

Sandia National Laboratories

Albuquerque, New Mexico 87185

WM DOCKET CONTROL CENTER

April 13, 1984

Mr. Peter M. Ornstein  
Geotechnical Branch  
Division of Waste Management  
U.S. Nuclear Regulatory Commission  
7915 Eastern Avenue  
Silver Spring, MD 20910

WM Record File  
A-1158

WM Project 10, 11, 16  
Docket No. \_\_\_\_\_  
PDR X  
LPDR B, N, S

Distribution: \_\_\_\_\_  
ORNSTEIN SECRET  
PA...  
(Return to W.M. 623-55) \_\_\_\_\_ 15

Dear Mr. Ornstein:

Enclosed is the monthly report on FIN A-1158, Repository Site Description and Technology Transfer for March 1984. In addition, a table of Milestones for 1984-86 is attached.

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

Sincerely,

*Robert M. Cranwell*

Robert M. Cranwell, Supervisor  
Waste Management Systems  
Division 6431

RMC:6431:jm

Enclosure

Copy to:  
Office of the Director, NMSS  
Attn: Program Support  
Robert Browning, Director  
Division of Waste Management  
Malcolm R. Knapp  
Division of Waste Management  
Cal Belote  
Division of Risk Analysis  
John Randall  
Health Siting & Waste Management Division  
6431 R. M. Cranwell  
6431 R. V. Guzowski  
6431 R. L. Hunter  
6431 M. D. Siegel  
6431 K. K. Wahi  
6431 G. E. Runkle

8409120031 840413  
PDR WMRES EXISANL  
A-1158 PDR

PROGRAM: Repository Site Data and Technology Transfer FIN#: A-1158  
CONTRACTOR: Sandia National Laboratories BUDGET PERIOD: 10/83 - 9/84  
NMSS PROGRAM MANAGER: P. M. Ornstein BUDGET AMOUNT: \$570K  
CONTRACT PROGRAM MANAGER: R. M. Cranwell FTS PHONE: 844-8368  
PRINCIPAL INVESTIGATORS: R. L. Hunter FTS PHONE: 846-5421  
M. D. Siegel FTS PHONE: 846-5448

### PROJECT OBJECTIVES

The first objective is to insure through technical support, problem definition, and documentation the timely, thorough, and efficient transfer of the information, analysis techniques, and analysis tools developed for the U.S. Nuclear Regulatory Commission (NRC) by the methodology program. The second objective is to develop reference repositories in media other than bedded salt (i.e., basalt, domed salt, welded tuff, and granite).

### ACTIVITIES DURING MARCH 1984

#### Technology Transfer

The NRC comments to the SWIFT II Self-Teaching Curriculum were received on March 21, 1984. These useful comments are being combined with those from the Sandia staff to prepare a revised version of the report. As indicated, the text requires major revision to increase clarity and understanding of the sample problems. This is currently underway and is expected to take approximately 2 months.

The SWIFT II Version 12.83 computer code was received from Geotrans, Inc. and installed on the Sandia computer system during the latter part of March. The first sample problem has been executed on this version of the code. Resolution of the minor differences in the output data are being investigated. The remaining 8 sample problems need to be run and the results compared to those provided by Geotrans as part of the review process for the self-teaching curriculum. As this process nears completion, a firm date for providing the camera-ready copy of the report will be established with the PM.

Due to the commitments that Dr. Karsten Pruess of Lawrence Berkeley Laboratories has at this time, preparation of the TOUGH self-contained documentation will not be initiated until September 1, 1984 and is expected to be completed in approximately 7 months thereafter. The contractual agreements, milestones and cost estimates for the TOUGH documentation are currently being prepared by Sandia and K. Pruess.

### Short Term Technical Assistance

The technical report entitled "State of the Art and Application of Population Balance to Transport of Colloids in Waste Management" and a letter report entitled "Recommendations on Short- and Long-Term Activities for studying Colloid Transport in High-Level Waste Management" were reviewed by E. Bonano. Additional review by the coauthors is expected to be completed in April.

In addition, E. Bonano began preparation of a paper on colloids to be presented at the ANS meeting in June 1984 at New Orleans and a paper on the transport of colloids for the 1984 MRS meeting.

### Geochemistry Subtasks

Subtask 1. Completion of scoping exercises for sensitivity study to assess the importance of colloid transport of radionuclides.

Drafts of the letter report and technical position paper required under this task were prepared for in-house review. An outline for the paper "A Population Balance for Radiocolloid Transport" described in last month's monthly report was prepared.

Subtask 2. Calculations of sensitivity of radionuclides to rate constants for reactions between radionuclide species with different retardation factors.

A poster session describing the results of this subtask was presented at the Waste Management '84 conference in Tucson, Arizona March 14. Forty-one requests were received for reprints of the paper associated with the poster session (see monthly report for February, 1984). Further development of the methodology to include radioactive decay and multiple radionuclide species of Am, Pu and Cm will be included in a paper entitled "Geochemical Sensitivity Analyses.

I. Radionuclide Speciation" and will be presented at the American Nuclear Society Meeting in New Orleans on June 5.

Subtask 3. Calculations of radionuclide solubility in basaltic ground water.

Two weeks of work were authorized for this subtask; therefore, calculations will probably be limited to Am, Pu, Np and Cm. The data base used in previous SNLA solubility calculations for these elements is being checked for errors and compared to data

bases published by Rockwell Hanford Operations and Lawrence Berkeley Laboratories. A revised deadline for the letter report describing progress in this effort was set for April 30, 1984.

#### Attendance at Meetings

Malcolm Siegel and Kenneth Erickson (1511) presented a poster session (see attachment 1) at the Waste Management '84 meeting in Tucson, Arizona on March 14, 1984. A trip report describing this meeting will be forwarded to the NRC under a separate cover.

#### Repository Site Data (RSD)

Meetings were held among SNLA staff and contract personnel to review and respond to the NRC's comments and recommended additions to the Program Plan for an RSD report for unsaturated tuff. Responses to the comments were sent in a letter to P. Ornstein on March 29. Included with the responses was a preliminary table of contents and a listing of the staff and contract personnel who are responsible for each topic.

Rough drafts of appendices on the following topics were compiled during March:

1. Properties of selected zeolites
2. Hydration and dehydration of a clinoptilolite - bearing core from Yucca Mountain
3. Effects of mineralogy on weight and volume change in selected tuff samples on heating to 400°C.

Because of the schedule for this report and the fact that new publications are becoming available each month, the write-ups for each of the topics covered to date are being left as rough drafts for the time being.

Additional topics reviewed but not completed in March are paleoclimate, the behavior of water in saturated tuff in response to heater experiments and the possible application to unsaturated tuff, the volcano-tectonic history of the Yucca Mountain area, and the preliminary assessment of the aspects of magmatic disruption of a repository.

Anticipated Problems

None.

# POTENTIAL VIOLATIONS OF THE PROPOSED EPA STANDARD BY RADIONUCLIDES WITH MULTIPLE AQUEOUS SPECIES.

M.D. SIEGEL AND K.L. ERICKSON SANDIA NATIONAL LABORATORIES, ALBUQUERQUE, N.M.

## INTRODUCTION

- Significant waste repository performance assessment calculations require simple algorithms to estimate radionuclide transport
- Use of retardation factors calculated from batch sorption data can cause underestimation of radionuclide discharge and require possible violation of proposed EPA Standard (40 CFR 191)

## OBJECTIVE

- Develop method to identify physicochemical conditions where dispersion modeling used for assessment is not conservative to ensure compliance with EPA Standard

## EXAMPLE: <sup>237</sup>Np

- Assume <sup>237</sup>Np is released within an aquifer & has equilibrium solubility of 10<sup>-10</sup> g/l and sorption isotherm is given by linear function of  $C_p$

$$C_s = K_d C_p + C_{oc}$$

- Use retardation factor  $R = 1 + K_d \rho_b$  to estimate delay for <sup>237</sup>Np, which enters the aquifer at constant discharge rate for 1000 y and is then discharged at constant rate

- $R = 100$  at these conditions using representative distribution coefficient of 10000 during the duration of the 1000 year EPA regulatory period (10<sup>4</sup> years)

$$C_{oc} = 10^{-10} \text{ g/l} + 10000 \times 10^{-10} \text{ g/l} = 10^{-6} \text{ g/l}$$

$$C_{oc} = 10^{-6} \text{ g/l} \times 100 = 10^{-4} \text{ g/l}$$

- To compare  $C_{oc}$  and  $C_{oc} R$  to determine conservatism of  $R$ , note that  $C_{oc} R$  is constant at 10<sup>-4</sup> g/l

## METHOD

- The purpose of estimating water bound to radionuclide discharge involves solving multiple chemical species of a radionuclide with an equilibrium by expressions of form

$$\sum_{i=1}^n C_i = C_{total}$$

where  $C_i$  is reaction rate constant for  $i$ th reaction  
 $C$  is concentration of  $i$ th species of radionuclide

### Steps

1. Determine reaction form for chemical reaction for each species
2. Write equations and integrate to obtain expression for discharge rate to EPA and EPA regulatory period
3. Run discharge of chemical species to radionuclide and set equal to EPA release limit
4. Solve equation to determine concentrations of parameters which cause violation of EPA Standard

- Use case of discharge discharge of 1000 g to  $C_{oc}$  in EPA release rate to  $C_{oc}$  as  $C_{oc}$  is  $10^{-6}$  g/l

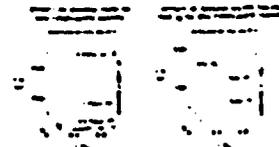
$$C_{oc} = 10^{-6} \text{ g/l} \times 1000 \text{ g} = 10^{-3} \text{ g}$$

$$C_{oc} = 10^{-3} \text{ g} \times 100 = 10^{-1} \text{ g}$$

Note  $C_{oc}$  with constant value for regulatory period but the release rate that through both is concentration of 10<sup>-4</sup> g/l

## RESULTS

- Analysis of  $C_{oc}$  vs  $C_{oc} R$  can be done for different parameters which cause up and down release rate to EPA release rate  $C_{oc}$  and  $C_{oc} R$  are constant and  $C_{oc}$  is  $10^{-6}$  g/l,  $C_{oc} R$  is 10<sup>-4</sup> g/l



- Analytical solution  $C_{oc}$  vs  $C_{oc} R$  for different release rates and parameters can be done using the EPA release rate  $C_{oc}$  and  $C_{oc} R$  is 10<sup>-4</sup> g/l



## CONCLUSIONS

- Conservative estimates can be made by estimating release of  $C_{oc}$  from available by sorption data. Minimum and maximum  $C_{oc}$  values have been accepted for several geologic media. Papers below show corresponding chemical species ( $C_{oc}$ ) for sorption capacity  $K_d$  and  $C_{oc}$  required for compliance with EPA Standard and 10 CFR 191, 10 CFR 192, 10 CFR 193, 10 CFR 194 & 10 CFR 195 corresponding to several geological release rates of 10<sup>-10</sup> g/l



- A wide range of parameters can be used to identify conditions where dispersion modeling used for assessment is not conservative to ensure compliance with EPA Standard



- General radionuclide species transport uncertainty to existing compliance of 10 CFR 191, 10 CFR 192, 10 CFR 193, 10 CFR 194 and 10 CFR 195 (10 CFR 191)

- Analytical dimensional data can be used to provide information needed to identify geochemical and physicochemical conditions where operation must be assessed

- A minimum necessary chemical model can be described for radionuclide species sorption in secondary or field studies which will ensure compliance with EPA Standard