

A1756

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LPDR- Wm-10 (2)
Wm-11 (2)
Wm-16 (2)WM DOCKET CONTROL
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May 15, 1987

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

Dear Mr. Kelly:

Enclosed is the monthly report on FIN A-1756, Geochemistry Sensitivity Analysis for April 1987. Please feel free to contact me at (FTS) 844-8368 or Malcolm Siegel at (FTS) 864-5448 if you have any questions or comments.

Sincerely,



Robert M. Cranwell, Supervisor
Waste Management Systems
Division 6416

RMC:6416

Enclosure

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A-1756 PDR

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WM-RES
WM Record File
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WM Project 10, 11, 16
Docket No. _____

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Distribution:

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WM Project: WM-10, 11, 16

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WM Record File: A1756

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PROGRAM: Geochemical Sensitivity Analysis

FIN#: A-1756

CONTRACTOR: Sandia National
Laboratories

BUDGET PERIOD: 10/86 -
9/87

NMSS PROGRAM MANAGER: W. Kelly

BUDGET AMOUNT: 200K

CONTRACT PROGRAM MANAGER: R. M. Cranwell

FTS PHONE: 844-8368

PRINCIPAL INVESTIGATORS: M. D. Siegel

FTS PHONE: 846-5448

PROJECT OBJECTIVE

The objective of this project is to provide technical assistance to the NRC in determining the sensitivity of performance assessment calculations to uncertainties in geochemical 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, sorption and kinetic 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 in Task III. Short-term technical assistance will be carried out under Task IV and the codes and data bases developed under this project will be transferred to the NRC under Task V.

ACTIVITIES DURING MARCH 1987

Task I. Uncertainty in Integrated Radionuclide Discharge

Subtask IA. Conceptual Models for Repository Sites.

During April, calculations of integrated radionuclide discharge using the LHS, NEFTRAN and EPACDF (CCDPLT) codes were continued on the VAX computer system. The LHS program was used to sample 20 values of ground-water travel times from the distribution suggested by R. Codell of the NRC (Codell, 1985). Kd values for radionuclide transport were obtained from the Sandia Sorption Data Base. For this set of simulations, the lowest reported Kd for each element for any rock/water combination was used. In cases where no Kd data were available, a value of zero was used. The effects of matrix diffusion were ignored and a porous medium was assumed. Figure 1 compares the CCDF obtained from these calculations with the no-retardation case reported in the March progress report. In this month's simulations, we have again assumed that the travel time through the disturbed zone is equal to zero; hence these calculations assume a worst-case hydrologic scenario for sites that comply with the Groundwater Travel Time Requirement of 10CFR60 as interpreted by Codell (1985). Future calculations will examine the sensitivity of the results to the

effects of dual-porosity flow, matrix diffusion and radionuclide source term.

Reference: Codell, R., 1985, Draft Generic Technical Position on Ground-water Travel Time (GWTT). U. S. N. R. C.

Subtask IB. Solubility/Speciation Effects.

Preparation of the final draft of "Thermodynamic Tables for Use in Performance Assessment of High-Level Waste Repositories. Volume 1. Aqueous Solutions Data Base," NUREG/CR-4864, SAND87-0323 was started during April.

Preparation of the paper 'Development of an Integrated Geochemical Data Base for Modeling and Sensitivity Analysis in Nuclear Waste Repository Performance Assessment Studies' which will be presented on May 12 at the 'International Conference on Thermodynamics of Aqueous Systems With Industrial Applications' continued.

Coding of several programs which allow transfer of data between the Aqueous Solutions Database and the MINEQL speciation code was completed. In addition, a code interface which reads sets of logK values from a LHS run and produces multiple input decks for MINEQL was written. These codes are discussed under Task 5 below.

Subtask IC. Sorption Effects.

The first set of calculations of the variation of the degree of sorption of uranium and neptunium onto hydrous oxides in oxic waters and selenium onto substrates in oxic and anoxic waters has been completed by the subcontractors at Stanford University. A letter report is in preparation. Additional calculations will be carried out at SNLA in the next few months.

Subtask IE. Coupled/Dynamic Effects

Earlier derivations of approximate methods to calculate radionuclide discharge in porous media with fractured plates are being extended to other geometries.

Task IV. Short-Term Technical Assistance.

No activity to report.

Task V. Technology Transfer

Development of a preprocessor which creates a file of complexation constants from data in the Aqueous Solutions Database for the MINEQL code continued. The preprocessor can be used either for single speciation calculations or for multiple runs in uncertainty/sensitivity analyses. Figures 2 and 3 describe the components of the ASD/MINEQL system and its use in sensitivity studies.

Trips

M. D. Siegel met with N. R. C. staff in Silver Spring, Maryland to discuss the status of FIN A-1756 on April 28-29. After giving a briefing on the results of the project, Siegel met with staff from the Geochemistry and Hydrology Sections and with R. Ballard, the new chief of the Technical Review Branch.

Allocation of Resources

Task I.....50%
Task V.....50%

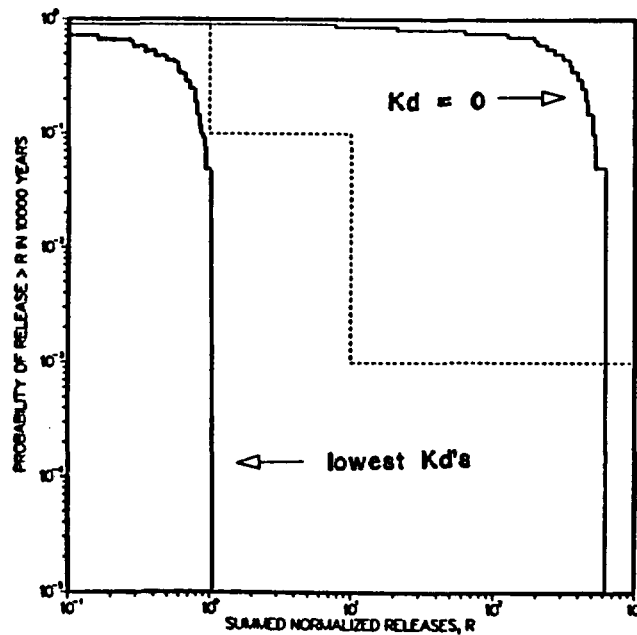


Figure 1. Complementary Cumulative Distribution Functions (CCDF) for discharge of radionuclides from repository complying with the ground water travel time, containment and release criteria of 10CFR60. Results are given for calculations in which no retardation ($K_d=0$) and for which the lowest reported K_d for basalt samples were used.

THERMODYNAMIC DATABASE FOR GSA

- ASD FORMAT 1: GHS and C_p data
- ASD FORMAT 2: $\log K$ for specific reaction
- ADDREACT: add new reaction to FORMAT 2
- COMPLOGK: compute $\log K \pm \sigma$ for reaction
- BRIDGE: produce new MINEQL database from ASD data with $\log K \pm \sigma$ and $\Delta H_r \pm \sigma$
- LHSMIN: prepare file for multiple runs of MINEQL for different $\log K$
- MINQLMLT: carry out multiple MINEQL runs and write specified results to a file for post-processing

Figure 2. Components of the ASD/MINEQL pre-processor.

**FUNCTIONS OF ASD PREPROCESSOR
IN SPECIATION SENSITIVITY ANALYSIS**

1. Reads ΔG values and σ from ASD for basis species
2. Calculates log K's and uncertainties for input to LHS
3. Uses LHS to produce nxm array of log K values
- 4.1 Reads vector of log K's input for a single calculation
- 4.2 Performs speciation calculation and writes results to a file
- 4.3 Chooses important species and writes their concentrations or other parameters to a file
- 4.4 Repeats for each vector
5. Prepares input for sensitivity analysis on results by graphical or other methods

Figure 3. Example of potential use of the ASD/MINEQL preprocessor in uncertainty/sensitivity analysis.

PRIAM ClusterTower
HOST ADAPTER - CHA
INSTALLATION INSTRUCTIONS

PRIAM Systems Division
20 West Montague Expressway
San Jose, California 95134

* INSTALLATION INSTRUCTIONS *

These instructions describe how to install the PRIAM ClusterTower Host Adapter (CHA) into an IBM PC/XT/AT or COMPAC system unit. A PRIAM ClusterTower Host Adapter (CHA) circuit card must be installed in each personal computer that is to be connected to the ClusterTower.

1. Insure that the power is disconnected from the system unit and all externally attached devices.

2. Remove the IBM AT system unit cover. If you are installing the CHA in an IBM PC or XT go to step 3.

Unlock the Key Lock on the front panel of the AT system unit (turn the key counterclockwise and remove the key). The padlock-like emblems beside the Key Lock on the unit's front panel indicate the unlocked and locked positions.

A plastic back panel may be attached to the system unit with plastic hook and loop fastener strips. If the panel is present, pull on the plastic panel until it comes loose, revealing the metal back panel of the system unit. Remove the five cover mounting screws on the metal back panel of the system unit. Pull the cover off by sliding it forward. Be careful not to pull out any internal cables when removing the cover.

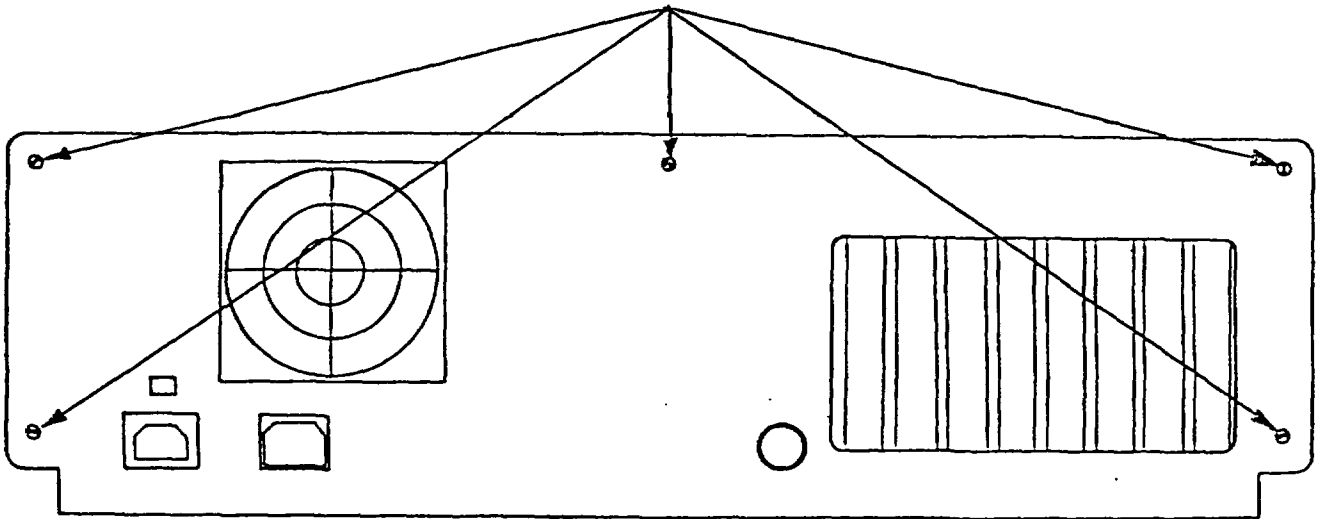
PRIAM ClusterTower CHA INSTALLATION

3. Remove the IBM PC/XT system unit cover.

Remove the five cover mounting screws on the metal back panel of the system unit, as shown on the diagram below. Save the screws for eventual reinstallation.

Remove the cover by sliding it forward and tilting up. Be careful not to pull out any internal cables when removing the cover.

Remove These Screws



System Unit Back Panel

4. Check the CHA switch settings.

The CHA board has two red DIP switches labeled MEM and I/O. Check these switches to ensure that they are set at the default values shown below (open or closed positions are indicated by "O" or "C").

	Position:	1	2	3	4	5	6	7	8
I/O - I/O Port Base Address:		C	O	O	C	C	O	O	-
I/O - BIOS ROM Ena/DIS:		-	-	-	-	-	-	-	O
MEM - BIOS ROM Base Address:		C	C	C	O	C	C	O	O

The default values shown correspond to an I/O Port Base Address of 330 Hex and a BIOS ROM Base Address of C8000 Hex with the BIOS ROM disabled.

PRIAM ClusterTower CHA INSTALLATION

5. If the system unit contains an internal or external hard disk that is used as the boot device, the BIOS ROM must be disabled by setting the I/O switch 8 to open.

6. If the system unit does not contain a bootable device and you want the ClusterTower to be the boot device, the BIOS ROM must be enabled by setting the I/O switch 8 to closed.

Installation of certain other accessories or expansion cards may require changes to the switch settings for correct operation. We suggest that you install the CHA as described, and see whether these default settings work for your system. The Superuser's manual defines the jumper functions and discusses possible conflicts with other accessories in the system. If it is necessary to change the jumpers, note the new configuration of the card in the space provided below.

I/O - I/O Port Base Address: Preset to 330H, New Setting _____
I/O - BIOS ROM Ena/Dis: Preset to Disabled, New Setting _____
MEM - BIOS ROM Base Address: Preset to C8000H, New Setting _____

7. Install the CHA in the system unit.

Select a free expansion slot, and remove the metal bracket that covers the panel cutout for that slot. Save the mounting screw.

If you are installing the CHA in an IBM PC or XT, locate the black plastic card guide that comes with your interface card. Find the inside front panel of your system unit chassis (near the speaker). Notice the two holes in the front inside panel that are aligned with the slot you have chosen. Turn the card guide so the "fingers" (in the channel on the card guide) are pointing down, and press the card guide's two mounting pegs into the two holes in the front panel.

Position the interface card so that the interface cable connector is at the rear of the system unit, and the expansion slot edge connector is pointing down. Then, using an even pressure, push the male edge connector into the female expansion slot connector.

Using the screw that you saved, attach the connector panel on the end of the card to cover the cutout in the rear panel.

8. Replace the system unit cover.

Push the cables in the system unit down and out of the way. The cables should be below the top of the power supply in order to slide the system unit's cover back on. Verify that ALL connectors are fully seated. Make sure that the lower inside lip of the cover is under the side rails of the system unit. Lift the cover up against the rails and slide it onto the system. Be careful not to disturb the cables. Install the five cover mounting screws on the back panel. Replace the plastic back panel of the system unit by pressing it into place.

PRIAM ClusterTower CHA INSTALLATION

9. Connect the ClusterTower to CHA cable.

Connect one end of the cable supplied in the CHA installation kit to the CHA. Connect the other end to any of the eight port connectors located on the back panel of the ClusterTower. Be sure the cable is firmly attached.

PRIAM ClusterTower SOFTWARE INSTALLATION PROCEDURE

These instructions setup the station for ClusterTower operation. The ClusterTower Superuser's manual defines how to customize the ClusterTower configuration for special applications.

STATIONS THAT HAVE THE CHA ROM BIOS ENABLED

If the BIOS ROM is enabled so that the system unit will boot from the ClusterTower, you should obtain the system disk that was created during the ClusterTower Setup and run the SSETUP program.

- o Boot from the disk created during the ClusterTower setup process.
- o Type SSETUP<Enter>.
- o Follow the prompts.

If the station does not have a hard disk and a floppy is not inserted in drive A, the station will boot from the ClusterTower. The station's boot volume may be selected by the Superuser (refer to the Superuser's Manual).

If a floppy disk is inserted in drive A, the system will boot from the floppy disk when the station is powered on or reset. To access the ClusterTower, the floppy disk must contain:

- o The DOS system files.
- o The ClusterTower device driver (CLUDVR.SYS)
- o The CONFIG.SYS file must contain the statement "DEVICE=CLUDVR.SYS"

PRIAM ClusterTower CHA INSTALLATION

STATIONS THAT HAVE THE ROM BIOS DISABLED

If the station has a hard disk the system will boot from the hard disk if a floppy is not inserted in drive A.

To access the ClusterTower, the boot device (floppy or hard disk) must contain:

- o The DOS system files
- o The ClusterTower device driver (CLUDVR.SYS)
- o The CONFIG.SYS file must contain the statement
"DEVICE=CLUDVR.SYS"

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A-1756
1646.010
April 1987

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY
SANDIA'S ACCOUNTING DEPARTMENT.

	Current Month -----	Year -to- Date ----
I. Direct Manpower (man-months of charged effort)	0.9 ---	4.2 ---
II. Direct Loaded Labor Costs	11	36
Materials and Services	0	7
ADP Support (computer)	3	9
Subcontracts	29	147
Travel	0	1
G & A	12	6
Other (computer roundoff)	0	0
	---	---
TOTAL COSTS	55	206

III. Funding Status

Prior FY Carryover -----	FY 87 Projected Funding Level -----	FY 87 Funds Received to Date -----	FY 87 Funding Balance Needed -----
29K	229K	200K	None