SOIL-BIOTIC-HYDROLOGIC PROCESSES GOVERNING MOBILITY AND BIOLOGICAL AVAILABILITY OF RADIONUCLIDES IN COMMERCIAL LOW-LEVEL WASTE DISPOSAL SITES

PROGRESS REPORT
NOVEMBER 1, 1984 to APRIL 30, 1985

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Pacific Northwest Laboratory
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Richland, Washington 99352

TABLE 2. Physical and chemical characteristics of soils separately associated with barren soil and greasewood shrub

LOCATION	DEPTH	Concentration of Soluble Al	Fe	Mn	Org C	pH	Eh
	cm	µg soluble/g soil			mgC/g		+mv
Soil	0-1	0.66	2.30	3.12	1.56	6.57	174
	1-5	2.14	3.08	0.18	0.41	6.84	227
	5-16	5.62	3.96	0.08	0.27	7.29	180
	16-26	6.12	3.16	0.02	0.21	7.75	178
	26-36	6.32	3.12	0.02	0.16	7.68	191
	36-46	8.48	3.52	0.02	0.10	7.88	162
Soil under Greasewood	Litter	2.58	21.20	12.80	18.80	8.59	94
	0-1	19.10	15.00	1.04	1.93	8.83	150
	1-5	31.20	19.00	0.78	1.08	9.24	150
	5-16	36.20	15.90	0.30	0.38	9.46	114
	16-26	26.80	8.78	0.22	0.40	9.61	127
	26-36	40.60	17.90	0.40	0.42	9.37	67
	36-46	36.60	11.60	0.28	0.37	9.31	73

Thus, Eh and soluble organic C played a role, via complexation, in the solubilization of hydrolyzable cations which have soil chemistries analogous to several important radionuclides.

MINTEQ Model Parameterization

In order to enhance the capability to model the movement of trace elements and radionuclides in ground water and to better estimate the proportion of the radionuclide or trace element complexed by organic compounds, thermodynamic data for Co and Am (different chemistries) and the organic compounds, EDTA (strong complexing agent) and citrate (weak complexing agent) were added to the MINTEQ thermodynamic database. The Co data was taken from a compilation by S. Peterson and L. E. Eary (Earth Sciences Department, PNL, personal communication) and includes the basic

thermodynamic data (i.e., free energy, enthalpy, and entropy) for each component and complex as well as the calculated Log K values. The Am thermodynamic data was taken from a compilation by Kerrisk (1984) and included the basic thermodynamic data as well as the calculated Log K values. The EDTA and citrate thermodynamic data was taken from the compilations of Martell and Smith (1974) and Martell and Smith (1977), respectively. The Log K values for complexation of EDTA and citrate with trace elements and radionuclides contained in these compilations were added to the MINTEQ thermodynamic data base without further review. Future geochemical modeling work will use the thermodynamic data for EDTA and citrate to bracket, but not predict, the effect of organic complexation by single compounds (not complex mixtures) on the aqueous chemistry of specific trace elements and radionuclides. The research described above, inconjunction with a formal thermodynamic data review process will ultimately provide the basis for prediction of soil solution chemistry and linkage with hydrologic transport models.

November 7, 1984

OFFICE OF RESOURCE MANAGEMENT
DIVISION OF AUTOMATED INFORMATION SERVICES

REQUIREMENTS FOR USE OF MICROCOMPUTERS BY NRC CONTRACTORS

These requirements cover the use of microcomputers by NRC contractors to produce machine-readable contract deliverables. The purpose of the guidelines is to assure that such deliverables (e.g., programs, documents, graphs, data, etc.) will be usable on NRC equipment.

All deliverables intended for use on NRC microcomputers should meet the following criteria:

1. All diskettes should be capable of use on an IBM PC using one of the software packages supported by the NRC Division of Automated Information Services (see attachment).

2. In particular, documents (e.g., reports) should be produced with IBM DisplayWrite 2 word processing software. This will allow them to be used both on NRC microcomputers and word processing equipment.

3. Failing criteria 1 or 2 above, data or text should be produced as ASCII files in standard IBM PC diskette format.

Questions concerning the above requirements should be addressed to the ITS Support Center, (301) 492-4160 (FTS 492-4160).

*Use of IBM DisplayWrite 2 mandatory.

APPENDIX A

NRC Scientific Software Submittal Package Description Form

Program Name:

Programming Languages(s) Used:

Machine:

Core Storage Requirements for Sample Problem:

Approximate Execution Time for Sample Problem:

Package Contents (items 1-8 are mandatory):

___1. Abstract

___2. Documentation consisting of the items described in the space below:

___3. Source program on ___ cards ___ tape ___ diskette.

___4. Sample problem input on ___ cards ___ tape ___ diskette.

___5. Compilation of the source program (item 3).

___6. Listing of the sample problem input (item 4).

___7. Output from an execution of the sample problem input, item 4, using the source code provided in item 3, including plots, if any.

___8. For tape submittals, a copy of the output for the job that created the tape.

___9. Other (describe other materials such as data libraries, control information, etc., in the space below).

Code Portability Information:

1. Provide name and description of required system library routines not included in the submittal, and indicate where these routines are called (subroutines name, line).

2. Provide name and description of required FORTRAN library routines (internal or external) which may differ between mainframes, and indicate where these routines are called (subroutine name, line).

3. Describe any special compiler or loader options used, such as:
    1. core present to zero or other values (CDC PRESET=ZERO)
    2. compiler optimization level
    3. rounding or truncation options

4. Provide any special instructions regarding execution time or core storage requirements, such as:
    1. special core storage requirements for loading or executing
    2. instructions for adjusting required core storage by increasing or decreasing array dimensions.
    3. estimates of relation of execution time to critical input parameters

5. Identify all input and output unit numbers and their purpose. List all locations of end-of-file tests.

If tapes are used for submittal, please use the attached tape description form. Be sure to include a copy of the job that created the tape. Where possible, we would prefer to receive tapes with the following format: 9 track, 1600 bpi, unlabeled, in EBCDIC character format, with fixed length block or unblocked records.

If diskettes are used for submittal, they should be 5.25" and MS-DOS compatible.

Office of Resource Management
Division of Automated Information Services

Scientific Software Development, Distribution and Submittal Requirements for NRC Contractors

This document provides requirements for contractors developing scientific software for the Nuclear Regulatory Commission (NRC). Its purpose is to assure that any such software can be readily implemented and used by staff at NRC headquarters and can, if required, be easily disseminated through the National Energy Software Center or transferred to other data processing sites. This implies the use of standard software packages, programming languages, and compilers as well as adherence to good programming and documentation practices.

Sections 1-4 below provides requirements for programming languages and practices, code documentation, distribution and submittal to the NRC.

1. Programming Languages and Practices

All new mainframe or minicomputer programs developed or converted for NRC shall be written in American National Standards (ANS) FORTRAN (ANSI Standard X3.9-1978) unless justified and cleared in advance by NRC, including concurrence by the NRC Division of Automated Information Services. All microcomputer software developed for the NRC shall be capable of running under MS-DOS. Source programs provided must be compatible with IBM PC BASIC or FORTRAN. In accordance with good programming practices, we recommend use of structured design principles, meaningful variable names, and modularity to enhance code transportability, readibility, and maintenance. It is imperative that all major variables and program logic structure be clearly described through liberal use of comments in the code.

Proprietary software packages should be avoided except where standard readily available packages exist and are supported for use at NRC-accessible computer facilities or on microcomputers by the NRC ITS Support Center. Machine-dependent and installation-specific packages and features including assembly language should not be used unless justified and cleared in advance by NRC, including concurrence by the NRC Division of Automated Information Services. Information about software supported for use on NRC-accessible computer facilities and microcomputers may be obtained from the NRC ITS Support Center, (301) 492-4160 (FTS 492-4160).

Mainframe programs which generate plots must do so using the Display Integrated Software System and Plotting Language (DISSPLA) or CALCOMP plot software (DISSPLA is a standard at all DOE laboratories).

2. Documentation

All scientific computer codes shall be documented in conformance with ANSI standard N-413, "Guidelines for Documentation of Digital Computer Programs."

This standard is specifically oriented toward computer programs prepared for scientific and engineering computations. The major documentation requirements included in the standard are:

a) Computer Program Abstract
b) Application Information (User's Guide)
c) Problem or Function Definition (Theoretical Development)
d) Programming Information (Programmer's Guide)

A copy of this standard may be obtained for $8.50 plus $2.00 shipping and handling from:

The American National Standards Institute
1430 Broadway
New York, New York 10018
ATTN: Sales Department

In addition to or instead of conforming to ANSI Standard N-413, documentation for large codes or complex systems may be required to conform to FIPS Pub 38 (02/12/78), "Documentation of Computer Programs and Automated Systems." Applicability of FIPS Pub 38 will be determined by the Office of Resource Management, Division of Automated Information Services in consultation with the NRC Project Manager. Specific documentation requirements under FIPS Pub 38 shall be decided at the discretion of the NRC Project Manager depending on project size and complexity.

Each program developed for the Nuclear Regulatory Commission should include the following program title block and disclaimer in the main program:

Program Title:

Developed for: U.S. Nuclear Regulatory Commission
Office of (fill in NRC Office)
Division of (fill in NRC Division)

Date:

NRC Contact(s): Phone:

Code Developer: Phone:

This program was prepared for an agency of the United States Government. Neither the United States Government no any agency thereof; or any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for any third party's use, or the results of such use, of any portion of this program or represents that its use by such third party would not infringe privately owned rights.

3. Code Distribution

In general, all computer codes developed with federal funds are in the public

domain and as such, must be made available for distribution to requestors such as utilities, vendors and universities. Each NRC contract involving code development should contain a task requiring the contractor to submit completed codes to the National Energy Software Center for subsequent distribution upon request:

U.S. Department of Energy
National Energy Software Center (NESC)
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439
Telephone: (Commercial) 312-972-7250
(FTS) 972-7250

4. Code Submittal to the NRC

If specified in the contract or DOE laboratory agreement that a code is to be transmitted to the NRC, Appendix A, "NRC Scientific Submittal Package Description Form" must be used. The form is designed to describe the contents of a standard software submittal package which must be used when transmitting completed codes to the NRC. All information on the form must be supplied, even if the contractors themselves are performing the code installation on NRC-accessible computer facilities.

ATTACHMENT

Microcomputer software support by the NRC Division of Automated Information Services:

Operating System:	PC DOS
Programming Languages:	IBM BASIC and IBM FORTRAN 2.0
Data Base:	dBASE III
Spreadsheet:	LOTUS 1-2-3
Graphics:	CHARTMASTER and SIGNMASTER
Project Management:	PERTMASTER
Word Processing:	DISPLAYWRITE 2
Communications:	CROSSTALK XVI (asynchronous) DISPLAYCOMM (bisynchronous)

LINDA

NNWSI Project/NRC Waste Package Meeting

Proposed Agenda - July 23-24, 1985

Introductions	1/4 hour
NRC Participants	
DOE/LLNL Participants	
Others	
Meeting Objective & Agenda Overview	1/4 hour
NRC Objectives	
DOE/LLNL Objective	
Agenda Overview	
Update on Conceptual Designs	1 1/2 hours
Emplacement Geometry	
Spent Fuel Internal Configurations	
WV/DHLW Containers	
MRS Packaging & Storage Implications	
Part 60 Excluded Materials	1/2 hour
Discussion of NRC Intent	
Rationale for Implementing Criteria	

Waste Form Testing - Spent Fuel — 3 hours

- Approach to Testing
- Release Rates
  - Cladding Degradation
  - Fuel Oxidation
- Results to date
  - Comparison with Part 60 Objectives
- Isotopes of Concern
- Discussion of Fuel Population
  - Proposed Test Matrix
  - Adequacy of Sampling
- Planned Testing
- Modeling of Releases

Waste Form Testing - Glass — 1 1/2 hours

- Unsaturated Testing
  - Procedure Development
  - Results to Date
  - Planned Testing
- Supporting Tests
- Modeling of Release Mechanisms

Container Material Testing — 3 hours

- Conceptual Model for Corrosion in Tuff
- Environmental Conditions
- General & Localized Corrosion Testing
- Stress Corrosion Testing
- Planned Testing

Reliability Considerations — 1 hour

Discussion of NRC Approach to

"substantially complete"

Approach to Reliability for Containment

Summary and Development of Minutes — 1 hour

DRAFT AGENDA FOR TBEG DATA REVIEW.

Date: August 5-9, 1985

Place: Austin City Limits

5 Aug AM — Travel DC-Austin

5 Aug PM — Orientation

Introductions NRC, TBEG, DOE

Objectives of data review/workshop: [NRC] Review and examine the geologic data base of TBEG relevant to proposed high level waste storage facility in Deaf Smith and Swisher Counties. Data to be reviewed includes core and logs from DOE drilled wells, geophysical surveys, borehole testing, hydrological testing (surface and subsurface), maps and cross sections, remote sensing information and the results of laboratory investigations.

Purpose of data review/workshop: [NRC] Familiarize the NRC staff with the data and data interpretations available to TBEG to support their presentation of the geologic, hydrologic and geochemical conditions in the area of the proposed high level waste sites.

General overview of TBEG program [TBEG] Brief overview of program areas to focus on types of information available, status of the information (raw data, interpretive data, draft reports, final reports), significant findings and QA program as implemented by TBEG.

6 Aug — Stratigraphy of Site Area

Topics for review:

- Examination of cores-DOE wells
- Depositional system, Permian sequence-Palo Duro Basin
- Continuity and distribution of units
- Facies relationships
- Diagenetic History
- Clay mineralogy
- Properties of host rock

Data: Cores from J. Friemel, Zeeck, Mansfield, Well logs
Mineralogical analysis of clays in host rock;
identification of alterations of clays and halite;
chemistry of brine inclusions, including isotopic data

Relevant TBEG WBS#: 332FG, 332GM IV, 332GP II, 332GP IV, 332GP V

Example Reports: Fisher, R.S. Geochemical and textural evidence of primary and altered halite; Texas Bureau of Economic Geology 1983 Annual Report

BMI/SRP-5017, 1984, Summary Well Report DOE-Gruy Federal No. 1 Grabbe: Unanalyzed Data; Texas Bureau of Economic Geology

Hovorka, S.D., 1983, Carbonate-Anhydrite-Halite Cycles San Andres Formation (Permian) Palo Duro Basin, Texas, Texas Bureau of Economic Geology

7 Aug AM — Geology/Hydrology of near surface units

Topics for Review:

- Stratigraphy of Dockum/Ogallalla/Quaternary deposits
- Depositional/erosional history of Dockum/Ogallala
- Lacustrine and eolian deposits: history, age, distribution.
- Paleoclimate
- Material properties
- Playas
- Hydrology of near surface units
- Relationship of Dockum to Ogallala and deeper Aquifers

Data: Data base to evaluate Plio-pliestocene lake basins, Tule formation, such as along Tierra Blanca Creek, Tule Creek.
Water Quality Data
Isopach and lithofacies maps
Structure contour maps of pre-Ogallala Surface
Maps of Ogallala Distibutional channels

Relevant TBEG WBS#: 332GN I, 332GN III, 332GM I, 332GM II, 332GM IX, 332GM III, 332GM VI,

[SCR 3.1.2.(BEG 3.4.2.1.), SCR 3.1.3.(BEG 3.4.2.2.), SCR 3.2.1.(BEG 3.5.7.) CSR 332FH(BEG 3.1)]

Example Reports: Seni, S.J.. 1980, Sand Body Geometry and Depositional Systems, Ogallala Formation, Texas: Texas Bureau of Economic Geology Report of Investigations no. 105

Gustavson, T.C. and R.T. Budnik, 1984,Salt Dissolution: Examples From Beneath the Southern High Plains; Texas Bureau of Economic Geology Report OF-WTWI-1984-3

Gustavson, T.C. and R.J. Finley, 1984,Late Cenozoic Geomorphic Evolution of the Texas Panhandle and Northeastern New Mexico: Case Studies of the Structural Controls of the Regional Drainage Development: Texas Bureau of Economic Geology Report OF-WTWI-1984-39

7 Aug PM

Dissolution

Topics for review:

- Location of known/suspected active dissolution
- Location of known/suspected paleodissolution features
- Controlling mechanism
- Geomorphic-stuctural-stratigraphic indicators
- Rates

Data: Structure contour maps and cross sections in areas of known and suspected dissolution; hydrochemistry of surface and ground water; petrographic-mineralogic-geochemical data from cores; geomorphic and paleogeomorphic evidence of dissolution

Relevant TBEG WBS#: 332GM V, 332GN IV, 332GM III,

Example Reports: Goldstein, A.G. and E.A. Collins, 1984, Deformation of the Permian Strata Overlying a Zone of Salt Dissolution and Collapse in the Texas Panhandle: Geology, Vol 12, pp 314-317

Gustavson, T.C., R.J. Finley and K.A. McGillis, 1980, Regional Dissolution of the Permian Salt in the Anadarka, Dalhart, and Palo Duro Basins of the Texas Panhandle; Texas Bureau of Economic Geology Report of Investigations no. 106

OF-WTWI-1984-3

(Work in progress) Petrographic, Stratigraphic and Structural Evidence for Dissolution of Upper Permian Bedded Halite, Palo Duro Basin, Texas, Texas Bureau of Economic Geology

Gustavson, T.C., and R.T. Budnik, (work in progress), Structural Influences on Geomorphic Processes and Physiographic Features, Texas Panhandle; Technical Issues in the Siting of a Nuclear Waste Repository, Texas Bureau of Economic Geology

Dutton, A.R., Water Sampling and Hydrologic testing in the Salt Dissolution Zone of the Texas Panhandle; Texas Bureau of Economic Geology 1983 Annual Report

8 Aug session A: Regional Geology

Topics for review:

- Structure and Tectonics of Palo Duro Basin
- Amarillo-Wichita-Ouachita Uplift
- Matador Uplift
- Seismotectonics
- Regional Stress field
- Meers Fault zone

Data: Cross sections and maps along with supporting borehole, geophysical, remote sensing and surface mapping information; in situ stress measurements.

Relevant TBEG WBS#: 332GM VII, 332GM VIII, 332GM X [CSR 332FH(C.1)(BEG 3.3.1), CSR 332FH(E.2)(BEG 3.3.2), CSR 332FH(BEG 3.5)]

Example Reports: McGooky, Gustavson and Hoadley, 1984, Regional Structural Cross Sections, Mid-Permian to Quaternary Strata, Texas Bureau of Economic Geology Portfolio of Cross-Sections, 20 pages, 12 Plates.

8 Aug session B: Hydrology

Topics for Review

- Groundwater flow modeling

Mechanism of flow thru San Andres
Evidence/effect of fracture flow
Leakeage Through Evaporite Aquitard
Recharge/disharge
Hydrogeologic parameter values for Basin units

Data: Isotopic, Hyrdochemical, Fracture data(core), permiability data

Relevant TBEG WBS#: 332GN II, 332GN V
[CSR 332FI]

Example Reports: Kreitler, C.W., Hydrologic Characterization of an Evaporite Aquitard

Smith, P.G., G.W. Page, and J.K. Downing, Regional Lithopermeability Determinations for the Permian Basin Area of Texas and New Mexico

Picking, L.W. and D.E. Wilton, Testing the Hydraulic Characteristics of Low Permiability Carbonates, Palo Duro Basin, Texas

Richter, B. and C.W. Kreitler, Geochemical and Hydrological Characteristics of Salt Springs and Shallow Subsurface Brines in the Rolling Olains of North-Central Texas and Southwest Oklahoma: Texas Bureau of Economic Geology Report of Investigations

Dutton, A.R. Hyrogeology of the San Andres Formation, Texas Bureau of Economic Geology Report of Investigation

Fisher, R.S. and C.W. Kreitler, Isotopic and Geochemical Composition of Deep Basin Brines, Palo Duro Basin, Texas, Geological Society of America, Abstracts with Program

Variations of Porosity in the Wolfcamp Aquifer

8 Aug session C Geochemistry

Topics for review:

Detailed geochemistry/petrology/minerology
Brine Geochmistry

Data: Petrographic and Mineralogic Analysis for host rock (Halite and Clays) and surrounding strata, Chemistry of groundwaters and brine inclusions, including isoltopic data; volume of brines in inclusions; sorptive capabilities of minerals; brine migration data (if applicable)

Relevant TBEG WBS#: 332GP ALL
[CSR 332 FJ(BEG 6.1)]

Example Reports: Fisher R. S., Water Content of Bedded Salt, Texas Burea of Economic Geology 1983 Annual Report

Fisher, R. S. Clay Mineral Assemblages in evaporite Host Rocks; Texas Bureau of Economic Geology 1983 Annual Report

Fisher, R.S. Hydrogeochemistry of the Palo Duro Basin, Texas Panhandle, OF-WTWJ-1983-13.

Fisher; Hovorka. Textural and Chemical Zones in Bedded Halite, Permian Lower San Andres Formation, Palo Duro Basin, OF-WTWJ-1984-48

9 Aug Continuation of sessions as needed:

Wrap-up and preparation of meeting notes

Travel Austin-DC

NOTE: LISTING OF TBEG WBS# IS GIVEN AS AN AID TO TYPES OF INFORMATION WHICH IS EXPECTED TO BE DISCUSSED IN EACH SESSION. IT IS NOT TO BE AN ALL INCLUSIVE LISTING. DUPLICATE LISTINGS ARE TO IMPLY THAT THE SUBJECT WILL BE DISCUSSED IN GENERAL IN EARLY SESSIONS, BUT IN MUCH MORE DETAIL IN LATER SESSIONS.