

MEMORANDUM

TO: Dr. Philip Justus
Division of High Level Waste
Management
U.S. Nuclear Regulatory Commission
Washington, DC 20555

December 14, 1987

FROM: Dr. Bob Duff



SUBJECT: Trip Report
CNWRA Attendance at the Geochemistry Program Review
December 3, 1987

Dates, Place of Trip: December 3, 1987
Wiltsie Building
Silver Spring, Maryland

Persons Present:

NRC

Dr. Philip Justus
Mr. David Brooks
Dr. John Bradbury
Mr. Paul Bembia
and others

SNL

Dr. Malcolm Siegel
Ms. Christine Leigh

LBL

Dr. Sidney Phillips

CNWRA

Dr. Bob Duff
Mr. Mark Logsdon (NWC)

Background and Purpose of Trip:

Dr. Philip Justus (NRC) requested Dr. Bob Duff (CNWRA) and Mr. Mark Logsdon (NWC) to attend the annual review of contract FIN A-1756, "Geochemical Sensitivity Analysis for Performance Assessment," presented by Dr. Malcolm Siegel (SNL). Mr. Logsdon attended this meeting as the CNWRA's geochemist, and Dr. Duff attended as the Chief Scientist of the CNWRA. The opportunity was also taken for Mr. Brooks and Dr. John Bradbury to present a briefing on the NRC Geochemistry program. The purpose of the trip as expressed in Dr. Justus's Technical Direction #1 was - "to learn the technical basis of the work performed and to become cognizant of the data bases, methods, models and codes utilized and available through FIN-A-1756. This is in anticipation of the transfer of all technologies, databases and codes from SNL to the CNWRA by the end of F/Y 1988.

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A-1756 PDR

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NH Project: NH-10, 11, 16
PDR w/encl
(Return to NH, 623-55)

NH Record File: A-1756
LPDR w/encl

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Summary of Pertinent Points:

Mr. David Brooks and Dr. John Bradbury of the NRC/HLTR Geochemistry Section presented an overview of the NRC geochemistry program, with an emphasis on the licensing group's activities and current technical assistance contractors. Following this briefing a project review of contract FIN A-1756, "Geochemical Sensitivity Analysis for Performance Assessment." The Principal Investigator for the subject project is Dr. Malcolm Siegel (Sandia National Laboratories); the NRC Project Manager is Mr. Paul Bembia. In addition to Dr. Siegel, the A-1756 project team was represented at the project review by Dr. Sidney Phillips (LBL) and Ms. Christine Liegh (SNL). The CNWRA was represented at the meeting by Dr. Bob Duff and Mr. Mark Logsdon (NWC). The NRC Staff were represented by numerous technical staff and managers from both HLTR and RES.

Following the formal presentation, informal discussions of technical matters with emphasis of methods for transfer of technologies, databases, and codes from SNL to the CNWRA.

Summary of Activities:

A complete summary of the presentations and discussion is presented in Mr. Logsdon's letter report to Dr. Bob Duff dated December 7, 1987. This letter report is included as an attachment to this trip report.

Recommendations:

As a result of this trip it is recommended that Mr. Logsdon and Dr. Siegel should arrange for transfer of reports and other relevant documentation to the CNWRA. Following review of the documentation by Mr. Logsdon and with NRC approval Mr. Logsdon should visit SNL for further discussions and arrangement for transfer of actual codes to the CNWRA where this is appropriate on establishing access of the CNWRA to codes which may remain resident on other computers at SNL or LBL.

lf

Attachment

cc: J. Bunting
M. Mace

ATTACHMENT

December 7, 1987

Center for Nuclear Waste
Regulatory Analysis
Southwest Research Institute
P.O. Drawer 28510
San Antonio, Texas 78284

9904/GS/TR.001
NRC-02-88-005
Communication No. 001

Attn: Dr. Robert Duff, Director - Technology Division/CNWRA

Re: Trip Report - Geochemistry Program Review, December 3, 1987

Dear Dr. Duff:

This letter constitutes my trip report to the CNWRA concerning the geochemistry project review at the Willste Building, Silver Spring, Maryland on December 3, 1987. I attended the meetings as directed by Dr. Philip Justus (NRC) in Technical Direction #1, dated 12/01/87. The activity is considered to be chargeable to Task 1.2 - Geologic Setting under the current contract between the CNWRA and NRC.

BACKGROUND

With respect to the CNWRA, the purpose of the meeting was to learn the technical basis of the work performed and to become cognizant of the data bases, methods, models and codes utilized and available to the NRC through FIN A-1756, "Geochemical Sensitivity Analysis for Performance Assessment." The Principal Investigator for the subject project is Dr. Malcolm Siegel (Sandia National Laboratories); the NRC Project Manager is Mr. Paul Bembia. In addition to Dr. Siegel, the A-1756 project team was represented at the project review by Dr. Sidney Phillips (LBL) and Ms. Christine Leigh (SNL). The CNWRA was represented at the meeting by Dr. Robert Duff and Mr. Mark Logsdon (NWC). The NRC Staff were represented by numerous technical staff and managers from both HLTR and RES.

Prior to the A-1756 project review, Mr. David Brooks and Dr. John Bradbury of the NRC/HLTR Geochemistry Section presented an overview of the NRC geochemistry program, with an emphasis on the licensing group's activities and current technical assistance contracts. Because you also received copies of all handouts, they will not be attached to this trip report. However, Attachment 1 is a listing of all the handouts that I received; please contact me if your records do not correspond with this listing, and I will transmit copies to you.

ACTIVITIES

In brief, my principal activities (in approximate chronological order) included:

- o Preparation for the meeting through review of SNL and NRC Staff geochemistry documents in the NWC library and telephone discussions with Dr. Siegel;
- o Participation in the HLTR geochemistry briefing;
- o Attendance at the SNL project review;
- o Participation in the data base demonstrations by Drs. Phillips and Siegel;
- o Participation in the wrap-up discussions between the SNL team, Mr. Bemba, and the CNWRA team;
- o Preparation of the trip report.

In addition, there were informal discussions of technical matters with NRC Staff and SNL team members and some final program management discussions with Dr. Duff and Dr. Justus.

ANALYSIS

The work conducted under the SNL project (FIN A-1756) is directly relevant to assessing geochemical information needs for the HLW program. First, the SNL group has developed two very effective data bases of critically evaluated geochemical information (the Sandia Sorption Data Management System, which is available for microcomputers, and the Aqueous Solutions Database, which is resident at LBL). The development and implementation of these databases appears to be fully consistent with the approach to databases that has been articulated previously to the NRC by NWC:

- o databases should be designed for specific uses by (or at least in conjunction with) the analysts who need the information;
- o databases should be as simple as possible (i.e., in format, input/editing and manipulation) and must be user-friendly;
- o databases should include an explicit evaluation of the quality (or uncertainty) of the data and must include sufficient information to allow the input to be traced to original sources;
- o analyses which may later be used to support NRC positions should depend to the maximum extent possible on data that derives from the NRC databases (for reasons of both independence and quality control).

Secondly, the SNL group has developed a methodology for geochemical sensitivity analyses that is directly related to the style of performance assessments that the NRC Staff likely will need to conduct throughout pre-licensing and licensing activities. That is, the SNL methodology can produce the CCDF's that are needed for comparison to the EPA Standards; at least as importantly, these results can be produced efficiently and through models and codes which are comprehensible conceptually to the "informed layman" as well as to the technical community. In addition, the group has critically explored alternative methods (including models and codes) and has established the relative strengths and weaknesses of the different approaches. In particular, they have shown that the data (and to some extent the theory) needed to reliably model geochemical interactions during transport using the more heuristically oriented approaches do not now exist. For example, electrostatic models for sorption (such as those being pursued at Stanford) offer theoretical advantages over strictly empirical (Kd) approaches to sorption, but to date there is actual data for only a handful of solid species (oxides and oxyhydroxides) and metallic species (uranyl and neptunyl) of interest. As I understand it, the triple-layer model experiments are difficult and quite time consuming, and it is not to be expected that there would be a body of experimental information sufficient to address licensing concerns related to HLW for several, perhaps many years. The extension of the experimental data to "real" systems (in which the mineralogy can be expected to be non-stoichiometric and incompletely to perhaps poorly defined in space and the solution chemistry complex and time-variant) for the purpose of transport modeling and performance assessment would require still more time and technical and programmatic uncertainty.

Thus, I concur with Dr. Siegel's conclusion that it is prudent to proceed with simpler approaches which can be implemented now and refined as needed in the future. Additionally, I am inclined to support empirical approaches to geochemistry, particularly when they can be extended to scales approaching those that are needed for licensing, for example through large-scale reactive tracer tests (e.g., Wallick (1986); NWC (1986)) and/or carefully selected and evaluated natural analogue studies. I consider that the "informed laymen" who are likely to make up licensing boards, intervenor groups and delegations of public officials are apt to find empirical data (for example, on the partitioning of radionuclides between aqueous and solid phases) more reliable than computer-generation predictions of future conditions based on thermodynamic and hydraulic principles as implemented in a mathematical model. After many years as both a student and a teacher, it is clear to me that very few people understand thermodynamics (particularly as it applies to complex, potentially irreversible systems), but that most people can understand the style of cook-and-look experiment that is used to generate a Kd.

Finally, I consider that the results generated by the SNL team for BWIP indicate that there is now available a substantial body of knowledge about the geochemistry of the relevant radionuclides with respect to transport from a deep geologic repository. In particular, the SNL results can be used to identify the ranges of source-term limitations (chemical and/or physical), advective-dispersive (-diffusive) transport, and attenuation along the flow path that must

be shown to make strong demonstrations of compliance with the EPA Standards. The principal use of the databases and models at this time is not, of course, pre-decisional statements about likelihood of licenseability, but rather the identification of data needs during the remainder of the national program. For example, for the range of source-terms and flow properties used in the analyses presented on December 4, 1987, it is clear that not all radionuclides in the HLW inventory are of equal concern with respect to their sorptive behavior, and it is equally clear that great precision in K_d (or other measure of sorptive potential) probably is not required for any of them, so long as it is possible to group them in order-of-magnitude sets. Finally, compared to the sometimes many orders-of-magnitude uncertainties that are present in hydrologic parameters or basic thermochemical data, it seems likely that very robust estimates of system response can be generated from valid simplifications of geochemistry in transport models.

In conclusion, I consider that the SNL program has demonstrated considerable success in its goal of defining criteria for valid simplifications of transport models. This programmatic goal has great merit in terms of practical developments in a pro-active licensing program, such as that being conducted by the NRC. If the NRC is to provide timely guidance to the DOE, then it would seem prudent for the Staff to push forward with the tools and data that are currently available, provided, of course, that they can be shown to be reliable for the evaluations that are required at this time. These are precisely the sorts of tool and data that the A-1756 team have developed for the NRC: relatively simple models and critically evaluated data that can be used to bound likely performance ranges and to assess and prioritize remaining data needs.

As an example of how these tools can be utilized promptly by the CNWRA, consider the NRC-proposed research initiative in actinide thermodynamics. NWC considers that the A-1756 program fits very nicely indeed with the recommendations that we forwarded to you on December 4, 1987 concerning the research program. In particular, the NWC recommendations included the following tasks:

- o Assemble geochemical task team. In light of the technology transfer aspect to the remaining work under A-1756, we consider that the task team should include representation from and close interaction with Dr. Siegel's team.
- o Compile database and evaluate available data. This task seems largely complete (at least up to this time), based on the Aqueous Solutions Database developed for A-1756 by Dr. Phillips at LBL.
- o Use simple models to assess sensitivity of performance measures to current ranges of solubility data. NEFTRAN, the SNL code used in the A-1756 work can be applied to this approach with little or no difficulty. The technology transfer from SNL to the CNWRA can use this application as a practical step in developing our familiarity with NEFTRAN. (Note: NEFTRAN is the newest generation of NWFT/DVM, which was cited in our December 4 memorandum.)

Based both on the BWIP results presented by Dr. Siegel and on work that we have been pursuing independently, NWC considers that it is very likely that this approach can be used to focus geochemical research quite narrowly. As you know from our previous discussions, we are very concerned about the need to focus research as narrowly as possible, in order to produce data in a timely fashion (with respect to the US HLW program) and in order to be responsible with fiscal resources.

RECOMMENDATIONS

Based on the meeting and the discussions with Mr. Bembia and the SNL team at the end of the sessions, NWC has the following recommendations:

- o The databases and modeling approaches of A-1756 are likely to provide significant support to the NRC Staff and should be maintained and developed further.
- o The SSDMS is highly portable and can be transferred with ease to any and all potential users. The ASD is a somewhat different matter. NWC recommends strongly that the ASD be maintained at LBL, rather than transferred to the CNWRA or elsewhere. Because of the cost-sharing nature of the LBL initiative, the "best buy" for the Government would appear to be to maintain the ASD where hardware, software, and quality-control matters are already in the hands of people familiar with the matter; retraining new people and developing new expertise at the CNWRA would not appear to be cost-effective or necessary. There would appear to be no practical advantage to transferring the database in terms of accessibility, since the ASD is accessible through regular modem communications. The only concern to NWC in this is the matter of software QA, particularly the code-custody and editing/updating issues. NWC recommends an early meeting with the CNWRA QA team to discuss this matter, with subsequent interactions with NRC QA staff and SNL/LBL as needed.
- o SNL proposes, and NWC concurs, that the most efficient way to transfer the A-1756 codes and databases is for SNL to make them available to the NRC Staff and the CNWRA in their current state of development, with sufficient documentation and testing material for the CNWRA and the Staff to determine which models and codes they wish to go to final, quality-assured versions.
- o At the close-out meeting with Mr. Bembia, I proposed that SNL transfer to the CNWRA (via NWC) copies of all its technical reports under A-1756 for our critical evaluation. After reviewing these materials, NWC proposes to meet in Albuquerque with the relevant SNL staff for clarifications and discussions of the work and the work products. After NWC/CNWRA has completed

its review of the SNL work, Mr. Bembia would transmit to us any internal NRC Staff reviews of the SNL work. After assessing the points made by the NRC Staff, the CNWRA would prepare a brief report and program plan to the NRC concerning the technology transfer.

- o The technology transfer task of A-1756 calls for a workshop to address the development of the next generation of codes that may be needed for performance assessment. The close-out group considered that such a workshop should be scheduled for early next summer, probably at the CNWRA in San Antonio.

ACTION

Based on the meeting and Dr. Justus' direction of 12/03/87, there are the following action items:

- o Dr. Duff to transmit the CNWRA trip report, to which NWC anticipates that this letter report will be an attachment.
- o Dr. Siegel and M. Logsdon to arrange for transfer of reports and other relevant documentation to NWC. NWC subsequently to transmit copies of SNL materials to the CNWRA library in San Antonio.
- o Following review of SNL materials, NWC to visit SNL for follow-up discussions (scheduling to be arranged).
- o Mr. Bembia to transmit copies of SOW and 1089, as well as internal NRC reviews of A-1756 to the CNWRA via NWC.

- o The CNWRA to prepare review of databases, models and codes and to draft a technology-transfer program that will occur, at least in part, during FY88. The technology transfer program will ultimately be developed between the CNWRA and SNL, under NRC Staff direction. Key personnel are expected to include:

NRC: Paul Bembia; Phil Justus; David Brooks

SNL: Malcolm Siegel; Sid Phillips

CNWRA: Mark Logsdon (NWC); Robert Duff.

If you have any questions about this trip report, please contact me immediately.

Respectfully submitted,
NUCLEAR WASTE CONSULTANTS

Balan Basse for MJL

Mark J. Logsdon, Vice President

Att.

cc: file 9904

ATTACHMENT 1

LIST OF HANDOUTS RECEIVED

- o TECHNICAL DIRECTION #1, P.S. Justus, dated 12/1/87
- o NRC HLW GEOCHEMISTRY handout package, undated
- o GUIDE TO GEOCHEMISTRY REQUIREMENTS FOR THE SAFETY ANALYSIS REPORT, undated
- o KEY GENERIC AND SITE-SPECIFIC ACTIVITIES: GEOCHEMISTRY SECTION/HLTR, undated
- o DETERMINATION OF RADIOMETRIC SOLUBILITY IN GROUNDWATER FOR ASSESSMENT OF HIGH-LEVEL WASTE ISOLATION Technical Position, dated November, 1984
- o DETERMINATION OF RADIONUCLIDE SORPTION FOR HIGH-LEVEL NUCLEAR WASTE REPOSITORIES technical position, dated January, 1987
- o MISCELLANEOUS HLW GEOCHEMISTRY PAPERS handout of coversheets, various dates
- o LOG-ON PROCEDURES FOR AQUEOUS SOLUTIONS DATABASE, Sid Phillips, undated

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WM Record File
A1756
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WM Project 10, 11, 16
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* LPDR (B, N, S)

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