REPORT ON GEOGRAPHIC DATABASE DEVELOPMENT AND INVESTIGATIONS TO SUPPORT CDM DEVELOPMENT—GEOCHEMISTRY FY94

Prepared for

Nuclear Regulatory Commission
Contract NRC-02-93-005

Prepared by

David Turner
David Pickett

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

October 1994

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ABSTRACT

The Nuclear Regulatory Commission (NRC) and the Center for Nuclear Waste Regulatory Analyses (CNWRA) staff are in the process of developing Compliance Determination Methods (CDMs) to assign research priorities and ensure a timely review of the U.S. Department of Energy (DOE) License Application (LA) for Yucca Mountain (YM). For the purposes of developing the necessary background to evaluate DOE submittals, it is possible to use current levels of understanding to identify broad types of data that will be needed to complete the compliance reviews of the LA in the mandated time. Many of the required data, such as site geology, precipitation, and hydrostratigraphy, are site-specific in nature. Given the recent initiation of site characterization activities at YM, while it is possible to make a preliminary identification of specific data sources, much of the data currently available is sparse. Presumably many of the gaps will be filled in through ongoing and future site characterization activities. For many of these types of data, such as radionuclide thermodynamic data, there is little need to acquire site-specific data, and current data sources can be identified readily. Even in these cases, however, certain systems or parameters may be poorly characterized and subject to change as research proceeds and levels of understanding increase. This report is an initial attempt to identify specific data needs for each of the Compliance Determination Methods related to geochemical issues, and currently available sources for these data.

Many of the geochemical data that will be generated during DOE site characterization will be site-specific to Yucca Mountain and the surrounding area. For this reason, these data are most useful when tied to a geographic and geologic framework. Geographic Information Systems (GIS) such as ARC/INFO are powerful tools designed for presenting and interpreting data in a geographic context. By incorporating geochemical data in a GIS database, it is possible to analyze the data for spatial trends, identify relations among other geographic and geologic data, and identify gaps in the data collection. By superimposing different coverages such as geology, other geochemical and hydrologic data and political and regulatory boundaries, it is possible to develop figures and maps that can transmit a wide range of information.

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ACRONYMS

ATDTS	Automated Technical Data Tracking System
CDM	Compliance Determination Method
CDS	Compliance Determination Strategy
CNWRA	Center for Nuclear Waste Regulatory Analyses
DOE	U.S. Department of Energy
DRI	Desert Research Institute
EPA	U.S. Environmental Protection Agency
FAC	Favorable Condition
FCRG	Form and Content Regulatory Guide
GIS	Geographic Information System
GEMBOCHS	Geologic and Engineering Materials: Bibliography of Chemical Species
HLW	High-Level Radioactive Waste
KTU	Key Technical Uncertainty
LA	License Application
LANL	Los Alamos National Laboratory
LARP	License Application Review Plan
LBL	Lawrence Berkeley Laboratory
LLNL	Lawrence Livermore National Laboratory
NAS	National Academy of Sciences
NRC	Nuclear Regulatory Commission
NWPA	National Waste Policy Act
ORNL	Oak Ridge National Laboratory
PAC	Potentially Adverse Condition
PNL	Pacific Northwest Laboratory
PPA	Proposed Program Approach
QA	Quality Assurance
SAR	Safety Analysis Report
SER	Safety Evaluation Report
SNL	Sandia National Laboratories
TDB	Technical Data Base
TOP	Technical Operating Procedure
USGS	U.S. Geological Survey
YM	Yucca Mountain
YMPO	Yucca Mountain Project Office

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QUALITY OF DATA

DATA: Sources of data are referenced in this report. CNWRA-generated laboratory and field data cited in this report meet quality assurance requirements described in the CNWRA Quality Assurance Manual. Data from other sources however, is freely used. For data from non-CNWRA sources, their referenced sources should be consulted for determining their level of quality assurance.

ANALYSES AND CODES: The scientific/engineering computer code ARC/INFO is used in analyses contained in this report. ARC/INFO is commercial software and only the object code is available to the CNWRA.

1 INTRODUCTION

Tertiary ash-flow tuffs at Yucca Mountain (YM), Nevada are currently being considered as a potential location for a high-level radioactive waste (HLW) geologic repository. To maintain the public health and safety, the ability of this repository to isolate the waste from the accessible environment is of critical importance. Because a multiple-barrier design is called for in the regulatory requirements, the geologic setting will be relied upon to provide isolation of the waste should the engineered barrier system fail. The different subsystems of the geologic setting, including the hydrologic, geochemical, and climatology/meteorological systems all contribute as key factors controlling the isolation capabilities of the site.

Many of the geochemical data that will be generated during the U.S. Department of Energy (DOE) site characterization will be site-specific to YM and the surrounding area. For this reason, these data are most useful when tied to a geographic and geologic framework. Geographic Information Systems (GIS) such as ARC/INFO are powerful tools designed for presenting and interpreting data in a geographic context. By incorporating geochemical data in a GIS database, it is possible to analyze the data for spatial trends, identify relations among other geographic and geologic data, and identify gaps in the data collection. By superimposing different coverages such as geology, other geochemical and hydrologic data and political and regulatory boundaries, it is possible to develop figures and maps that can transmit a wide range of information.

1.1 REGULATORY BASIS

The Nuclear Waste Policy Act of 1982 (NWPA), as amended in 1987 charges the DOE, the Nuclear Regulatory Commission (NRC), and the Environmental Protection Agency (EPA) with particular responsibilities in the siting, licensing, construction, operation, and permanent closure of a HLW geologic repository. The NRC regulations governing waste isolation in a geologic repository are given principally in 10 CFR Part 60, while the limits imposed on radionuclide release to the accessible environment are established by the EPA in 40 CFR Part 191. The EPA standards are currently under evaluation by the National Academy of Sciences (NAS) in the context of the Energy Policy Act of 1992.

Through site characterization activities designed to meet the requirements in 10 CFR Part 60 and described in detail elsewhere (e.g., U.S.Department of Energy, 1988a-h), the License Application (LA) submitted by DOE is required to provide general information on the ability of YM to meet overall performance objectives. The LA must also include a Safety Analysis Report (SAR)[10 CFR 60.21(c)] containing both specific information on the hydrogeologic and geochemical properties of the system, and an analysis of the hydrogeology, geochemistry, climatology, and meteorology of the site. The analyses and evaluations of individual systems required for the SAR are covered in 10 CFR 60.21(c)(1)(ii)(B) and 10 CFR 60.21(c)(1)(ii)(C). Hydrogeologic, geochemical, and climatology/meteorology considerations are also identified in several places in the siting criteria identified in 10 CFR 60.122(b) and 10 CFR 60.122(c) as both favorable (FAC) and potentially adverse (PAC) conditions, respectively.

The overall system performance objective for the geologic repository after permanent closure is defined in 10 CFR 60.112 and requires that "...releases of radioactive materials to the accessible environment following permanent closure conform to such generally applicable environmental standards for radioactivity as may have been established by the Environmental Protection Agency with respect to both anticipated processes and events and unanticipated processes and events" (10 CFR 60.112).

Performance objectives for the engineered barrier and the geologic setting are described in 10 CFR 60.113. In 10 CFR 60.113(a)(2), the performance of the hydrogeologic system is described such that "...pre-waste-emplacement groundwater travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment shall be at least 1,000 years...," [10 CFR 60.113(a)(2)]. The role of geochemical processes in performance assessment is described in 10 CFR 60.113(b)(3). Specifically, "The geochemical characteristics of the host rock, surrounding strata, and groundwater...,"[10 CFR 60.113(b)(3)] can be a factor that the Commission may take into account if it decides to "...approve or specify some other radionuclide release rate, designed containment period, or pre-waste-emplacement groundwater travel time...," [10 CFR 60.113(b)]. Such a decision is contingent on the satisfaction of the overall system performance objective (10 CFR 60.112) as it relates to anticipated processes and events. For unanticipated processes and events, it may be necessary to specify additional requirements to satisfy the overall performance objective [10 CFR 60.113(c)].

1.2 OVERALL REVIEW STRATEGY AND THE LICENSE APPLICATION REVIEW PLAN (LARP)

The general nature of the review strategies for the LA that will be followed by NRC are described in Overall Review Strategy for the Nuclear Regulatory Commission's High-Level Waste Repository Program (Johnson, 1993). Stated simply, upon receiving the LA from DOE, NRC will be charged with evaluating the application and making a recommendation as to whether or not to grant a license for construction of the HLW repository. As described in 10 CFR 60.31, the decision to authorize construction will be based on consideration of three factors:

- Reasonable risk to the health and safety of the public [10 CFR 60.31(a)]
- Non-inimicability to the common defense and security [10 CFR 60.31(b)]
- Protection of environmental values [10 CFR 60.31(c)]

The statutory time period mandated by the NWPA for review of the LA is 3 years, including only 18 months for NRC staff to review the LA and prepare its safety evaluation report (SER).

Because of the complex nature of the technical issues that are to be addressed in the LA and the relatively short review time mandated by the NWPA, NRC has developed guidance to help streamline the review process. One such guidance document is the Draft Regulatory Guide DG-3003: Format and Content for the License Application for the High-Level Waste Repository (FCRG) to indicate what NRC staff consider acceptable format and content for the LA.

Additionally, NRC is iteratively developing the LARP. The LARP consists of more than 90 individual review plans that provide guidance relevant to the review of procedural and technical requirements identified in 10 CFR Part 60. As described in the Draft License Application Review Plan for the Review of a License Application for a Geologic Repository for Spent Nuclear Fuel and High-Level Radioactive Waste, Yucca Mountain, Nevada (NRC, 1993), the LARP is comprised of three parts. Part A describes the overall review strategy. Part B consists of eight individual review plans developed for review of general information in the LA. The final section (Part C) contains all other individual review plans for the technical information required as a part of the SAR [10 CFR 60.21(c)].

The individual review plans contained in the LARP follow a standard format. The first part identifies the applicable parts of 10 CFR Part 60 (regulatory requirements). The second part consists of the Compliance Determination Strategies (CDSs) developed by NRC and Center for Nuclear Waste Regulatory Analyses (CNWRA) staff to assess the compliance of DOE with the applicable 10 CFR Part 60 regulatory requirements. The last two parts of the individual review plan contains the procedure and acceptance criteria to be used in evaluating DOE's demonstrations of compliance.

NRC and CNWRA staff have completed the initial development of the CDSs. To streamline the review process and assure that important issues associated with the regulatory requirements are given appropriate emphasis, the review strategies specify review types of varying complexity. The following definitions are from the Technical Operating Procedure (TOP) for CDS development (TOP-001-11):

- A Type 1 Acceptance Review is designed to determine if the LA is complete and acceptable for further compliance reviews. It is not designed to determine the adequacy of the data in the LA. This type of review is required in all of the individual review plans.

- A Type 2 Procedural Review is designed to determine the adequacy of the compliance demonstrations for the procedural requirements of 10 CFR Part 60.

- A Type 3 Safety Review is the first level of review of the compliance demonstrations and systems descriptions related to radiological health and safety or waste isolation. The focus of the review is on the contents of the LA itself and is not designed to require detailed independent analysis beyond the use of standard formula or simple "back-of-the-envelope" calculations.

The most detailed types of review (Type 4 and 5) are associated with key technical uncertainties (KTUs), which are those technical issues that the staff believes pose the highest risk of noncompliance with a performance objective of 10 CFR Part 60. All of the review plans requiring Type 4 and/or 5 reviews also require a Type 3 Safety Review.

- A Type 4 review requires the detailed review of selected information, supported by analyses performed by the technical staff using "...methods, developed by DOE or other parties, that have been reviewed and found acceptable by the staff." (Johnson, 1993).

- A Type 5 review is given the highest priority, and requires the application of methods and analyses independently developed by the technical staff to those technical issues considered to be the most difficult to resolve.

The compliance Review Types 2 through 5 all require some evaluation of the technical adequacy of DOE compliance demonstrations. For this reason, these types of review will all require significant technical expertise on the part of NRC and CNWRA staff. This may include general expertise in a relevant field such as hydrology or geochemistry, as well as knowledge of information that is site-specific to YM or related to the repository design. The type of expertise and information that will be necessary to evaluate the adequacy of the LA are described in the Compliance Determination Methods (CDMs).

NRC and CNWRA staff have begun development of the CDMs that will contain the review procedures and acceptance criteria to be used by NRC in determining the compliance of DOE's LA with the performance objectives given in 10 CFR Part 60. It is this part of the LARP review plans that deals

specifically with the technical criteria for siting a repository. As part of the LARP, 28 of the more than 90 individual review plans are related to issues in hydrology, geochemistry, and climatology/meteorology. A listing of the different geochemistry CDMs and the current schedule for their completion is given in Table 1-1. The schedule may be modified depending on the Proposed Program Approach (PPA) adopted by DOE, where site suitability evaluations will be submitted to NRC beginning in FY 1998.

Table 1-1. Compliance Determination Methods for Geochemistry System

CDM	Individual System	Review Type	Schedule
3.1.3—Description of Geochemical System	Geochemistry	Types 1 and 3	FY94
8.1.3—Performance Confirmation: Geochemistry	Geochemistry	Types 1 and 3	FY95
3.2.3.6—(PAC) Not Reducing Groundwater	Geochemistry	Types 1 and 3	FY95
3.2.3.3—(FAC) Mineral Assemblages	Geochemistry	Types 1, 3, 4	FY96
3.2.3.7—(PAC) Gaseous Radionuclide Movement	Geochemistry	Types 1, 3, 4	FY97
3.2.3.1—(FAC) Nature and Rates: Geochemical Processes	Geochemistry	Types 1, 3, 5	FY98
3.2.3.2—(FAC) Geochemical Conditions	Geochemistry	Types 1, 3, 4	FY99
3.2.3.4—(PAC) Groundwater Conditions and EBS	Geochemistry	Types 1, 3, 4, 5	FY00
3.2.3.5—(PAC) Geochemical Processes	Geochemistry	Types 1, 3, 4, 5	FY00

2 COMPLIANCE DETERMINATION METHODS DATA NEEDS, METHODS, AND ANALYSES

2.1 DATA NEEDS FOR DIFFERENT LEVELS OF COMPLIANCE REVIEW

An important part of CDM/LARP section development is inclusion of rationales for the different procedures and acceptance criteria which the LA must meet to adequately demonstrate compliance. To aid in developing these criteria and rationales, it is desirable that NRC and CNWRA staff identify as early as possible technical data that will be necessary for the timely review of the LA. For many of the individual review plans the staff has considered the issues relatively well understood and has assigned only a Type 1 Acceptance Review and a Type 3 Safety Review. For these review plans, the types of data necessary for an effective review should be relatively well understood and the review can be largely confined to evaluating the information presented in the LA.

Although a Type 3 Safety Review will rely on information provided with the LA, there are advantages to identifying data needs within the context of CDM development and establishing a database of site specific data to prepare NRC/CNWRA staff for reviewing the LA. By allowing staff to become familiar with existing data and DOE approaches well in advance of receiving the LA, the Safety Review would be performed efficiently. In addition, information that either is pre-existing or is gathered outside of the DOE program through state and federal (other than DOE and NRC) agencies, international programs, universities, and private companies may be very useful in developing an understanding of the hydrologic, geochemical, and meteorological systems present at YM. This understanding is important to determine the uncertainties and limitations of these data and the effect on the computations that use them.

For those review plans that require the more detailed analysis of a Type 4 or Type 5 review, it may be more difficult to identify all of the data needs at this point in time. It is possible, however, to identify potential approaches that may be adopted by DOE through documents like the Site Characterization Plan (e.g., U.S.Department of Energy, 1988a,c-e,g-h), and DOE study plans (e.g., U.S. Department of Energy, 1988b). In addition, the Total System Performance Assessments conducted by DOE (e.g., Barnard et al., 1992; Eslinger et al., 1993; Wilson et al., 1994) provide details on the types of information that are currently available, the likely focus of DOE site characterization, and the types of information DOE is likely to use in future performance assessments. In addition to data needs, it is important to identify computer codes that are either likely to be used by DOE (Type 4 Review) or even those codes that may provide an independent alternative to DOE codes (Type 5 Review).

For the purposes of developing the necessary background, it is possible to use current levels of understanding to identify broad types of data that will be needed to complete the compliance reviews of the LA in a timely manner. Many of the required data, such as site geology, precipitation, and hydrostratigraphy, are site-specific in nature. Given the recent initiation of site characterization activities at YM, while it is possible to make a preliminary identification of specific data sources, much of the data currently available is sparse. Presumably many of the gaps will be filled in through ongoing and future site characterization activities. For many of these other types of data, such as radionuclide thermodynamic data, there is little need to acquire site-specific data, and current data sources can be identified readily. Even in these cases, however, certain systems or parameters may be poorly characterized and subject to change as research proceeds and levels of understanding increase.

Table 2-1 is an attempt to identify the broad data needs for the different CDMs related to geochemistry. There are three types of data at this high level that are important to CDM development:

- Basic data, such as thermodynamic and kinetic rate data that are applicable to all systems. These are informational in nature and do not carry site-specific information. These data are typically kept in electronic databases (e.g., GEMBOCHS; U.S. Department of Energy, 1993b) and are not suited for GIS storage and display.

- Site specific data that are necessary to define boundary and initial conditions at YM such as mineral and water chemistry. These data are currently being generated as part of the YM site characterization, and will presumably become available in on-line DOE databases such as Automated Technical Data Tracking System (ATDTS) and the Technical Data Base (TDB) being developed by the Yucca Mountain Project Office (YMPO) (Harloe, 1993). These are the data that carry information in a geographic context and are most effectively stored and displayed in a GIS database.

- Design data that are necessary to define the effects of the repository itself such as repository design and man-made materials. Many of these design issues are in development and final design decisions have not yet been made. In addition, most of these data do not have a specific geographic context, and are not best displayed in a GIS format.

It is important to note that there are several areas of data overlap, and computer codes that may be used for more than one LARP section. As will be shown in Section 3, each LARP section may require a specific type of data such as sorption data, or colloid chemistry data that is unique to that particular issue. In most cases, however, data such as water chemistry data or thermodynamic data will be applicable in more than one section and these sections of the databases can be shared.

2.2 CODES, METHODS, AND ANALYSES

Much of the LA will be based on computer analyses. Many of these codes are complex and require significant knowledge on the part of the user to develop a conceptual model and identify appropriate boundary and initial conditions. To evaluate model results, the reviewer must be familiar with the assumptions and limitations of the models. For those KTUs that require confirmatory or independent review, the reviewer should also be familiar either with the computer code(s) used by DOE in the analysis, or similar types of codes. Much in the same way that early identification of data will enhance the review of the LA, there is an advantage in the early identification of methods and computer codes, and to the extent possible, exercising these codes. Table 2-2 is a preliminary effort to identify methods that are likely to be used by DOE and for those CDMs/LARP sections that require a Type 4 or 5 review, a tentative listing of existing codes that address these issues.

In many cases, due to the complexities of natural systems, expert elicitation will be necessary to provide key information that is unavailable by more direct means. In all cases, conceptual and mathematical models are likely to be required, even for those CDMs/LARP sections that do not have associated KTUs. Thorough evaluation of DOE submittals will require that the reviewer is familiar with the assumptions and approximations that are made in constructing the models. It is important to note that the computer codes that are listed are meant only as examples of the types of codes that currently exist. In most cases, DOE has not yet identified the code(s) that it will use for the different sections of the LA, and in some cases, the codes that will be used have not yet been developed.

Table 2-1. Broad data needs for Compliance Determination Methods in geochemistry individual system

CDM\Data Needs: GEOCHEMISTRY	Thermodynamic Data	Kinetic rate Data	Temperature	Site Data: Water Chemistry	Site Data: Mineral Chemistry	Site Data: Gas Chemistry	Man-Made Materials	Waste Characteristics /Inventory
3.1.3—Description of Geochemical System			X	X	X	X		
8.1.3—Performance Confirmation-Geochemistry			X	X	X	X	X	X
3.2.3.6—(PAC) Not Reducing Groundwater			X	X	X	X		
3.2.3.3—(FAC) Mineral Assemblages	X	X	X	X	X	X		
3.2.3.7—(PAC) Gaseous Radionuclide Movement	X	X	X	X	X	X	X	X
3.2.3.1—(FAC) Nature & Rates - Geochemistry	X	X	X	X	X	X		
3.2.3.2—(FAC) Geochemical Conditions	X	X	X	X	X	X	X	
3.2.3.4—(PAC) Groundwater Conditions and Engineered Barrier System	X	X	X	X	X	X	X	X
3.2.3.5—(PAC) Geochemical Processes	X	X	X	X	X	X		

Table 2-2. Codes, methods, and analyses for Compliance Determination Methods in the Geochemistry Individual System

CDM\Possible Methods: GEOCHEMISTRY	Expert Elicitation	Conceptual Models	Mathematical Models	Computer Codes (Types, examples)
3.1.3—Description of Geochemical System	X	X	X	Type 1 only — No KTUs
8.1.3—Performance Confirmation-Geochemistry	X	X	X	Type 1 and 3 — No KTUs
3.2.3.6—(PAC) Not Reducing Groundwater	X	X	X	Type 1 and 3 — No KTUs
3.2.3.3—(FAC) Mineral Assemblages	X	X	X	Geochemistry — EQ3/6 (LLNL); PHREEQE (USGS); MINTEQA2 (EPA)
3.2.3.7—(PAC) Gaseous Radionuclide Movement	X	X	X	Geochemistry — EQ3/6 (LLNL); PHREEQE (USGS); MINTEQA2 (EPA) Two Phase Flow — PORFLOW (ACRI/ CNWRA); VTOUGH (LLNL); TRACR3D (LANL)
3.2.3.1—(FAC) Nature & Rates - Geochemistry	X	X	X	Geochemistry — EQ3/6 (LLNL); PHREEQE (USGS)
3.2.3.2—(FAC) Geochemical Conditions	X	X	X	Geochemistry — EQ3/6 (LLNL); PHREEQE (USGS); MINTEQA2 (EPA)
3.2.3.4—(PAC) Groundwater Conditions and Engineered Barrier System	X	X	X	Geochemistry — EQ3/6 (LLNL); PHREEQE (USGS); MINTEQA2 (EPA); Waste Inventory — ORIGEN2 (SNL) Waste Package — TWITCH/MARIANA (CNWRA); PANDORA (LLNL); WAPPA (LLNL)
3.2.3.5—(PAC) Geochemical Processes	X	X	X	Geochemistry — EQ3/6 (LLNL); PHREEQE (USGS); MINTEQA2 (EPA)

3 SPECIFIC DATA NEEDS AND EXISTING DATA SOURCES

In the matrices discussed in Section 2, broad data needs were outlined for those sections of the LARP related to technical issues in geochemistry. While these matrices show areas of overlap and similarities in data needs between the different LARP sections, there is also interest in examining on the cells of these matrices in more detail to identify more specific data needs, existing data sources, and the status of these data in the GIS database being developed at CNWRA.

Tables 3-1 through 3-9 are an initial attempt to identify specific data needs and geochemical (and other) data that are *currently* available from the different DOE programs and from the general literature. Since site characterization at YM will continue until license submittal (and beyond), much of this information should be viewed as preliminary and subject to change. The tables will be expanded and updated as site characterization proceeds and additional data become available. In addition, although most of the data referenced in Section 3 have been selected from the peer-reviewed literature, many of the data sets that are identified precede the development of approved procedures and have not been collected under DOE Quality Assurance (QA). It is expected that much of this will change as DOE Studies and Activities, conducted under DOE QA procedures, progress and additional data become available. Under these conditions, either DOE will bring existing data under QA control, or new data generated under appropriate QA will supersede those data sources listed here.

The format of Tables 3-1 through 3-9 includes:

- Column 1 — Specific Data Needs: These are specific types of data that the analyst believes are necessary to addressing this issue in developing the CDM. These subdivisions are typically constrained by the CDS developed by NRC/CNWRA staff.

- Column 2—Data Source(s): These are the references for the data identified in Column 1. Although some references identify DOE Study Plans that are designed to provide these types of data, emphasis has been placed on those data that are known to exist currently. Additional data may be added or supersede the data given here as site characterization proceeds.

- Column 3—Data Obtained?: This column simply indicates whether or not the current data have been acquired by NRC/CNWRA. In the current version, this is usually "Yes" since most of the data sources identified by the staff were based on hardcopies or electronic copies in their possession. It is expected that as electronic reference databases come on line (e.g., ATDTS), data sources will be identified that exist in the DOE program, but have not been obtained.

- Column 4—Entered in GIS?: This column indicates whether data have been entered in an electronic form into the GIS ARC/INFO database. As discussed in Section 2, only some of these data have the geographic context appropriate for GIS format. At present, only two data sets have been entered in ARC/INFO under this task: (i) the compilation of saturated water chemistry of McKinley et al. (1991), and (ii) the mineral chemistry data of Broxton et al. (1986). Other coverages may be available as part of other research projects (e.g., Stirewalt et al., 1994).

- Column 5—QA Status: Most of the data identified have been generated and gathered outside of the QA program developed by DOE for the YM Project. Where no indication is made in the report of the QA status, a question mark is entered next to the agency or laboratory that produced the data. It is assumed that as data are developed under the DOE program, many of these uncertainties in QA status can be updated.

The final row under each broad data need gives a short summary of why the specific data types are important in evaluating these parts of the LA. This type of information is useful in developing rationale language for the CDM.

Table 3-1. LARP Section 3.1.3—Geochemical Systems Description (FY94)

Broad Data Need—Temperature	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Temperature Distribution (Pre-emplacement)	1. Bently et al. (1983)	Yes	No	?USGS
	2. Craig and Reed (1991)	Yes	No	?USGS
	3. Erickson and Waddell (1985)	Yes	No	?USGS
	4. Lahoud et al. (1984)	Yes	No	?USGS
	5. Rush et al. (1983)	Yes	No	?USGS
	6. Thordarson (1983)	Yes	No	?USGS
	7. Whitfield et al. (1985)	Yes	No	?USGS
	8. DOE (1988a)	Yes	No	DOE
All chemical reactions are affected by temperature meaning that mineral and waste solubilities, reaction rates are all dependent on temperature conditions. Data on the temperature distributions through space (depth and distance) are necessary to establish baseline conditions for performance assessment.				
Broad Data Need—Water Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS**	**QA Status**
1. Saturated Zone Waters	1. Bently et al., (1983)	Yes	No	?USGS
	2. Craig and Reed (1991)	Yes	No	?USGS
	3. Craig et al. (1983)	Yes	No	?USGS
	4. Lahoud et al. (1984)	Yes	No	?USGS
	5. Rush et al. (1983)	Yes	No	?USGS
	6. Thordarson (1983)	Yes	No	?USGS
	7. Whitfield et al. (1985)	Yes	No	?USGS
	8. Whitfield et al. (1990)	Yes	No	?USGS
	9. McKinley et al. (1991)	Yes	No	?USGS
	10. Kerrisk (1987)	Yes	Yes	?LANL
	11. White et al. (1980)	Yes	No	?USGS
	12. Claassen (1985)	Yes	No	?USGS
	13. DOE (1988b)	Yes	No	DOE
	14. DOE (1988c)	Yes	No	DOE
	15. DOE (1992a)	Yes	No	DOE
2. Unsaturated Zone Waters	1. Yang et al. (1988)	Yes	No	?USGS
	2. White et al. (1980)	Yes	No	?USGS
	3. Yang et al. (1993)	Yes	No	?USGS
	4. DOE (1990)	Yes	No	DOE
	5. Kerrisk (1983)	Yes	No	?LANL
A complete description of the geochemical system at YM must include data on the water chemistries present. Since both the saturated and unsaturated zones are part of the geologic setting, chemistry on both types of water needs to be provided. These data are required to predict the solubility of minerals and mobility and wastes in groundwater and/or gases passing through and around the repository.				

Table 3-1. LARP Section 3.1.3—Geochemical Systems Description (FY94) (Cont'd)

Broad Data Need—Mineral Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Primary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. DOE (1989)	Yes	No	DOE
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. DOE (1988d)	Yes	No	DOE
2. Secondary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. Broxton et al. (1986)	Yes	Yes	?LANL
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. Carlos (1987)	Yes	No	?LANL
	5. Carlos et al. (1990)	Yes	No	?LANL
	6. Carlos et al. (1991)	Yes	No	?LANL
	7. Bish (1989)	Yes	No	?LANL
	8. Carlos (1989)	Yes	No	?LANL
	9. Broxton et al. (1987)	Yes	No	?LANL
A complete description of the geochemical system must include the solid phases present in the system. These data are required to predict the mobility of any wastes that enter groundwater flowing through or around the repository. Many sorption models require information on mineralogy and mineral chemistry.				
Broad Data Need—Gas Chemistry	**Data Source(s)**	**Data Obtained**	**Entered in GIS**	**QA Status**
1. Gas partial pressures (Pre-waste Emplacement)	1. Thorstenson et al. (1989)	Yes	No	?USGS
	2. Weeks (1987)	Yes	No	?USGS
	3. DOE (1991a)	Yes	No	DOE
	4. DOE (1988e)	Yes	No	DOE
In the unsaturated zone at YM, a complete description of the geochemical system must include information on the gas phase. Gas-phase compositions can be sensitive to repository-related chemical perturbations of the geochemical system. Baseline knowledge of pre-repository conditions is necessary.				

Table 3-2. LARP Section 8.1.3—Performance Confirmation of the Geochemical System (FY96)

Broad Data Need—Temperature	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Temperature Distribution (Pre-emplacement)	1. Bently et al. (1983)	Yes	No	?USGS
	2. Craig and Reed (1991)	Yes	No	?USGS
	3. Erickson and Waddell (1985)	Yes	No	?USGS
	4. Lahoud et al. (1984)	Yes	No	?USGS
	5. Rush et al. (1983)	Yes	No	?USGS
	6. Thordarson (1983)	Yes	No	?USGS
	7. Whitfield et al. (1985)	Yes	No	?USGS
	8. DOE (1988a)	Yes	No	?DOE
2. Temperature Distribution (post-emplacement)	1. O'Neal et al. (1984)	Yes	No	?LLNL
	2. Buscheck and Nitao (1993a)	Yes	No	?LLNL
	3. Buscheck and Nitao (1993b)	Yes	No	?LLNL
	4. Buscheck and Nitao (1993c)	Yes	No	?LLNL
	5. Pruess and Tsang (1993)	Yes	No	?LBL
	6. Wilson et al. (1994)	Yes	No	?SNL
Adequate confirmation of performance of the geochemical systems in assuring compliance requires monitoring geochemical conditions at and around the repository. It is also desirable to have a thorough database on pre-construction geochemical conditions to serve as a baseline for comparison with performance confirmation data. Temperature is an important variable in geochemical characterization, largely due to its effects on both equilibrium conditions and kinetic rates. Furthermore, it is likely to be significantly affected by repository construction and operation.				
Broad Data Need—Site Data: Water Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Saturated Zone Waters	1. McKinley et al. (1991)	Yes	Yes	?USGS
	2. Kerrisk (1987)	Yes	No	?LANL
	3. White et al. (1980)	Yes	No	?USGS
	4. Claassen (1985)	Yes	No	?USGS
	5. DOE (1988b)	Yes	No	DOE
	6. DOE (1988c)	Yes	No	DOE
	7. DOE (1992a)	Yes	No	DOE
2. Unsaturated Zone Waters	1. Yang et al. (1988)	Yes	No	?USGS
	2. White et al. (1980)	Yes	No	?USGS
	3. Yang et al. (1993)	Yes	No	?USGS
	4. DOE (1990)	Yes	No	DOE
	5. Kerrisk (1983)	Yes	No	?LANL
Again, a pre-repository geochemical baseline is desirable. Water chemistry is clearly a crucial geochemical parameter for assessing repository performance, since aqueous transport is a major mode of release of radionuclides and other contaminants.				

Table 3-2. LARP Section 8.1.3—Performance Confirmation of the Geochemical System (FY96) (Cont'd)

Broad Data Need—Site Data: Mineral Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Primary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. DOE (1989)	Yes	No	DOE
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. DOE (1988d)	Yes	No	DOE
2. Secondary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. Broxton et al. (1986)	Yes	Yes	?LANL
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. Carlos (1987)	Yes	No	?LANL
	5. Carlos et al. (1990)	Yes	No	?LANL
	6. Carlos et al. (1991)	Yes	No	?LANL
	7. Bish (1989)	Yes	No	?LANL
	8. Carlos (1989)	Yes	No	?LANL
	9. Broxton et al. (1987)	Yes	No	?LANL
Geochemical characterization necessitates knowledge of mineral compositions for accurate interpretation of hydrochemical data.				
Broad Data Need—Site Data: Gas Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Gas partial pressures (Pre-waste Emplacement)	1. Thorstenson et al. (1989)	Yes	No	?USGS
	2. Weeks (1987)	Yes	No	?USGS
	3. DOE (1991a)	Yes	No	DOE
	4. DOE (1988e)	Yes	No	DOE
Gas-phase compositions can be sensitive to repository-related chemical perturbations of the geochemical system. Baseline knowledge of pre-repository conditions is necessary.				
Broad Data Need—Man-Made Materials	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Waste package design	1. DOE (1993a)	Yes	n/a	DOE
2. Test data on package performance	1. Zimmerman et al. (1986)	Yes	n/a	?SNL
	2. Ramirez et al. (1991)	Yes	n/a	?LLNL
	3. Sridhar et al. (1994)	Yes	n/a	CNWRA
3. Materials Inventory	1. West (1988)	No	n/a	?LANL
	2. Meike and Wittwer (1994a)	Yes	n/a	?LLNL
	3. Meike and Wittwer (1994b)	Yes	n/a	?LLNL
	4. Meike (1994)	Yes	n/a	?LLNL
Performance confirmation also requires knowledge of the effect of man-made materials on the geochemical barriers. The reviewer should be aware of the nature of those materials and their possible responses to repository conditions. This will require an ongoing familiarity with evolving DOE design plans.				

Table 3-2. LARP Section 8.1.3—Performance Confirmation of the Geochemical System (FY96) (Cont'd)

Broad Data Need—Waste Characteristics and Inventory	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Waste Stream	1. DOE (1988f) ("MPA") 2. Andress and McLeod (1988)	Yes Yes	n/a n/a	DOE ?ORNL
2. Repository Layout	1. DOE (1988g)	Yes	n/a	DOE
3. Radionuclide Inventory	1. DOE (1992b) ("CDB") 2. DOE (1991b) ("IDB")	Yes Yes	n/a n/a	DOE DOE
Again, knowledge of waste characteristics is essential to performance confirmation. These are also changeable and the reviewer must keep track of evolving DOE plans.				
Broad Data Need—Repository Design	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Repository Heating	1. O'Neal et al. (1984) 2. Buscheck and Nitao (1993a) 3. Buscheck and Nitao (1993b) 4. Buscheck and Nitao (1993c) 5. Pruess and Tsang (1993) 6. Wilson et al. (1994)	Yes Yes Yes Yes Yes Yes	No No No No No No	?LLNL ?LLNL ?LLNL ?LLNL ?LBL ?SNL
2. Water Infiltration	1. Wilson et al. (1994) 2. Dodge and Green (1994)	Yes Yes	No No	?SNL CNWRA
3. Source Term Models	1. Manaktala (1993) 2. Codell and Weller (1994) 3. Ahola et al. (1994) 4. Wilson et al. (1994)	Yes Yes Yes Yes	n/a n/a n/a n/a	CNWRA NRC CNWRA ?SNL
During the period of performance confirmation, thermal and hydrologic conditions in the repository may be significantly altered. An understanding of these potential effects is necessary for reviewing the performance confirmation program. The listed references are not intended to be complete, but should provide sufficient background; see also data and model needs for RRTs related to hydrology.				

Table 3-3. LARP Section 3.2.3.6—(PAC) Not Reducing Groundwater (FY95)

Broad Data Need—Temperature	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Temperature Distribution (Pre-emplacement)	1. Bently et al. (1983)	Yes	No	?USGS
	2. Craig and Reed (1991)	Yes	No	?USGS
	3. Erickson and Waddell (1985)	Yes	No	?USGS
	4. Lahoud et al. (1984)	Yes	No	?USGS
	5. Rush et al. (1983)	Yes	No	?USGS
	6. Thordarson (1983)	Yes	No	?USGS
	7. Whitfield et al. (1985)	Yes	No	?USGS
	8. DOE (1988a)	Yes	No	DOE
2. Temperature Distribution (post-emplacement)	1. O'Neal et al. (1984)	Yes	No	?LLNL
	2. Buscheck and Nitao (1993a)	Yes	No	?LLNL
	3. Buscheck and Nitao (1993b)	Yes	No	?LLNL
	4. Buscheck and Nitao (1993c)	Yes	No	?LLNL
	5. Pruess and Tsang (1993)	Yes	No	?LBL
	6. Wilson et al. (1994)	Yes	No	?SNL
Estimation of aqueous redox state involves thermodynamic consideration of chemical conditions; temperature is an important variable in such estimations.				
Broad Data Need—Site Data: Water Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Saturated Zone Waters	1. McKinley et al. (1991)	Yes	Yes	?USGS
	2. Kerrisk (1987)	Yes	No	?LANL
	3. White et al. (1980)	Yes	No	?USGS
	4. Claassen (1985)	Yes	No	?USGS
	5. DOE (1988b)	Yes	No	DOE
	6. DOE (1988c)	Yes	No	DOE
	7. DOE (1992a)	Yes	No	DOE
2. Unsaturated Zone Waters	1. Yang et al. (1988)	Yes	No	?USGS
	2. White et al. (1980)	Yes	No	?USGS
	3. Yang et al. (1993)	Yes	No	?USGS
	4. DOE (1990)	Yes	No	DOE
	5. Kerrisk (1983)	Yes	No	?LANL
Chemical data on groundwater samples from the site and environs are a primary source of information on the redox conditions in the water. Specific measurements of interest include Eh, oxidation states of multivalent elements such as Fe, and dissolved oxygen.				

Table 3-3. LARP Section 3.2.3.6—PAC) Not Reducing Groundwater (FY95) (Cont'd)

Broad Data Need—Site Data: Mineral Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Primary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. DOE (1989)	Yes	No	DOE
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. DOE (1988d)	Yes	No	DOE
2. Secondary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. Broxton et al. (1986)	Yes	Yes	?LANL
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. Carlos (1987)	Yes	No	?LANL
	5. Carlos et al. (1990)	Yes	No	?LANL
	6. Carlos et al. (1991)	Yes	No	?LANL
	7. Bish (1989)	Yes	No	?LANL
	8. Carlos (1989)	Yes	No	?LANL
	9. Broxton et al. (1987)	Yes	No	?LANL
Host rock minerals may exert an influence on water redox conditions, particularly in the saturated zone. Secondary minerals may also exert influence on the waters in contact with them. Furthermore, diagenetic mineralization is indicative of past and present water-rock interaction the nature of which is strongly dependent on the oxidizing potential of the waters.				
Broad Data Need—Site Data: Gas Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Gas partial pressures (Pre-waste Emplacement)	1. Thorstenson et al. (1989)	Yes	No	?USGS
	2. Weeks (1987)	Yes	No	?USGS
	3. DOE (1991a)	Yes	No	DOE
	4. DOE (1988e)	Yes	No	DOE
The composition of the gas phase in the unsaturated zone at YM has a strong influence on the redox conditions in the waters which "see" those gases. Most importantly, the presence of O_2 in the gas phase will greatly increase the likelihood that groundwaters are oxidizing.				

Table 3-4. LARP Section 3.2.3.3—(FAC) Mineral Assemblages (FY96)

Broad Data Need—Thermodynamic Data	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Aqueous Thermodynamic Data	1. EQ3/6 Database (Wolery, 1992) 2. GEMBOCHS (DOE, 1993b) 3. Aqueous Solutions Database (Phillips et al., 1988)	Yes No Yes	n/a n/a n/a	?LBL DOE ?LBL
2. Solid Thermodynamic Data	1. EQ3/6 Database (Wolery, 1992) 2. GEMBOCHS (DOE, 1993b) 3. Aqueous Solutions Database (Phillips et al., 1988) 4. Murphy and Pabalan (1994)	Yes No Yes Yes	n/a n/a n/a n/a	?LBL DOE ?LBL CNWRA
3. Batch Sorption Data	1. DOE (1988h) 2. Wilson et al. (1994) 3. Thomas (1987)	Yes Yes Yes	n/a n/a n/a	DOE ?SNL ?LANL
One of the KTUs related to this RRT is the mineralogic/chemical response of host rock to repository heating. Prediction of this response involves thermodynamic calculations of equilibrium states; these require an accurate, comprehensive, internally consistent database of values for thermodynamic variables. The other KTU concerns the effect of that response on the favorable radionuclide retardation characteristics of the assemblages.; thus, data on sorption characteristics of minerals of interest are essential for this RRT. Batch sorption studies are currently being used by DOE to determine K_D values for empirical radionuclide sorption models (e.g., DOE, 1988h). Although there are alternative, more mechanistic models for sorption, suitable radionuclide sorption data are relatively scarce, and only recently have uniform modeling approaches been developed to take advantage of their capabilities (Turner, 1993; Pabalan and Turner, 1994)				
Broad Data Need—Kinetic Rate Data	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Reaction Rates - Silicate Minerals	1. Murphy and Helgeson (1989) 2. Sverdrup (1990) 3. Dove (1994) 4. Murphy and Pabalan (1994)	Yes Yes Yes Yes	n/a n/a n/a n/a	? ? ? CNWRA
Calculations of thermodynamic equilibrium states do not completely describe the response of a system to differing thermochemical conditions. Persistence of nonequilibrium conditions is possible if reaction rates are slow; thus, information on kinetics is necessary for accurate prediction of host rock alteration.				

Table 3-4. LARP Section 3.2.3.3—(FC) Mineral Assemblages (FY96) (Cont'd)

Broad Data Need—Temperature	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Temperature Distribution (Pre-emplacement)	1. Bently et al. (1983)	Yes	No	?USGS
	2. Craig and Reed (1991)	Yes	No	?USGS
	3. Erickson and Waddell (1985)	Yes	No	?USGS
	4. Lahoud et al. (1984)	Yes	No	?USGS
	5. Rush et al. (1983)	Yes	No	?USGS
	6. Thordarson (1983)	Yes	No	?USGS
	7. Whitfield et al. (1985)	Yes	No	?USGS
	8. DOE (1988a)	Yes	No	DOE
Data on pre-repository temperature distributions are important to modeling of repository thermal effects.				
Broad Data Need—Site Data: Water Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Saturated Zone Waters	1. McKinley et al. (1991)	Yes	Yes	?USGS
	2. Kerrisk (1987)	Yes	No	?LANL
	3. White et al. (1980)	Yes	No	?USGS
	4. Claassen (1985)	Yes	No	?USGS
	5. DOE (1988b)	Yes	No	DOE
	6. DOE (1988c)	Yes	No	DOE
	7. DOE (1992a)	Yes	No	DOE
2. Unsaturated Zone Waters	1. Yang et al. (1988)	Yes	No	?USGS
	2. White et al. (1980)	Yes	No	?USGS
	3. Yang et al. (1993)	Yes	No	?USGS
	4. DOE (1990)	Yes	No	DOE
	5. Kerrisk (1983)	Yes	No	?LANL
Hydrochemistry will have a profound effect on mineral alteration processes around the repository and must be characterized for thermodynamic modeling. Furthermore, water chemistry has an effect on sorption behavior. Models require an adequate baseline of pre-repository water chemical conditions and variations.				
Broad Data Need—Site Data: Mineral Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Primary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. DOE (1989)	Yes	No	DOE
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. DOE (1988d)	Yes	No	DOE

Table 3-4. LARP Section 3.2.3.3—(FC) Mineral Assemblages (FY96) (Cont'd)

Broad Data Need—Site Data: Mineral Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
2. Secondary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. Broxton et al. (1986)	Yes	Yes	?LANL
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. Carlos (1987)	Yes	No	?LANL
	5. Carlos et al. (1990)	Yes	No	?LANL
	6. Carlos et al. (1991)	Yes	No	?LANL
	7. Bish (1989)	Yes	No	?LANL
	8. Carlos (1989)	Yes	No	?LANL
	9. Broxton et al. (1987)	Yes	No	?LANL
Thermodynamic modeling of alteration processes and prediction of sorption behavior require complete information on mineral phase chemical compositions.				
Broad Data Need—Site Data: Gas Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Gas partial pressures (Pre-waste Emplacement)	1. Thorstenson et al. (1989)	Yes	No	?USGS
	2. Weeks (1987)	Yes	No	?USGS
	3. DOE (1991a)	Yes	No	DOE
	4. DOE (1988e)	Yes	No	DOE
Modeling must also include vapor phase components. Current conditions must be characterized for accurate prediction of response to repository heating.				

Table 3-5. LARP Section 3.2.3.7—(PAC) Gaseous Radionuclide Movement

Broad Data Need—Thermodynamic Data	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Aqueous and Gaseous Thermodynamic Data	1. EQ3/6 Database (Wolery, 1992) 2. GEMBOCHS (DOE, 1993b) 3. Aqueous Solutions Database (Phillips et al., 1988)	Yes No Yes	n/a n/a n/a	?LBL DOE ?LBL
2. Solid Thermodynamic Data	1. EQ3/6 Database (Wolery, 1992) 2. GEMBOCHS (DOE, 1993B) 3. Aqueous Solutions Database (Phillips et al., 1988) 4. Murphy and Pabalan (1994)	Yes No Yes Yes	n/a n/a n/a n/a	?LBL DOE ?LBL CNWRA
One of the KTUs with which this RRT is concerned is the volatility and stability of chemical species of radionuclides. Thermodynamic data are necessary for the required detailed analysis of this issue through modeling, with the goal of identifying those radionuclides with gaseous species that pose a potential risk of noncompliance.				
Broad Data Need—Kinetic Rate Data	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Reaction Rates - Carbonate Minerals				
2. Reaction Rates - Silicate Minerals	1. Murphy and Helgeson (1989) 2. Sverdrup (1990) 3. Dove (1994) 4. Murphy and Pabalan (1994)	Yes Yes Yes Yes	n/a n/a n/a n/a	? ? ? CNWRA
Modeling of gaseous radionuclide species stability is incomplete if only thermodynamic equilibrium is assumed. Kinetic and metastability effects must be considered in the context of the geochemical environment (e.g., metastability of CH_4 in air). It is likely that equilibrium will reasonably be assumed for gas-aqueous interaction.				
Broad Data Need—Temperature	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Temperature Distribution (Pre-emplacement)	1. Bently et al. (1983) 2. Craig and Reed (1991) 3. Erickson and Waddell (1985) 4. Lahoud et al. (1984) 5. Rush et al. (1983) 6. Thordarson (1983) 7. Whitfield et al. (1985) 8. DOE (1988a)	Yes Yes Yes Yes Yes Yes Yes Yes	No No No No No No No No	?USGS ?USGS ?USGS ?USGS ?USGS ?USGS ?USGS DOE

Table 3-5. LARP Section 3.2.3.7—(PAC) Gaseous Radionuclide Movement (Cont'd)

Broad Data Need—Temperature	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
2. Temperature Distribution (post-emplacement)	1. O'Neal et al. (1984)	Yes	No	?LLNL
	2. Buscheck and Nitao (1993a)	Yes	No	?LLNL
	3. Buscheck and Nitao (1993b)	Yes	No	?LLNL
	4. Buscheck and Nitao (1993c)	Yes	No	?LLNL
	5. Pruess and Tsang (1993)	Yes	No	?LBL
	6. Wilson et al. (1994)	Yes	No	?SNL
Pre-repository temperature structure is necessary for accurate thermodynamic and transport calculations.				
Broad Data Need—Site Data: Water Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Saturated Zone Waters	1. McKinley et al. (1991)	Yes	Yes	?USGS
	2. Kerrisk (1987)	Yes	No	?LANL
	3. White et al. (1980)	Yes	No	?USGS
	4. Claassen (1985)	Yes	No	?USGS
	5. DOE (1988b)	Yes	No	DOE
	6. DOE (1988c)	Yes	No	DOE
	7. DOE (1992a)	Yes	No	DOE
2. Unsaturated Zone Waters	1. Yang et al. (1988)	Yes	No	?USGS
	2. White et al. (1980)	Yes	No	?USGS
	3. Yang et al. (1993)	Yes	No	?USGS
	4. DOE (1990)	Yes	No	DOE
	5. Kerrisk (1983)	Yes	No	?LANL
Water chemistry data are important for two reasons. First, they are necessary for thermodynamic calculation of stability of gaseous species in the unsaturated zone. Second, features of water chemistry (e.g., dissolved carbon) may be important in determining the retardation potential of the unsaturated zone.				
Broad Data Need—Site Data: Mineral Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Primary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. DOE (1989)	Yes	No	DOE
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. DOE (1988d)	Yes	No	DOE
2. Secondary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. Broxton et al. (1986)	Yes	Yes	?LANL
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. Carlos (1987)	Yes	No	?LANL
	5. Carlos et al. (1990)	Yes	No	?LANL
	6. Carlos et al. (1991)	Yes	No	?LANL
	7. Bish (1989)	Yes	No	?LANL
	8. Carlos (1989)	Yes	No	?LANL
	9. Broxton et al. (1987)	Yes	No	?LANL

Table 3-5. LARP Section 3.2.3.7—(PAC) Gaseous Radionuclide Movement (Cont'd)

Solid phase chemistry is essential to calculation of gaseous species stability and gaseous radionuclide retardation potential.

Broad Data Need—Site Data: Gas Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Gas partial pressures (Pre-waste Emplacement)	1. Thorstenson et al. (1989) 2. Weeks (1987) 3. DOE (1991a) 4. DOE (1988e)	Yes Yes Yes Yes	No No No No	?USGS ?USGS DOE DOE

Pre-repository data on gas-phase chemistry and pressure provides information on the stability and mobility of species which may be important for radionuclide transport. Data on ^{14}C distributions would be useful for constraining models of gas transport directions and rates.

Broad Data Need—Man-Made Materials	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Waste package design	1. DOE (1993a)	Yes	n/a	DOE
2. Test data on package performance	1. Zimmerman et al. (1986) 2. Ramirez et al. (1991) 3. Sridhar et al. (1994)	Yes Yes Yes	n/a n/a n/a	?SNL ?LLNL CNWRA
3. Materials Inventory	1. West (1988) 2. Meike and Wittwer (1994a) 3. Meike and Wittwer (1994b) 4. Meike (1994)	No Yes Yes Yes	n/a n/a n/a n/a	?LANL ?LLNL ?LLNL ?LLNL

Because retardation of gaseous transport may be affected by the materials present in the repository and the heat generated by the waste, evaluation of gaseous radionuclide transport requires knowledge of the effect of man-made materials. This will require an ongoing familiarity with evolving DOE design plans.

Broad Data Need—Waste Characteristics and Inventory	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Waste Stream	1. DOE (1988f) ("MPA") 2. Andress and McLeod (1988)	Yes Yes	n/a n/a	DOE ?ORNL
2. Repository Layout	1. DOE (1988g)	Yes	n/a	DOE
3. Radionuclide Inventory	1. DOE (1992b) ("CDB") 2. DOE (1991b) ("IDB")	Yes Yes	n/a n/a	DOE DOE

Again, knowledge of waste characteristics is essential to evaluating the potential for gaseous radionuclide transport. These are also changeable and the reviewer must keep track of evolving DOE plans.

Table 3-5. LARP Section 3.2.3.7—(PAC) Gaseous Radionuclide Movement (Cont'd)

Broad Data Need: Repository Design	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Repository Heating	1. O'Neal et al. (1984)	Yes	No	?LLNL
	2. Buscheck and Nitao (1993a)	Yes	No	?LLNL
	3. Buscheck and Nitao (1993b)	Yes	No	?LLNL
	4. Buscheck and Nitao (1993c)	Yes	No	?LLNL
	5. Pruess and Tsang (1993)	Yes	No	?LBL
	6. Wilson et al. (1994)	Yes	No	?SNL
2. Source Term Models	1. Manaktala (1993)	Yes	n/a	CNWRA
	2. Codell and Weller (1994)	Yes	n/a	NRC
	3. Ahola et al. (1994)	Yes	n/a	CNWRA
	4. Wilson et al. (1994)	Yes	n/a	?SNL
Geochemical and hydrologic conditions are likely to be significantly altered by the heat generated by the repository. An understanding of potential temperature effects is necessary for reviewing the potential for gaseous radionuclide transport.				

Table 3-6. LARP Section 3.2.3.1—(FAC) Nature and Rates of Geochemical Processes (FY98)

Broad Data Need—Thermodynamic Data	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Aqueous and Gaseous Thermodynamic Data	1. EQ3/6 Database (Wolery, 1992)	Yes	n/a	?LBL
	2. GEMBOCHS (DOE, 1993b)	No	n/a	DOE
	3. Aqueous Solutions Database (Phillips et al., 1988)	Yes	na/	?LBL
2. Solid Thermodynamic Data	1. EQ3/6 Database (Wolery, 1992)	Yes	n/a	?LBL
	2. GEMBOCHS (DOE, 1993b)	No	n/a	DOE
	3. Aqueous Solutions Database (Phillips et al., 1988)	Yes	n/a	?LBL
	4. Murphy and Pabalan (1994)	Yes	n/a	CNWRA
Thermodynamic data on the various phases involved in geochemical processes are of critical interest in discussions on the nature and rates of these processes.				
Broad Data Need—Kinetic Rate Data	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Reaction Rates-Silicate Minerals	1. Murphy and Helgeson (1989)	Yes	n/a	?
	2. Sverdrup (1990)	Yes	n/a	?
	3. Dove (1994)	Yes	n/a	?
	4. Murphy and Pabalan (1994)	Yes	n/a	CNWRA
Kinetic rate data is necessary for determining the stability of waste forms such as spent fuel and synthetic glasses, as well as natural mineral phases that may be important in radionuclide transport. Minerals that are thermodynamically out of equilibrium with a given system may still be metastable for significant times if the reaction(s) governing its dissolution are kinetically inhibited. In a similar fashion, precipitation of mineral phases may be inhibited unless the aqueous phase is supersaturated by orders of magnitude.				
Broad Data Need—Temperature	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Temperature Distribution (Pre-emplacement)	1. Bently et al. (1983)	Yes	No	?USGS
	2. Craig and Reed (1991)	Yes	No	?USGS
	3. Erickson and Waddell (1985)	Yes	No	?USGS
	4. Lahoud et al. (1984)	Yes	No	?USGS
	5. Rush et al. (1983)	Yes	No	?USGS
	6. Thordarson (1983)	Yes	No	?USGS
	7. Whitfield et al. (1985)	Yes	No	?USGS
	8. DOE (1988a)	Yes	No	DOE
2. Temperature Distribution (post-emplacement)	1. O'Neal et al. (1984)	Yes	No	?LLNL
	2. Buscheck and Nitao (1993a)	Yes	No	?LLNL
	3. Buscheck and Nitao (1993b)	Yes	No	?LLNL
	4. Buscheck and Nitao (1993c)	Yes	No	?LLNL
	5. Pruess and Tsang (1993)	Yes	No	?LBL
	6. Wilson et al. (1994)	Yes	No	?SNL

Table 3-6. LARP Section 3.2.3.1—(FC) Nature and Rates of Geochemical Processes (FY98) (Cont'd)

All chemical reactions are sensitive to the effects of temperature. The current repository design calls for the emplacement while heat is still being generated by the waste. The overall temperature distribution through space and time is subject to many design issues such as waste burnup history, the age of the waste, and the distribution of the waste packages (thermal loading) planned for the repository.

Broad Data Need—Site Data: Water Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Saturated Zone Waters	1. McKinley et al. (1991)	Yes	Yes	?USGS
	2. Kerrisk (1987)	Yes	No	?LANL
	3. White et al. (1980)	Yes	No	?USGS
	4. Claassen (1985)	Yes	No	?USGS
	5. DOE (1988b)	Yes	No	DOE
	6. DOE (1988c)	Yes	No	DOE
	7. DOE (1992a)	Yes	No	DOE
2. Unsaturated Zone Waters	1. Yang et al. (1988)	Yes	No	?USGS
	2. White et al. (1980)	Yes	No	?USGS
	3. Yang et al. (1993)	Yes	No	?USGS
	4. DOE (1990)	Yes	No	DOE
	5. Kerrisk (1983)	Yes	No	?LANL

The most likely path for the transport of radionuclides from the repository to the accessible environment will be as dissolved constituents in groundwater or as a gaseous phase (i.e. ^{14}C in CO_2). Waste package stability, waste form degradation, radioelement solubility and radionuclide transport are all dependent on the chemistry of the water. In natural systems such as at YM, interactions between the gas, water, and solid phases control the water chemistry. At YM, the location of the repository in the hydrologically unsaturated zone requires additional information on these groundwaters. Saturated zone water compositions are necessary due to the inclusion of the saturated zone in transporting radionuclides to the accessible environment.

Broad Data Need—Site Data: Mineral Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Primary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. DOE (1989)	Yes	No	DOE
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. DOE (1988d)	Yes	No	DOE
2. Secondary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. Broxton et al. (1986)	Yes	Yes	?LANL
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. Carlos (1987)	Yes	No	?LANL
	5. Carlos et al. (1990)	Yes	No	?LANL
	6. Carlos et al. (1991)	Yes	No	?LANL
	7. Bish (1989)	Yes	No	?LANL
	8. Carlos (1989)	Yes	No	?LANL
	9. Broxton et al. (1987)	Yes	No	?LANL

Table 3-6. LARP Section 3.2.3.1—(FC) Nature and Rates of Geochemical Processes (FY98) (Cont'd)

Like water chemistry, radionuclide transport is a function of the mineral chemistry in both the fractures and matrix at YM. Both primary and secondary minerals may play a role in processes such as controlling the water chemistry (e.g., buffering reactions), radionuclide retardation through sorption, ion exchange, and precipitation dissolution. In addition, thermal, mechanical, and hydrological properties of the rock will depend, at least to some extent, on the constituent minerals.

Broad Data Need—Site Data: Gas Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Gas partial pressures (Pre-waste Emplacement)	1. Thorstenson et al. (1989)	Yes	No	?USGS
	2. Weeks (1987)	Yes	No	?USGS
	3. DOE (1991a)	Yes	No	DOE
	4. DOE (1988e)	Yes	No	DOE

Partial pressures of gases, particularly CO_2, can have an effect on both the chemistry of the waters at the site and the stability of the different minerals that make up the host units for the repository. There is also the possibility of the transport of certain radioelements such as ^{129}I and ^{14}C in the gaseous phase.

Table 3-7. LARP Section 3.2.3.2—(FAC) Geochemical Conditions (FY99)

Broad Data Need—Thermodynamic Data	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Aqueous and Gaseous Thermodynamic Data	1. EQ3/6 Database (Wolery, 1992) 2. GEMBOCHS (DOE, 1993b) 3. Aqueous Solutions Database (Phillips et al., 1988)	Yes No Yes	n/a n/a n/a	?LBL DOE ?LBL
2. Solid Thermodynamic Data	1. EQ3/6 Database (Wolery, 1992) 2. GEMBOCHS (DOE, 1993b) 3. Aqueous Solutions Database (Phillips et al., 1988) 4. Murphy and Pabalan (1994)	Yes No Yes Yes	n/a n/a n/a n/a	?LBL DOE ?LBL CNWRA
Thermodynamic data on the various phases involved in geochemical processes are of critical interest in discussions on the transport of radionuclides from the repository to the accessible environment.				
Broad Data Need—Kinetic Rate Data	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Reaction Rates-Silicate Minerals	1. Murphy and Helgeson (1989) 2. Sverdrup (1990) 3. Dove (1994) 4. Murphy and Pabalan (1994)	Yes Yes Yes Yes	n/a n/a n/a n/a	? ? ? CNWRA
RRT 3.2.3.2 is concerned with favorable conditions that may retard the transport of radioelements from the repository to the accessible environment. In this respect, kinetic rate data are necessary for determining the stability of natural phases that may be important in radionuclide transport. Sorptive (or nonsorptive) minerals that are thermodynamically out of equilibrium with a given system may still be metastable for significant times if the reaction(s) governing its dissolution are slow. In a similar fashion, precipitation processes that either exhibit strong sorption for radionuclides, or sequester radioelements through precipitation and coprecipitation of radionuclide bearing phases may be inhibited unless the aqueous phase is supersaturated with respect to the solid by orders of magnitude.				
Broad Data Need—Temperature	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Temperature Distribution (Pre-emplacement)	1. Bently et al. (1983) 2. Craig and Reed (1991) 3. Erickson and Waddell (1985) 4. Lahoud et al. (1984) 5. Rush et al. (1983) 6. Thordarson (1983) 7. Whitfield et al. (1985) 8. DOE (1988a)	Yes Yes Yes Yes Yes Yes Yes Yes	No No No No No No No No	?USGS ?USGS ?USGS ?USGS ?USGS ?USGS ?USGS DOE

Table 3-7. LARP Section 3.2.3.2—(FC) Geochemical Conditions (FY99) (Cont'd)

Broad Data Need—Temperature	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
2. Temperature Distributions (post-emplacement)	1. O'Neal et al. (1984)	Yes	No	?LLNL
	2. Buscheck and Nitao (1993a)	Yes	No	?LLNL
	3. Buscheck and Nitao (1993b)	Yes	No	?LLNL
	4. Buscheck and Nitao (1993c)	Yes	No	?LLNL
	5. Pruess and Tsang (1993)	Yes	No	?LBL
	6. Wilson et al. (1994)	Yes	No	?SNL
All chemical reactions are sensitive to the effects of temperature. The current repository design calls for emplacement while substantial heat is still being generated by the waste. The overall temperature distribution through space and time is subject to many design issues such as waste burnup history, the age of the waste, and the distribution of the waste packages (thermal loading) planned for the repository that have not been settled on in final form.				
Broad Data Need—Site Data: Water Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Saturated Zone Waters	1. McKinley et al. (1991)	Yes	Yes	?USGS
	2. Kerrisk (1987)	Yes	No	?LANL
	3. White et al. (1980)	Yes	No	?USGS
	4. Claassen (1985)	Yes	No	?USGS
	5. DOE (1988b)	Yes	No	DOE
	6. DOE (1988c)	Yes	No	DOE
	7. DOE (1992a)	Yes	No	DOE
2. Unsaturated Zone Waters	1. Yang et al. (1988)	Yes	No	?USGS
	2. White et al. (1980)	Yes	No	?USGS
	3. Yang et al. (1993)	Yes	No	?USGS
	4. DOE (1990)	Yes	No	DOE
	5. Kerrisk (1983)	Yes	No	?LANL
3. Colloid Chemistry	1. Buddemeir and Hunt (1988)	Yes	No	?
	2. Kerrisk (1987)	Yes	No	?LANL
	3. Kingston and Whitbeck (1991)	Yes	No	?DRI
The most likely path for the transport of radionuclides from the repository to the accessible environment will be as dissolved constituents in groundwater or as a gas phase (i.e. ^{14}C in CO_2). Radionuclide transport is known to be dependent on the chemistry of the water. In natural systems such as at YM, interactions between the gas, water, and solid phases control the water chemistry. At YM, the location of the repository in the hydrologically unsaturated zone requires additional information on these groundwaters. Saturated zone water compositions are necessary due to the inclusion of the saturated zone in transporting radionuclides to the accessible environment.				

Table 3-7. LARP Section 3.2.3.2—(FC) Geochemical Conditions (FY99) (Cont'd)

Broad Data Need—Site Data: Mineral Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Primary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. DOE (1989)	Yes	No	DOE
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. DOE (1988d)	Yes	No	DOE
2. Secondary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. Broxton et al. (1986)	Yes	Yes	?LANL
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. Carlos (1987)	Yes	No	?LANL
	5. Carlos et al. (1990)	Yes	No	?LANL
	6. Carlos et al. (1991)	Yes	No	?LANL
	7. Bish (1989)	Yes	No	?LANL
	8. Carlos (1989)	Yes	No	?LANL
	9. Broxton et al. (1987)	Yes	No	?LANL
3. Batch Sorption Data	1. DOE (1988h)	Yes	n/a	DOE
	2. Wilson et al. (1994)	Yes	n/a	?SNL
	3. Thomas (1987)	Yes	n/a	?LANL
Like water chemistry, radionuclide transport is a function of the mineral chemistry in both the fractures and matrix at YM. Both primary and secondary minerals may play a role in processes such as controlling the water chemistry (e.g., buffering reactions), radionuclide retardation through sorption, ion exchange, and precipitation/dissolution.				
Broad Data Need—Site Data: Gas Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Gas partial pressures (Pre-waste Emplacement)	1. Thorstenson et al. (1989)	Yes	No	?USGS
	2. Weeks (1987)	Yes	No	?USGS
	3. DOE (1991a)	Yes	No	DOE
	4. DOE (1988e)	Yes	No	DOE
Partial pressures of gases, particularly CO_2, can have an effect on both the chemistry of the waters at the site and the stability of the different minerals that make up the host units for the repository. There is also the possibility of the transport of certain radioelements such as ^{129}I and ^{14}C in the gaseous phase.				
Broad Data Need—Site Data: Man-Made Materials	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Waste package design	1. DOE (1993a)	Yes	n/a	DOE
2. Test data on package performance	1. Zimmerman et al. (1986)	Yes	n/a	?SNL
	2. Ramirez et al. (1991)	Yes	n/a	?LLNL
	3. Sridhar et al. (1994)	Yes	n/a	CNWRA

Table 3-7. LARP Section 3.2.3.2—(FC) Geochemical Conditions (FY99) (Cont'd)

Broad Data Need—Site Data: Man-Made Materials	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
3. Materials Inventory	1. West (1988) 2. Meike and Wittwer (1994a) 3. Meike and Wittwer (1994b) 4. Meike (1994)	No Yes Yes Yes	n/a n/a n/a n/a	?LANL ?LLNL ?LLNL ?LLNL
Introduced materials such as cements, organic drilling fluids, resins, and metals may have a significant effect on the performance of the geologic setting, especially with regard to radionuclide transport. These effects may include the generation of colloids, elevated pH, organic chelation, and localized oxidation/reduction.				

Table 3-8. LARP Section 3.2.3.4—(PAC) Groundwater Conditions and the Engineered Barrier System (FY00)

Broad Data Need—Thermodynamic Data	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Aqueous and Gaseous Thermodynamic Data	1. EQ3/6 Database (Wolery, 1992) 2. GEMBOCHS (DOE, 1993b) 3. Aqueous Solutions Database (Phillips et al., 1988)	Yes No Yes	n/a n/a n/a	?LBL DOE ?LBL
2. Solid Thermodynamic Data	1. EQ3/6 Database (Wolery, 1992) 2. GEMBOCHS (DOE, 1993b) 3. Aqueous Solutions Database (Phillips et al., 1988) 4. Murphy and Pabalan (1994)	Yes No Yes Yes	n/a n/a n/a n/a	?LBL DOE ?LBL CNWRA
Thermodynamic data on the various phases involved in geochemical processes are of critical interest in discussions on the stability of the waste package containers, the alteration of the waste form, and the solubility and retardation of radionuclides in the engineered barrier system (EBS).				
Broad Data Need—Kinetic Rate Data	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Reaction Rates-Silicate Minerals	1. Murphy and Helgeson (1989) 2. Sverdrup (1990) 3. Dove (1994) 4. Murphy and Pabalan (1994)	Yes Yes Yes Yes	n/a n/a n/a n/a	? ? ? CNWRA
2. Corrosion processes and Corrosion Rates for Waste Package Materials	1. Stahl and Miller (1986) 2. Stephens et al. (1986) 3. O'Connell (1990)	Yes Yes Yes	n/a n/a n/a	? ? DOE
3. Spent Fuel dissolution	1. Forsyth and Werme (1992) 2. Wronkiewicz et al. (1992) 3. Wilson (1990a) 4. Wilson (1990b) 5. Veleckis and Ho (1991)	Yes Yes Yes Yes Yes	n/a n/a n/a n/a n/a	?Swedish DOE DOE DOE DOE
4. Glass dissolution	1. Bates et al. (1992) 2. Buck et al. (1993) 3. Ebert and Bates (1992)	Yes Yes Yes	n/a n/a n/a	DOE DOE DOE
RRT 3.2.3.4 is concerned with potentially adverse conditions that may have a deleterious effect on the ability of the EBS to effectively isolate waste from the groundwater and prevent radionuclide release to the geologic setting. In this respect, kinetic rate data is necessary for determining the stability of the waste packages (metal corrosion), the waste forms (glass, spent fuel), and natural phases that may be important in retarding radionuclide transport. In addition, the precipitation/dissolution of primary and secondary phases will control, to a large extent, the groundwater chemistry in the immediate vicinity of the waste package.				

Table 3-8. LARP Section 3.2.3.4—(PAC) Groundwater Conditions and the Engineered Barrier System (FY00) (Cont'd)

Broad Data Need—Temperature	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Temperature Distribution (Pre-emplacement)	1. Bently et al. (1983)	Yes	No	?USGS
	2. Craig and Reed (1991)	Yes	No	?USGS
	3. Erickson and Waddell (1985)	Yes	No	?USGS
	4. Lahoud et al. (1984)	Yes	No	?USGS
	5. Rush et al. (1983)	Yes	No	?USGS
	6. Thordarson (1983)	Yes	No	?USGS
	7. Whitfield et al. (1985)	Yes	No	?USGS
	8. DOE (1988a)	Yes	No	DOE
2. Temperature Distributions (post-emplacement)	1. O'Neal et al. (1984)	Yes	No	?LLNL
	2. Buscheck and Nitao (1993a)	Yes	No	?LLNL
	3. Buscheck and Nitao (1993b)	Yes	No	?LLNL
	4. Buscheck and Nitao (1993c)	Yes	No	?LLNL
	5. Pruess and Tsang (1993)	Yes	No	?LBL
	6. Wilson et al. (1994)	Yes	No	?SNL
All chemical reactions are sensitive to the effects of temperature. The current repository design calls for the emplacement while heat is still being generated by the waste. The overall temperature distribution through space and time is subject to many design issues such as waste burnup history, the age of the waste, and the distribution of the waste packages (thermal loading) planned for the repository that have not been settled on in final form. The effects of temperature will be especially pronounced in the EBS and in the near-field, where the thermal effects of the waste are likely to be the most pronounced. In this region, the interactions between groundwater and the waste package will be significantly influenced by temperature.				
Broad Data Need—Site Data: Water Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Saturated Zone Waters	1. McKinley et al. (1991)	Yes	Yes	?USGS
	2. Kerrisk (1987)	Yes	No	?LANL
	3. White et al. (1980)	Yes	No	?USGS
	4. Claassen (1985)	Yes	No	?USGS
	5. DOE (1988b)	Yes	No	DOE
	6. DOE (1988c)	Yes	No	DOE
	7. DOE (1992a)	Yes	No	DOE
2. Unsaturated Zone Waters	1. Yang et al. (1988)	Yes	No	?USGS
	2. White et al. (1980)	Yes	No	?USGS
	3. Yang et al. (1993)	Yes	No	?USGS
	4. DOE (1990)	Yes	No	DOE
	5. Kerrisk (1983)	Yes	No	?LANL

Table 3-8. LARP Section 3.2.3.4—(PAC) Groundwater Conditions and the Engineered Barrier System (FY00) (Cont'd)

The corrosion of the waste package is controlled by the interaction of groundwater with the waste package material. In addition, once the waste package has failed, the groundwater chemistry will control the rate of dissolution of the waste form, the release of radionuclides, and their sorption in and near the EBS. Through interactions between the EBS (waste packages, waste forms, backfill, etc) and the local environments at elevated temperatures, the chemistry of the groundwaters in the EBS and in the near-field is likely to be significantly different from the far-field groundwaters measured during site characterization. Nevertheless, current groundwater compositions are a necessary starting point in modeling these interactions and predicting their effects on the performance of the EBS.

Broad Data Need—Site Data: Mineral Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Primary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. DOE (1989)	Yes	No	DOE
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. DOE (1988d)	Yes	No	DOE
2. Secondary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. Broxton et al. (1986)	Yes	Yes	?LANL
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. Carlos (1987)	Yes	No	?LANL
	5. Carlos et al. (1990)	Yes	No	?LANL
	6. Carlos et al. (1991)	Yes	No	?LANL
	7. Bish (1989)	Yes	No	?LANL
	8. Carlos (1989)	Yes	No	?LANL
	9. Broxton et al. (1987)	Yes	No	?LANL
3. Batch Sorption Data	1. DOE (1988h)	Yes	n/a	DOE
	2. Wilson et al. (1994)	Yes	n/a	?SNL
	3. Thomas (1987)	Yes	n/a	?LANL

Mineral chemistry will have a significant effect on the chemical evolution of groundwaters near and within the EBS. Both primary and secondary minerals may play a role in controlling water chemistry (e.g., buffering), and radionuclide retardation through sorption, ion exchange, and precipitation/dissolution.

Broad Data Need—Site Data: Gas Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Partial Gas Pressures/ Pre-Waste Emplacement	1. Thorstenson et al. (1989)	Yes	No	?USGS
	2. Weeks (1987)	Yes	No	?USGS
	3. DOE (1991a)	Yes	No	DOE
	4. DOE (1988e)	Yes	No	DOE

Partial pressures of gases, particularly CO_2, can affect both the chemistry of the waters and the stability of the different minerals of the host units. It is also possible that the presence of gases such as CO_2 will lead to the formation of salts (e.g., Na_2CO_3) that may adversely affect the performance of the EBS. There is also the possibility of the transport of certain radioelements such as ^{129}I and ^{14}C in the gaseous phase.

Table 3-8. LARP Section 3.2.3.4—(PAC) Groundwater Conditions and the Engineered Barrier System (FY00) (Cont'd)

Broad Data Need—Site Data: Man-Made Materials	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Waste Package Design	1. DOE (1993a)	Yes	n/a	DOE
2. Test Data on Package Performance	1. Zimmerman et al. (1986) 2. Ramirez et al. (1991) 3. Sridhar et al. (1994)	Yes Yes Yes	n/a n/a n/a	?SNL ?LLNL CNWRA
3. Materials Inventory	1. West (1988) 2. Meike and Wittwer (1994a) 3. Meike and Wittwer (1994b) 4. Meike (1994)	No Yes Yes Yes	n/a n/a n/a n/a	?LANL ?LLNL ?LLNL ?LLNL
Introduced materials such as cements, drilling fluids, resins, and metals may have a significant effect on EBS performance, especially with regard to radionuclide transport. These effects may include modifying system water chemistry, the generation of colloids, elevated pH, organic chelation, and localized oxidation/reduction.				
Broad Data Need—Waste Characteristics/Inventory	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Waste Stream	1. DOE (1988f) ("MPA") 2. Andress and McLeod (1988)	Yes Yes	n/a n/a	DOE ?ORNL
2. Repository Layout	1. DOE (1988g)	Yes	n/a	DOE
3. Radionuclide Inventory	1. DOE (1992b) ("CDB") 2. DOE (1991b) ("IDB")	Yes Yes	n/a n/a	DOE DOE
Again, knowledge of waste characteristics is essential to modeling the performance of the EBS. This will help to determine what processes are important to controlling radionuclide releases from the EBS to the geologic setting. These are also changeable and the reviewer must keep track of evolving DOE plans.				

Table 3-9. LARP Section 3.2.3.5—(PAC) Geochemical Processes (FY00)

Broad Data Need—Thermodynamic Data	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Aqueous and Gaseous Thermodynamic Data	1. EQ3/6 Database (Wolery, 1992) 2. GEMBOCHS (DOE, 1993b) 3. Aqueous Solutions Database (Phillips et al., 1988)	Yes No Yes	n/a n/a n/a	?LBL DOE ?LBL
2. Solid Thermodynamic Data	1. EQ3/6 Database (Wolery, 1992) 2. GEMBOCHS (DOE, 1993b) 3. Aqueous Solutions Database (Phillips et al., 1988) 4. Murphy and Pabalan (1994)	Yes No Yes Yes	n/a n/a n/a n/a	?LBL DOE ?LBL CNWRA
Thermodynamic data on the various phases involved in geochemical processes are of critical interest in discussions on the potential adverse effects on radionuclide sorption, degradation in rock strength, or the performance of the Engineered Barrier System (EBS).				
Broad Data Need—Kinetic Rate Data	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Reaction Rates-Silicate Minerals	1. Murphy and Helgeson (1989) 2. Sverdrup (1990) 3. Dove (1994) 4. Murphy and Pabalan (1994)	Yes Yes Yes Yes	n/a n/a n/a n/a	? ? ? CNWRA
2. Corrosion Processes and Corrosion Rates for Waste Package Materials	1. Stahl and Miller (1986) 2. Stephens et al. (1986) 3. O'Connell (1990)	Yes Yes Yes	n/a n/a n/a	? ? DOE
3. Spent Fuel Dissolution	1. Forsyth and Werme (1992) 2. Wronkiewicz et al. (1992) 3. Wilson (1990a) 4. Wilson (1990b) 5. Veleckis and Ho (1991)	Yes Yes Yes Yes Yes	n/a n/a n/a n/a n/a	?Swedish DOE DOE DOE DOE
4. Glass Dissolution	1. Bates et al. (1992) 2. Buck et al. (1993) 3. Ebert and Bates (1992)	Yes Yes Yes	n/a n/a n/a	DOE DOE DOE

Table 3-9. LARP Section 3.2.3.5—(PAC) Geochemical Processes (FY00) (Cont'd)

RRT 3.2.3.5 is concerned with potentially adverse conditions that may have a deleterious effect on the ability of the geologic setting to retard radionuclide transport, a degradation of rock strength, or the ability of the EBS to effectively isolate waste. In this respect, kinetic rate data is necessary for determining the stability of natural phases that may be important in radionuclide transport. Sorptive (or nonsorptive) minerals that are thermodynamically out of equilibrium with a given system may still be metastable for significant times if the reaction(s) governing its dissolution are kinetically inhibited. In a similar fashion, precipitation processes that either exhibit strong sorption for radionuclides, or sequester radioelements through precipitation and coprecipitation of radionuclide bearing phases are likely to be controlled by reaction rates. Kinetic rate data is also necessary for determining whether or not alteration of the rock to a given suite of secondary minerals will result in a degradation of the overall rock strength. Finally, the stability of the waste packages (metal corrosion), the waste forms (glass, spent fuel), and natural phases that may be important in retarding radionuclide transport are all measures of the performance of the EBS for waste isolation.

Broad Data Need—Temperature	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Temperature Distribution (Pre-emplacement)	1. Bently et al. (1983)	Yes	No	?USGS
	2. Craig and Reed (1991)	Yes	No	?USGS
	3. Erickson and Waddell (1985)	Yes	No	?USGS
	4. Lahoud et al. (1984)	Yes	No	?USGS
	5. Rush et al. (1983)	Yes	No	?USGS
	6. Thordarson (1983)	Yes	No	?USGS
	7. Whitfield et al. (1985)	Yes	No	?USGS
	8. DOE (1988a)	Yes	No	DOE
2. Temperature Distributions	1. O'Neal et al. (1984)	Yes	No	?LLNL
	2. Buscheck and Nitao (1993a)	Yes	No	?LLNL
	3. Buscheck and Nitao (1993b)	Yes	No	?LLNL
	4. Buscheck and Nitao (1993c)	Yes	No	?LLNL
	5. Pruess and Tsang (1993)	Yes	No	?LBL
	6. Wilson et al. (1994)	Yes	No	?SNL

All chemical reactions are sensitive to the effects of temperature. This includes chemical processes that may have adverse effects on radionuclide sorption, degradation in rock strength, or the performance of the EBS. The current repository design calls for the emplacement while heat is still being generated by the waste. The overall temperature distribution through space and time is subject to many design issues such as waste burnup history, the age of the waste, and the distribution of the waste packages (thermal loading) planned for the repository.

Broad Data Need—Site Data: Water Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Saturated Zone Waters	1. McKinley et al. (1991)	Yes	Yes	?USGS
	2. Kerrisk (1987)	Yes	No	?LANL
	3. White et al. (1980)	Yes	No	?USGS
	4. Claassen (1985)	Yes	No	?USGS
	5. DOE (1988b)	Yes	No	DOE
	6. DOE (1988c)	Yes	No	DOE
	7. DOE (1992a)	Yes	No	DOE

Table 3-9. LARP Section 3.2.3.5—(PAC) Geochemical Processes (FY00) (Cont'd)

Broad Data Need—Site Data: Water Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
2. Unsaturated Zone Waters	1. Yang et al. (1988)	Yes	No	?USGS
	2. White et al. (1980)	Yes	No	?USGS
	3. Yang et al. (1993)	Yes	No	?USGS
	4. DOE (1990)	Yes	No	DOE
	5. Kerrisk (1983)	Yes	No	?LANL
The most likely path for the transport of radionuclides from the repository to the accessible environment will be as dissolved constituents in groundwater or as a gas phase (e.g. ^{14}C in CO_2). Waste package stability, waste for degradation, radioelement solubility and radionuclide transport are all dependent on the chemistry of the water. In natural systems such as at YM, interactions between the gas, water, and solid phases control the water chemistry. At YM, the location of the repository in the hydrologically unsaturated zone requires additional information on these groundwaters. Saturated zone water compositions are necessary due to the inclusion of the saturated zone in transporting radionuclides to the accessible environment.				
Broad Data Need—Site Data: Mineral Chemistry	**Data Source(s)**	**Data Obtained?**	**Entered in GIS?**	**QA Status**
1. Primary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. DOE (1989)	Yes	No	DOE
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. DOE (1988d)	Yes	No	DOE
2. Secondary Mineral Assemblages	1. Warren et al. (1984)	Yes	No	?LANL
	2. Broxton et al. (1986)	Yes	Yes	?LANL
	3. Bish and Chipera (1989)	Yes	No	?LANL
	4. Carlos (1987)	Yes	No	?LANL
	5. Carlos et al. (1990)	Yes	No	?LANL
	6. Carlos et al. (1991)	Yes	No	?LANL
	7. Bish (1989)	Yes	No	?LANL
	8. Carlos (1989)	Yes	No	?LANL
	9. Broxton et al. (1987)	Yes	No	?LANL
Like water chemistry, radionuclide sorption is a function of the mineral chemistry in both the fractures and matrix at YM. Both primary and secondary minerals will also play a role in controlling the water chemistry (e.g., buffering reactions), and thereby having an effect on the performance of the EBS (e.g., waste package stability, waste form dissolution, near-field sorption). In addition, thermal, mechanical, and hydrological properties of the rock will depend, at least to some extent, on the constituent minerals and their susceptibility to alteration.				

Table 3-9. LARP Section 3.2.3.5—(PAC) Geochemical Processes (FY00) (Cont'd)

Broad Data Need—Site Data: Gas Chemistry	Data Source(s)	Data Obtained?	Entered in GIS?	QA Status
1. Gas Partial Pressures (Pre-waste Emplacement)	1. Thorstenson et al. (1989) 2. Weeks (1987) 3. DOE (1991a) 4. DOE (1988e)	Yes Yes Yes Yes	No No No No	?USGS ?USGS DOE DOE
Because the proposed repository is to be located in the unsaturated zone, partial pressures of gases, particularly CO_2, can have an effect on both the chemistry of the waters at the site and the stability of the different minerals that make up the host units for the repository. There is also the possibility of the transport of certain radioelements such as ^{129}I and ^{14}C in the gaseous phase.				

4 ARC/INFO COVERAGES AND SYSTEM CAPABILITIES - EXAMPLES

In a geologic system such as YM, much of the data generated during site characterization is most useful when tied to a geographic/geologic framework. GIS systems such as ARC/INFO are powerful tools for presenting and interpreting data in a geographic context. By superimposing different coverages such as geology, political boundaries, and geochemical/hydrologic data, it is possible to develop figures and maps that can transmit a wide range of information. In addition, the ARC Macro Language (AML) provides the capability to manipulate the data and display quantitative information in ways that may help in interpreting trends and tendencies.

In the initial stages of data compilation and entry into ARC/INFO format, the task on investigations of issues in hydrology, geochemistry, and climatology/meteorology have produced electronic forms of two geochemical data sources and entered them into the ARC/INFO database currently being constructed at CNWRA. These include:

- Broxton, D.E., R.G. Warren, R.C. Hagan, and G. Luedemann. 1986. *Chemistry of Diagenetically Altered Tuffs at a Potential Nuclear Waste Repository, Yucca Mountain, Nye County, Nevada.* LA-10802-MS. Los Alamos, NM: Los Alamos National Laboratory.

- McKinley, P.W., M.P. Long, and L.V. Benson. 1991. *Chemical Analyses of Water for Selected Wells and Springs in the Yucca Mountain Area, Nevada and Southeastern California.* USGS Open File Report 90-355. U.S. Geological Survey.

Additional DOE data on stable isotope (^{13}C, ^{18}O, deuterium) and radiogenic isotopes (^{87}Sr, ^{14}C) has been converted to electronic form, but is not yet available in ARC/INFO.

The ARC/INFO database was initially developed for projects conducted by CNWRA for both NRC/NMSS tasks and NRC Research projects. As part of these projects, a great deal of information has been entered as coverages into ARC/INFO (Center for Nuclear Waste Regulatory Analyses, 1994). These coverages continue to evolve as part of ongoing efforts in these research projects. Where possible, the current effort will take advantage of existing coverages to provide a strong geological framework for the current effort in Investigations of Issues in Hydrology, Geochemistry, and Climatology/Meteorology, and to enhance display and interpretation of hydrologic, geochemical and climatological data.

4.1 EXISTING COVERAGES

Figures 4-1 through 4-3 are examples of the types of geologic coverages that are currently available in the ARC/INFO database being developed at CNWRA. These coverages can be overlain with hydrologic, geochemical, and climatological data, perhaps to relate geologic structures with spatial trends in the data.

4.2 DATA DISPLAY CAPABILITIES

AML is a powerful tool for developing data display capabilities that aid in the interpretation of the data in a geological and geographical context. Figures 4-4 and 4-5 show sample locations for the water chemistry data of McKinley et al. (1991) and the mineral chemistry data of Broxton et al. (1986)

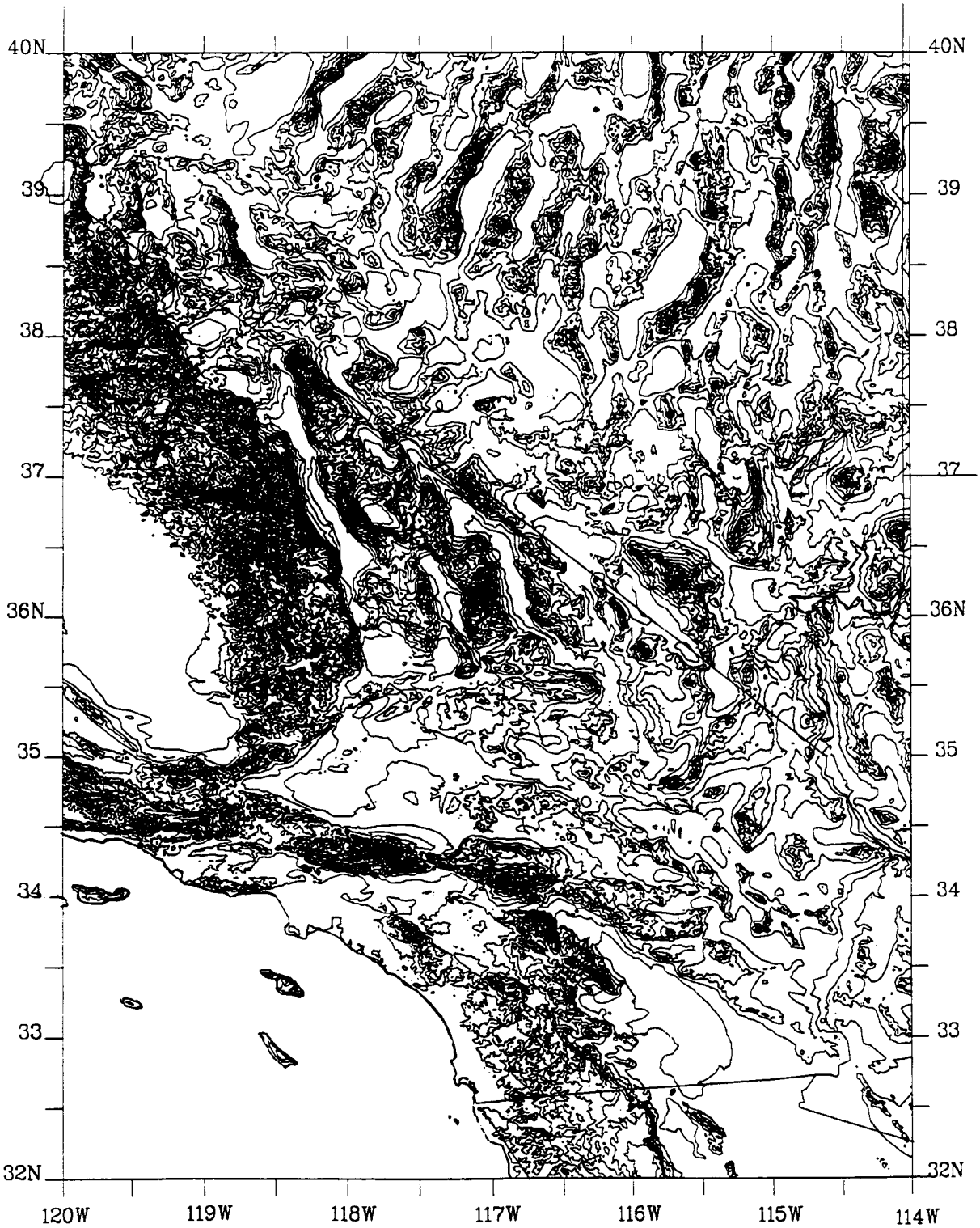


Figure 4-1. Topographic coverage for the southern Nevada/California region. Contours are from processed Digital Elevation Model (DEM) data collected by the U.S. Geologic Survey.

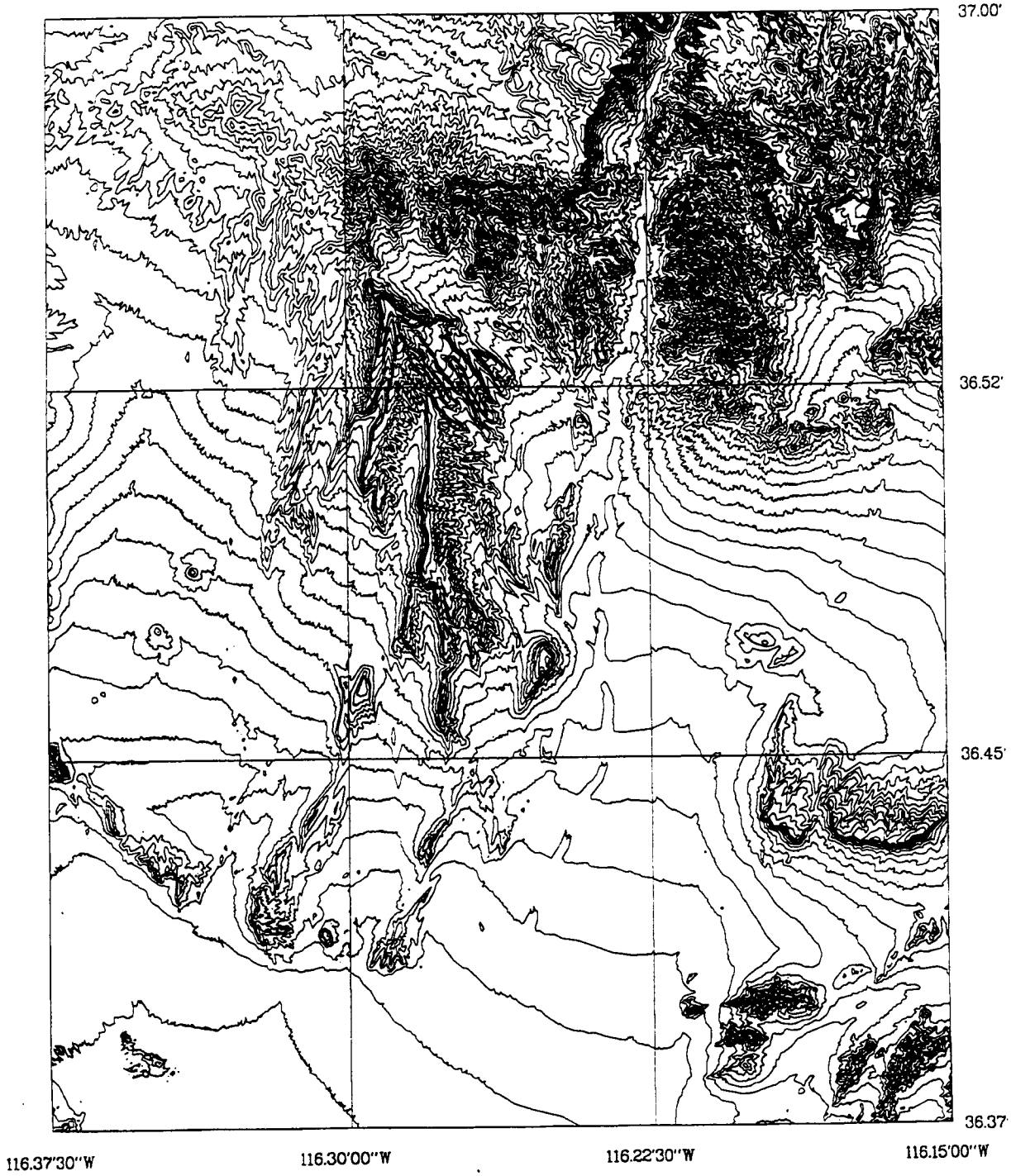


Figure 4-2. Local topography for the Yucca Mountain region

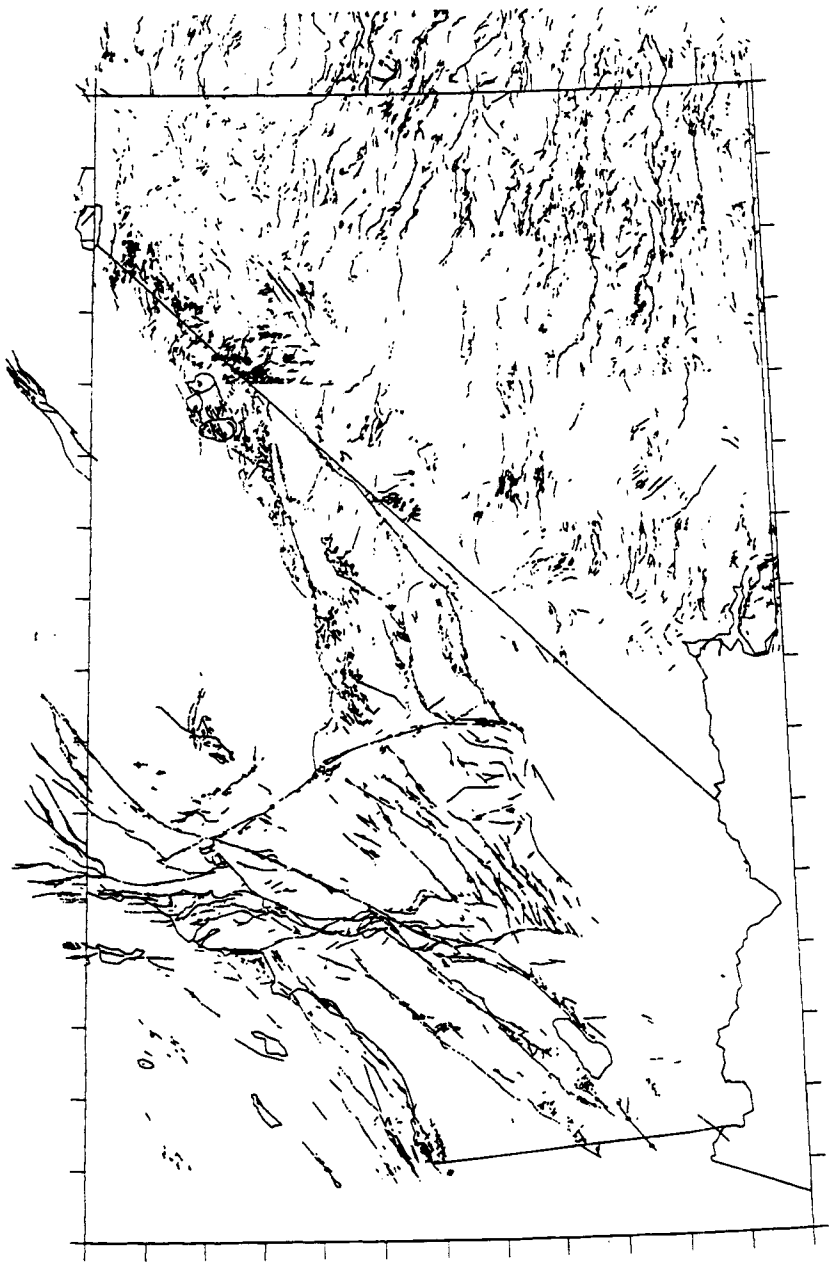


Figure 4-3. Composite of fault coverages for the southern Nevada/California region

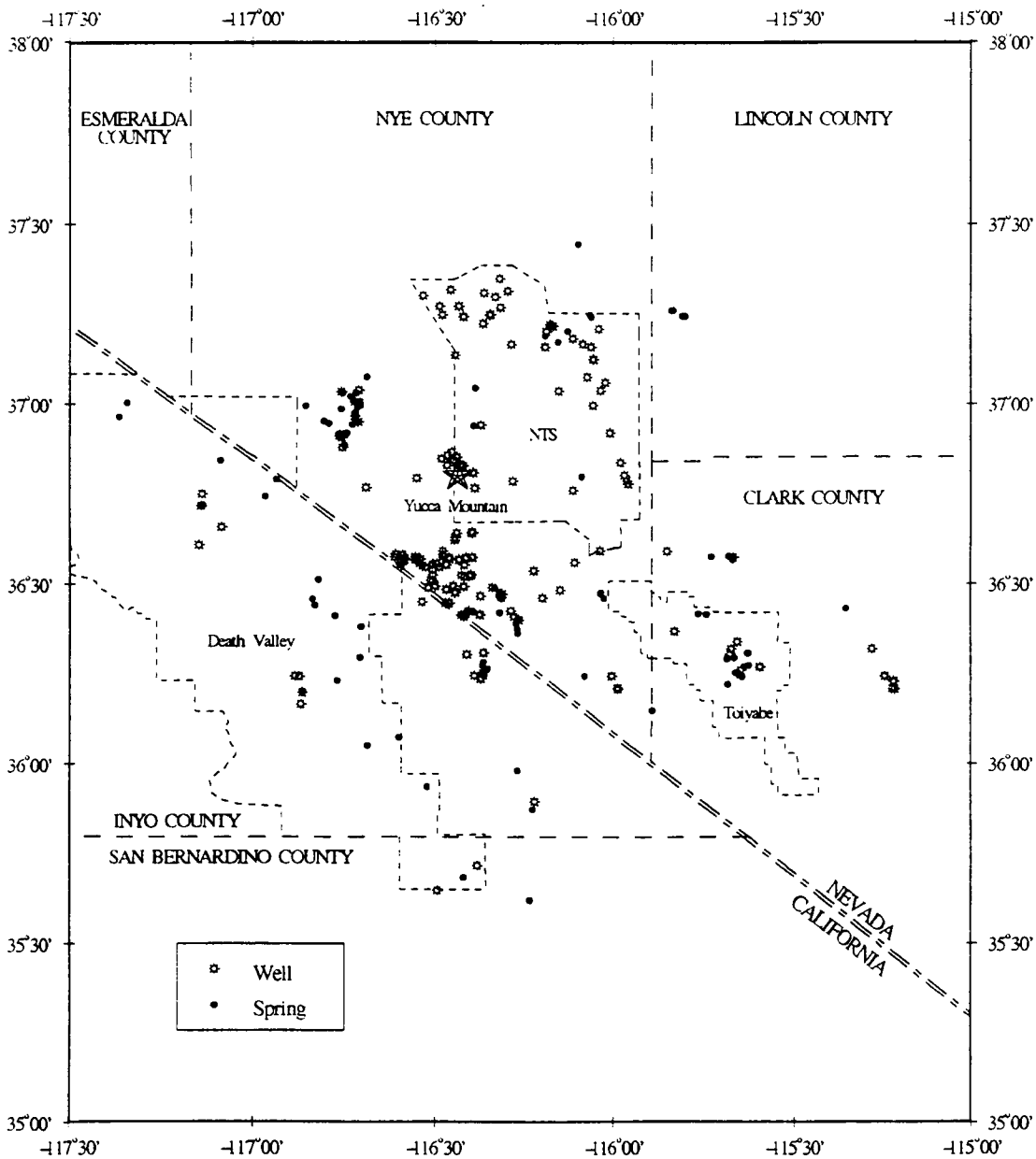


Figure 4-4. Locations of 279 wells and springs in the southern Nevada/California region for which water chemistry data are available in ARC/INFO. Data from McKinley et al. (1991).

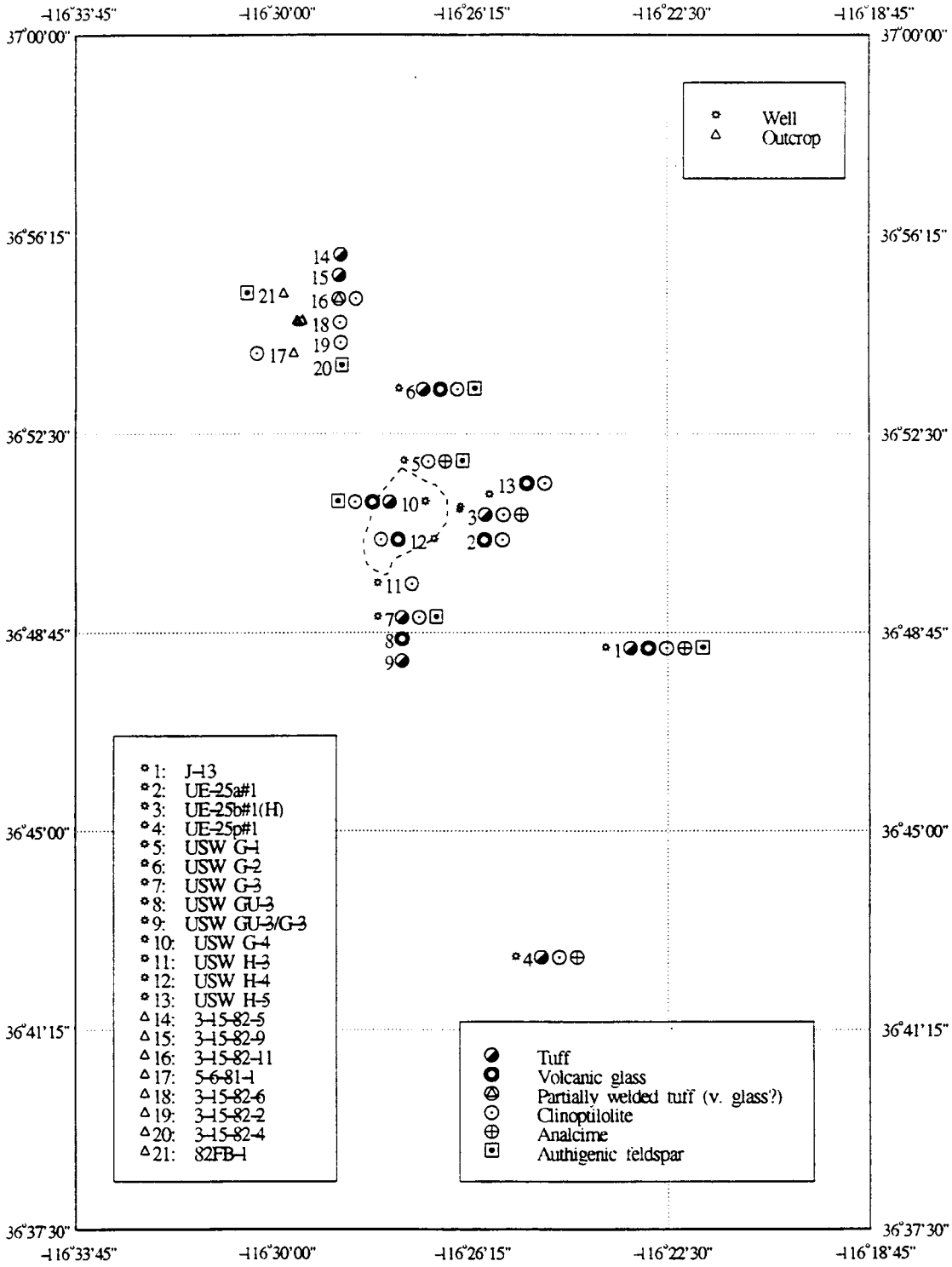
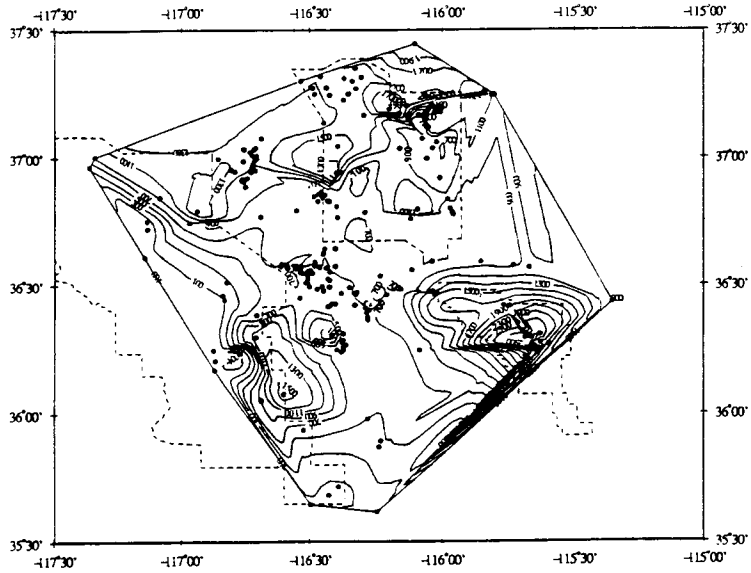


Figure 4-5. Site locations in the local Yucca Mountain Region for which mineral chemistry data are available in ARC/INFO. The outline of the repository block is shown by the dashed line. Data are from Broxton et al. (1986).

that are currently available in ARC/INFO. Using the data of McKinley et al. (1991), Figures 4-6 and 4-7 demonstrate the contouring that is possible using the AML. It is also possible to write programs in AML that combine and transform different data attributes and plot simple graphics such as the Stiff diagrams shown in Figure 4-8.

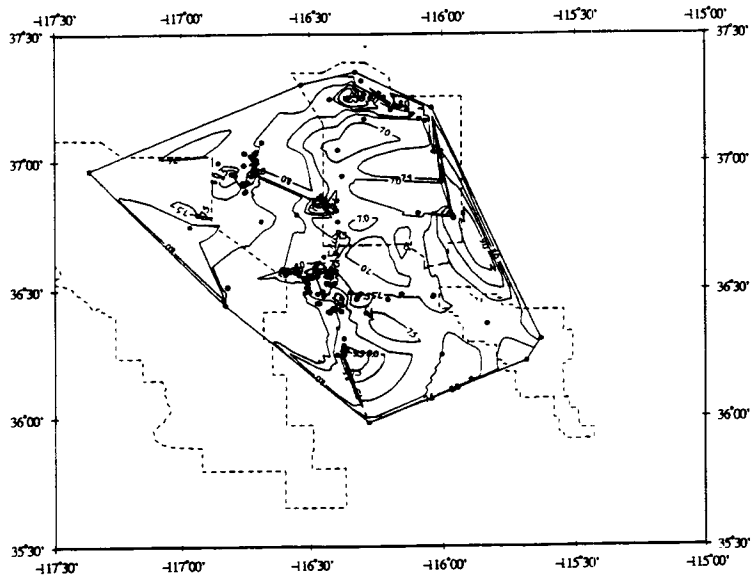
It is important to note that the geopolitical boundaries that are plotted in Figures 4-4 and 4-5 were acquired from databases developed by DOE and forwarded in electronic format to NRC/CNWRA. This provides some assurance that it is possible to acquire data in electronic form from DOE, reducing the need to reenter data from hard copy. This data exchange capability is likely to become even more important, and hopefully more efficient, as computerized DOE databanks such as ATDTS come on-line and more data are available.

Water Table Elevation
-100 – 3048 m. Contour Interval = 200 m



(a)

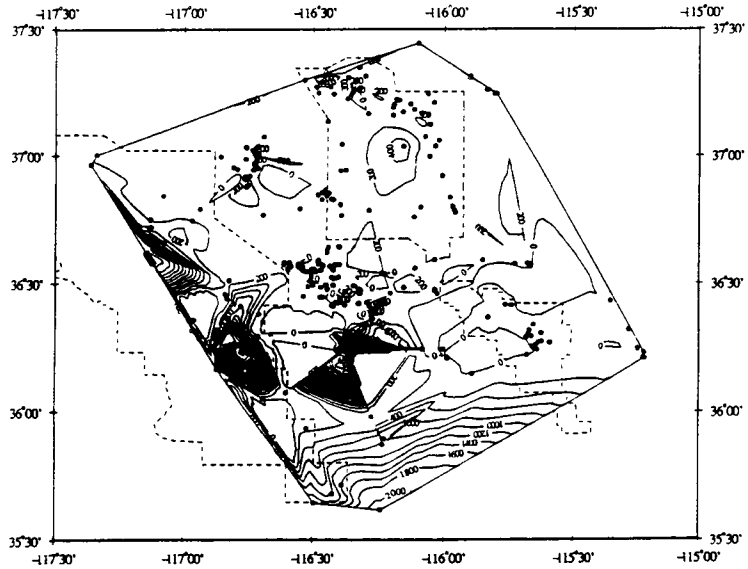
Field pH
6.5 – 10.0 units, Contour Interval = .5 units



(b)

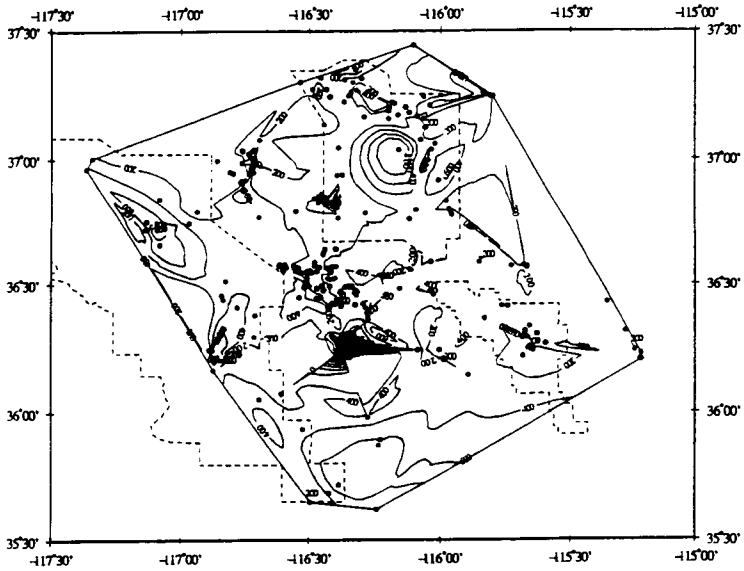
Figure 4-6. (a) Water table elevation (meters); (b) Field pH. The NTS, Death Valley National Monument, and Toiyabe National Forest are for reference. Data from McKinley et al. (1991).

Sodium
0 – 28000 mg/L; Contour Interval = 200 mg/L



(a)

Alkalinity as HCO3
0 – 16000 mg/L, Contour Interval = 200 mg/L



(b)

Figure 4-7. (a) Sodium concentration (mg/L); (b) Alkalinity as bicarbonate (mg/L). The NTS, Death Valley, and Toiyabe National Forest are for reference. Data from McKinley et al. (1991).

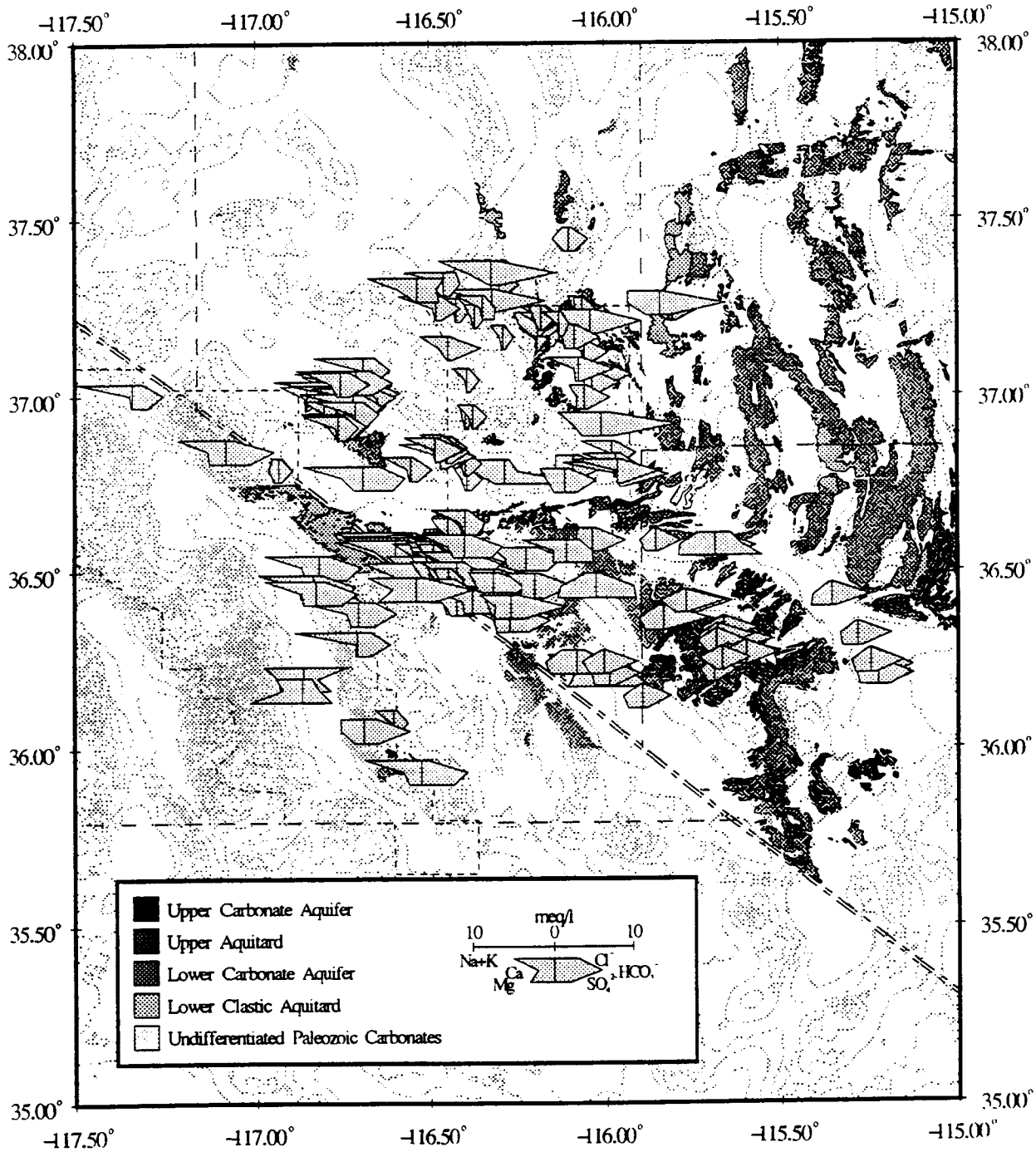


Figure 4-8. Stiff diagrams for hydrochemical data from McKinley et al. (1991). Axes clockwise from upper left are: Na+K, Cl, HCO_3, SO_4, Mg, and Ca. Units in meq/L.

5 SUMMARY AND CONCLUSIONS

5.1 CURRENT STATUS

Technical issues related to geochemistry represent a significant portion of the sections currently in development for the License Application Review Plan and many of the KTUs identified during the development of CDSs. To assure timely review of the geochemical aspects of the License Application, it is reasonable to identify the data needs and computer codes that will be used during the review process as early as possible. This will enable NRC/CNWRA staff to become familiar at an early stage with data and methods that are likely to be presented by DOE. This approach will also have the advantage of identifying areas of overlap between the different LARP sections, as well as providing background information that is critical to the development of the geochemical CDMs that make up the LARP. The disadvantage in this approach is the premature selection of data and/or computer codes in the absence of final indications by DOE.

In this letter report, an initial attempt has been made to identify broad data needs for those CDMs/LARP sections related to geochemistry. Based on this effort, there are three types of data at this relatively high level that are important to CDM development. These include:

- Basic data that are applicable to systems outside of YM, but are necessary for calculations such as thermodynamic data, kinetic rate data. These data are informational in nature and do not carry site-specific spatial information.

- Site specific data that are necessary to define the boundary and initial conditions at YM. These data are currently being generated as part of YM site characterization, and will presumably become available in on-line DOE databases such as Automated Technical Data Tracking System (ATDTS) and the Technical Data Base (TDB) being developed by the YMPO (Harloe, 1993). These are the data that carry information in a geographic context and are best stored and displayed in a GIS database.

- Design data that are necessary to define the effects of the repository itself such as repository design and man-made materials. Many of these design issues are in development and final design decisions have not yet been made.

Once the broad data needs are identified, the next step is to identify specific data needs and the existing sources for these data. At this time, this effort has been conducted by CNWRA staff using their familiarity with the current literature. Where they are known, the appropriate DOE study plans have been identified as a future data source. As the capability to access on-line electronic databases improves, the effort can focus more tightly on data generated under these study plans.

In identifying specific data needs, several points can be noted:

- Geochemical and related data have tended to come out in a number of small reports and papers rather than as large compilations. This is particularly true with regard to site-specific data, which tend to be reported in the proceedings for conferences, such as the annual International High Level Radioactive Waste Management or the Materials Research

Symposia on the Scientific Basis for Nuclear Waste Management, or as USGS Open-File Reports.

- Some of the specific data like water chemistry and pre-emplacement temperature are measured values. However, some of the data such as post-emplacement temperature distribution are derived from models. Extrapolation of limited data may also be required to provide the desired spatial coverage. Such extrapolation may be as simple as contouring the existing data (Section 4), or may require more detailed modeling such as kriging or stochastic analysis.

- Many of the different CDM/LARP sections can use the same data. Identifying these sources at this stage will help to reduce the amount of duplication in developing any database. It may be appropriate to identify these cross-linkages explicitly.

- The QA status of many of these data is uncertain. Many of the data were gathered prior to the development of DOE QA procedures, but in most cases, they are the only data currently available. As site characterization proceeds, it may be appropriate for DOE to bring these existing data into compliance with QA procedures, or for results from current site characterization activities to supersede these data. It is important for NRC/CNWRA staff to keep current with regard to these issues so that QA status can be monitored and data can be updated accordingly in the databases being developed.

Because of the spatial nature of a geologic HLW repository, much of the site-specific data is best displayed in a GIS database. At present, only a small amount of geochemical data (Broxton et al., 1986; McKinley et al., 1991) have been converted to electronic format and entered into the CNWRA GIS database as a part of this task. These data have been used in this report to demonstrate some of the capabilities of the ARC/INFO software.

5.2 FUTURE EFFORTS

Future efforts will continue to focus in several areas:

- Continue to identify specific data sources. As on-line databases become available, these will be used to identify the most current data sources, and obtain electronic copies where possible.

- Specific data sources identified will be obtained. For those data that are best displayed in a geographic context, data will be entered into the CNWRA GIS database. For those data that are not already available in electronic format (from DOE or other agencies), some effort will be needed to convert these data for GIS entry. For those data such as thermodynamic databases or design information, hard copies and electronic copies, where appropriate, will be maintained at CNWRA.

- It may be appropriate to develop a limited bibliographic database to monitor the status of the database and to indicate cross-references between different LARP sections.

- Methods and Computer codes tentatively identified in Table 2-2 will be investigated in more detail. Where DOE has indicated a "code of choice," it may be appropriate to obtain versions of these codes for installation and adaptation to NRC/CNWRA computer facilities.

- Results from these efforts will be used to help in CDM development. Data justification, uncertainty, and limitations will all be used to help develop the rationale sections for the different CDMs. In the future, computer codes and the existing databases will be used to test the suitability of proposed CDM approaches.

It is important to remember that effort will focus on those CDMs that are scheduled for completion in the relatively short-term. Less effort will be spent on those scheduled for completion in out years. Any changes to the CDM completion schedule that may result from the DOE Proposed Program Approach will require additional changes in scheduling for work performed under this task.

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