++}, Al^{+++}, $I_2O_5(cr)$ and the recent work by Vivian Parker on Sr^{++}. I am certainly interested in coordinating closely with the CODATA Task Group on Thermodynamic Tables, and will be delighted to know more about the activities. The Task Group might add (if not already done) the following to a list of substances for evaluation and recommendation: $e(aq)$, $Fe^{++}(aq)$, $Fe^{+++}(aq)$, $Al^{+++}(aq)$, $U^{++++}(aq)$ and $Tl^{+}(aq)$. Also, I have read CODATA Bulletin 51 "Guide for the preparation of Thermodynamic Tables and Correlations of the Fluid State," as well as Bulletins 19, 30 and 39.

Currently, I am evaluating chemical thermodynamic data for iodine, e.g., $I_2O_5(cr)$, $NH_4I(cr)$, $IO_3^-(aq)$. A preliminary listing of selected substances of iodine is attached (I), together with a tabulation of key data (II), and two examples of an expected format (III) for publishing recommended values. Publication date is during the second quarter of FY 1986, contingent on the size of staff permitted by FY 1986 funding.

With best wishes.

Sincerely,

Sid

Sidney L. Phillips
Principal Investigator
Aqueous Solutions Database
Computer Science Research Dept.
Mail Stop: 50B-3238
Telephone: 486-6865

SLP:wc

Enclosures

ATTACHMENT 3

Proposed Outline

Development of LBL/NRC/BES Thermochemical Data Base:
Interim Report

I. Technical Fundamentals
   A. Definitions of thermochemical variables
   B. Review of procedures to extract thermochemical constants from experimental data
      1. Experimental methods
      2. Data reduction

II. Propagation of Uncertainties in Thermochemical Calculations

III. Internal Consistency

IV. Criteria for Data Selection

V. Outline of Contents of Data Base
   A. Elements
   B. Formats

VI. Future Data Needs

VII. Summary of Peer Review Comments and Responses

Appendix I. Report of Activities of Technical Peer Review Committee

Appendix II. Peer Review Comments

Appendix III Responses to Peer Review Comments

ATTACHMENT 1

UNITED STATES DEPARTMENT OF COMMERCE
National Bureau of Standards
Gaithersburg, Maryland 20899

June 26, 1985

S. L. Phillips
Aqueous Solutions Database
Lawrence Berkeley Laboratory
1 Cyclotron Road
Berkeley, CA 94720

Dear Sid:

In answer to your letter on criteria for selection of reference data, I have the following comments.

In general, I think your plans are good. Since you intend to take evaluated data from a number of proven sources which are not thermodynamically consistent among themselves, you will probably have some trouble reaching the level of consistency you would like. You will, of course, need to connect all data to a common base of units, conventions, reference states, etc. But after this has been done, there will still be inconsistencies about which you can do very little.

Having said this, let me say that given the circumstances, I don't think you can do much else. It will be an interesting experiment to see what kinds of inconsistency problems you do run into.

I might point out that there is a system to develop data consistent with the CODATA Key Values and with one another via the activities of the CODATA Task Group on Chemical Thermodynamic Tables. This system is beginning to be used by groups including the one under Anthony Muller of the OECD which is also interested in nuclear waste. However, it does require direct evaluation and close coordination with the CODATA Task Group so that the time per evaluated data point is greater than you may wish to spend. I think we talked some about this at Oak Ridge, but if you want to know more about it, let me know.

Best regards.

Sincerely,

Howard J. White, Jr.
Office of Standard Reference Data