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Dr. King Stablein
U.S. Nuclear Regulatory Commission
7915 Eastern Avenue
Silver Spring, Maryland 20910

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Dear Dr. Stablein:

It was a pleasure talking with you earlier this month in Maryland. Enclosed is a copy of my trip report for the Sorption Workshop at Los Alamos, New Mexico.

We have completed our investigations of those analytical equipment necessary to accurately provide geochemical and hydrogeochemical assessment of several Yucca Mountain characterization issues. And we have settled on a Tandetron using mass and charge analysis (MACS) coupled with nuclear reaction analysis (NRA). At this point in time, we are actively seeking assistance in locating funds for acquisition of this new laboratory, which would operate on a time/share basis. It is felt that this mode of analysis will allow us to investigate the full spectrum of hydrogeochemical concerns relevant to licensing criteria.

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I am in the process of revising our technical reports into a DRI-WRC report series. We have placed you on our mailing list so that you will receive these reports as they are made available.

Sincerely yours,

A handwritten signature in cursive script, appearing to read "Maury Morgenstein", written over a horizontal line.

Maury Morgenstein
DRI-WRC

MEM:gt

cc/M. Mifflin
C. Johnson



TRIP REPORT

YUCCA MOUNTAIN REVIEW PROJECT

Maury Morgenstein, Desert Research Institute

Informal Workshop on Sorption Geochemistry Relating to
Yucca Mountain NNWSI Project.

Location: Los Alamos, NM.
Date: 26 September 1985.
Sponsors: U.S. NRC, U.S. DOE.

INTRODUCTION:

The purpose of the workshop was to provide a forum for the exchange of current ideas and concerns with respect to sorption geochemistry relating to the Yucca Mountain NNWSI Project. The contributing attendees were from the Los Alamos Sorption Group representing U.S. DOE and the Chemical Technology Division of Oak Ridge National Laboratory representing U.S. NRC. A. D. Kelmars from Oak Ridge provided two presentations during the morning session:

1. "Concerns Relative to the Applicability of the Yucca Mountain Sorption Information For Site Performance Assessment Purposes." ORNL WS-41351.
2. "Application of Radionuclide Sorption Information For Prediction of Retardation in Fracture-Flow Geologic Systems." ORNL-WS 41476.

Unfortunately, both of these excellent presentations were rushed apparently due to time constraints. The afternoon session was a laboratory excursion through the ongoing experiments at Los Alamos. Both sponsors concluded that the workshop was beneficial in breaking the communications gap between active research and the publication of results. Additional workshops with fewer numbers of individuals handling specific topics in sorption geochemistry would be beneficial to the NNWSI Program.

SPECIFIC COMMENTS:

- A. First presentation (ORNL WS-41351) by A. D. Kelmers relating to a letter report LR-287-7 of July 15, 1985.
1. Lack of compilation and synthesis of sorption information.
 - a. This concern can apparently be rectified by higher levels of communication between the Los Alamos group and NRC, if DOE would provide a workable format in their management system.
 2. Timelines of reporting.
 - a. The need for rapid information exchange has been made obvious.
 3. Absence of performing assessment strategy for the Yucca Mountain Site.
 - a. The reasoning for the abundance of Sr, Cs, and Ba sorption information is because their behavior is easier to assess than the more critical radionuclides (Am, Pu, and Tc).

b. This technological drawback is highly significant since there seems to be a paucity of knowledge concerning the basic behavioral elements during sorption of other than Sr, Cs, and Ba. Therefore, if this gap in knowledge is not overcome in a relatively short period of time, the information developed by the Los Alamos Sorption Group would probably not be acceptable for performance assessment purposes.

c. Since the rudimentary understanding of sorption behavior is presently being addressed, the general absence of performance assessment strategy for Yucca Mountain is understandable. This facet of concern is critical especially in light of the apparent pressure placed on the Los Alamos Sorption Group by Sandia Performance Assessment Group for retardation numbers for stratigraphic horizons.

4. Uncertain applicability of sorption information for modeling fracture-flow geologic systems.

a. The ORNL position indicates that:

- 1) Reliance on K_d and R_f concepts leads to inaccurate and nonconservative predictions of radionuclide releases to the environment for fracture-flow systems.
- 2) Use of crushed rock does not represent fracture-flow minerals.
- 3) Use of saturated conditions does not model Yucca Mountain Repository.
- 4) Key radionuclides have not been emphasized in the published information.

b. We concur with the above ORNL position and further bring to the attention of those concerned:

Anacker, W. W. and R. Kopelman, 1984.
FRACTURAL CHEMICAL KINETICS : SIMULATIONS
AND EXPERIMENT, J. Chem. Phys., vol. 81,
no. 12, pt. 11, pp. 6402-6403.

According to Anacker and Kopelman's (1984) work, the classical diffusion-limited chemical reactions appear to be anomalous in fractured media. Although this may not play an important role in ion exchange reactions, this may be very important with respect to surface reactions and hence the key radionuclides.

5. Unevaluated methodology.

The ORNL concerns are well founded and may be partially alleviated by higher levels of interaction - such as in future workshops.

6. Ground-water instability.

- a. The ground-water used in the sorption tests are not representative of in situ conditions.
- b. A discussion of bacterial and fungal experiments indicates that Los Alamos is on top of the biotic problems with respect to hydrogeochemistry.
- c. A draft report was made available by Los Alamos concerning J-13, UE-25p#1, and H-3 water used during sorption experiments.
- d. Vadose hydrogeochemistry is unavailable at present even though a sample of vadose water has been collected. The Los Alamos Sorption Group were unaware of this sample.
- e. Actual in situ vs. laboratory measured water chemistry may vary due to CO₂ loss.
- f. Eh measurements are highly suspect.
- g. We feel that the actual stratigraphic location of the collected saturated zone water is in many cases undetermined, as there can be multiple lenses which can mix at the well point. Consequently, individual lense hydrogeochemistry is not confidently attained.
- h. The Sorption - program is greatly hindered by the lack of a comprehensive hydrogeochemical program.

7. The ORNL conclusions are:

- a. Published Yucca Mountain sorption may be both inaccurate and nonconservative.
- b. Information may not be acceptable for performance assessment purposes for site characterization or license application.

B. Second presentation (ORNL-WS 41476) by A. D. Kelmers.

1. This presentation reviewed assumptions underlying K_d and R_f concepts for modeling radionuclide sorption and migration. Limitations and inaccuracies in applying K_d and R_f concepts to fracture-flow systems and actinide elements were identified. Some recent European publications were reviewed.
2. Key radionuclides were identified as: Am, Pu, Tc, and Np, (where $\text{NRC}10^{-5}$ release rate from waste package exceeds EPA release to environment).
3. Sorption isotherms are better modes for describing sorption than K_d as there is certainly a point in sorption site saturation.
4. In a fracture-flow system, the ground-water velocity can be greater than the rate of diffusion of radionuclides into bulk rock, thus K_d is nonconservative.
5. The R_f concept does not predict concentrations released to environment as a function of time and it can not deal with competition for sorption sites.
6. There are problems in extrapolating laboratory sorption measurements to repository behavior over geologic times:
 - a. Ground-water/rock ratios.
 - b. Reactions of primary, secondary, and accessory minerals.
 - c. Ground-water/host-rock reactions.
 - d. Thermal and radiation pulse effects.
 - e. Reaction kinetic limitations on time extrapolation.
 - f. Radionuclide speciation effects.

7. The European publications of interest are:

- a. NERETNIEKS, J. Geophys. Res. 85, 4379 (1980).
- b. CHAPMAN and Sargent, AECL-8361 (1984).
- c. MORENO, et al., Water Resources Res. 21, 951 (1985).
- d. MCKINLEY and Haderman, Swiss TR 84-40 (1985).
- e. HADERMAN and Roesel, Swiss TR 85-40 (1985).

DISCUSSION:

There are certain significant realizations which have either been reinforced by the workshop or are a consequence of it:

1. The present sorption research of the NNWSI needs to continue with several significant modifications which would incorporate the concerns of the ORNL Group. In particular, the K_d and R_f concepts appear to be poorly reconcilable to in situ conditions. Sorption isotherms appear more realistic. In addition, the European studies seem to point towards various concerns which could be beneficial if heeded.
2. In addition to this particular research direction, two other directions appear to be warranted:
 - a. Specific mineral and radionuclide sorption reaction-studies using MACS (Tandetron) analysis in the presence of whole-rock tuff buffers.
 - b. In situ retardation experiments utilizing underlying nuclear test locations (which could be specified) and heater-sorption thermal experiments.

3. The realizations acquired by the NNWSI Sorption - Fracture experiments (SATURATED ZONE) with respect to fracture flow and sorption should be made public in a preliminary data and discussion report.
4. The DOE needs to find a workable mechanism to communicate to the NRC and the State of Nevada, such that ongoing research and results are made public sooner than the present filtered report process allows.
5. Sorption experiments have to be run for VADOSE fracture-flow under both near-field and far-field conditions, in order for the sorption data to be conservative and have utility in the assessment process.
6. If there is insufficient resource, in the present sorption NNWSI project to accomplish the necessary tasks in a timely manner, the DOE should augment the present program with that which is needed and required, in order to meet licensing criteria for characterization.
7. It is imperative that the Sandia Performance Modeling Group not use data which is at an inappropriate confidence level. Scientific validity must precede modeling before modeling can be viable for licensing purposes.
8. Additional informal workshops are warranted to focus investigative programs.