

308 --- Q199702060008
Radionuclide Transport
Scientific Notebook #157A

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Task 20-5702-826

Investigate Issues in Hydrology/Geochemistry/Climatology
Technical Assessment

Due to CNWRA Reorganization, converted
to Task 20-5708-871 - Radianuclide Transport effective
1/20/96

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157 AC
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157A DRJ
12/12/96 DRJ

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12/10/96 to correct
misnumbering in
scientific notebook log.

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DRJ

David E. Turner

Sr. Research Scientist

Task 20-5702-826: Investigate Issues in Hydrology, Geochemistry, Climatology

The purpose of this project is to provide technical assessment methods for that will aid NRC/CNWRA staff in the review of the DOE LA for the HLW repository. The focus of this project is to be on issues in hydrology, geochemistry, and climatology that will have an impact on repository performance. The work presented here consists largely of projects that have been proposed by CNWRA either formally or informally to NRC/DWM/PAHB and have received verbal approval from the NRC section leader. A basic understanding of chemical and/or hydrological principles, as well as computer hardware and software are necessary requirements for most of the work outlined here. Specific knowledge requirements, data sources, computer hardware and software, as well as potential sources of error and uncertainty are described in more detail in the summaries provided here.

10/3/9

JRM

Starting in FY96, the Hydrology aspects of this technical assessment project were split off at CNWRA under the management of A. Gureghian.

1/30/96
DRJ The objectives of this Task are largely adopted for this new
Task 20-5708-871 KTI on Radionuclide Transport resulting
from NRC/CNWRA reorganization (see pg 49 this volume).
Focus is on using geochemical and hydrologic data to describe
and place bounding limits on radionuclide transport processes
such as mixing & dilution. Much of the purpose of this
scientific notebook is to identify sources of hydrochemical
data and provide a trace on the original sources to
the extent possible. Relatively little effort is devoted to
QA control of the original data packages, and the quality of
these data, the reader is referred to the original report
as identified here.

1/16/96 DRJ

Initial Entry DRJ 1/17/97

Saturated Zone Water Chemistry - Data Sources and GIS Entry

One of the goals of this task is to acquire existing hydrological and geochemical data for the Yucca Mountain region and use it to populate the Geographic Information System (GIS) database being developed at CNWRA as a part of other research projects.

The initial data source for saturated zone water chemistry identified for this technical assessment activity includes:

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. Denver, CO: U.S. Geological Survey.

This report is a USGS document prepared as a hydrochemical compilation of data collected over the past several decades at Yucca Mountain. These data were not generally collected under a DOE-approved QA program, but are freely used. The sources referenced in McKinley et al. (1991) should be consulted for determining the quality of the data.

Well and spring ID numbers (1-279) that are used by McKinley et al. (1991) are internal to the report. These sampling locations are shown in the maps included in this scientific notebook. Original data sources cited by McKinley et al. (1991) are also included.

The data included here are originally entered using a ~~Lotus 1-2-3~~ spreadsheet. This allows exporting an ASCII-comma delimited format for inclusion in GIS and 3D graphics systems like ArcInfo and EarthVision. In the tables, concentrations are given in units of mg/L. The notation -1111 means not reported, while -9999 indicates below detection limits.

Excel, 4.0 for Windows DRJ 1/17/96

Sampling locations-McKinley et al. (1991)

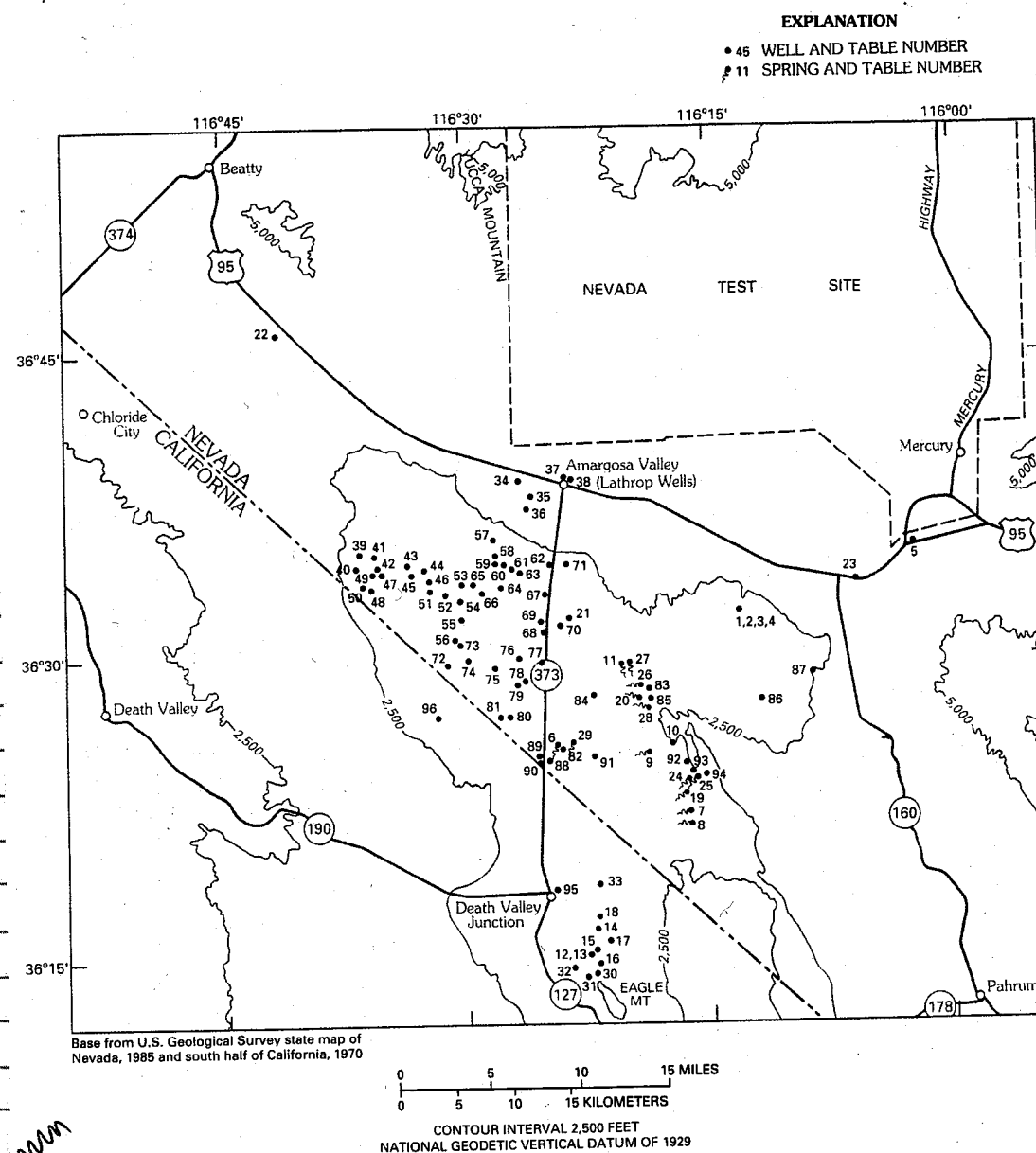
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Figure 2.--Location of wells and springs in the Amargosa Desert area.

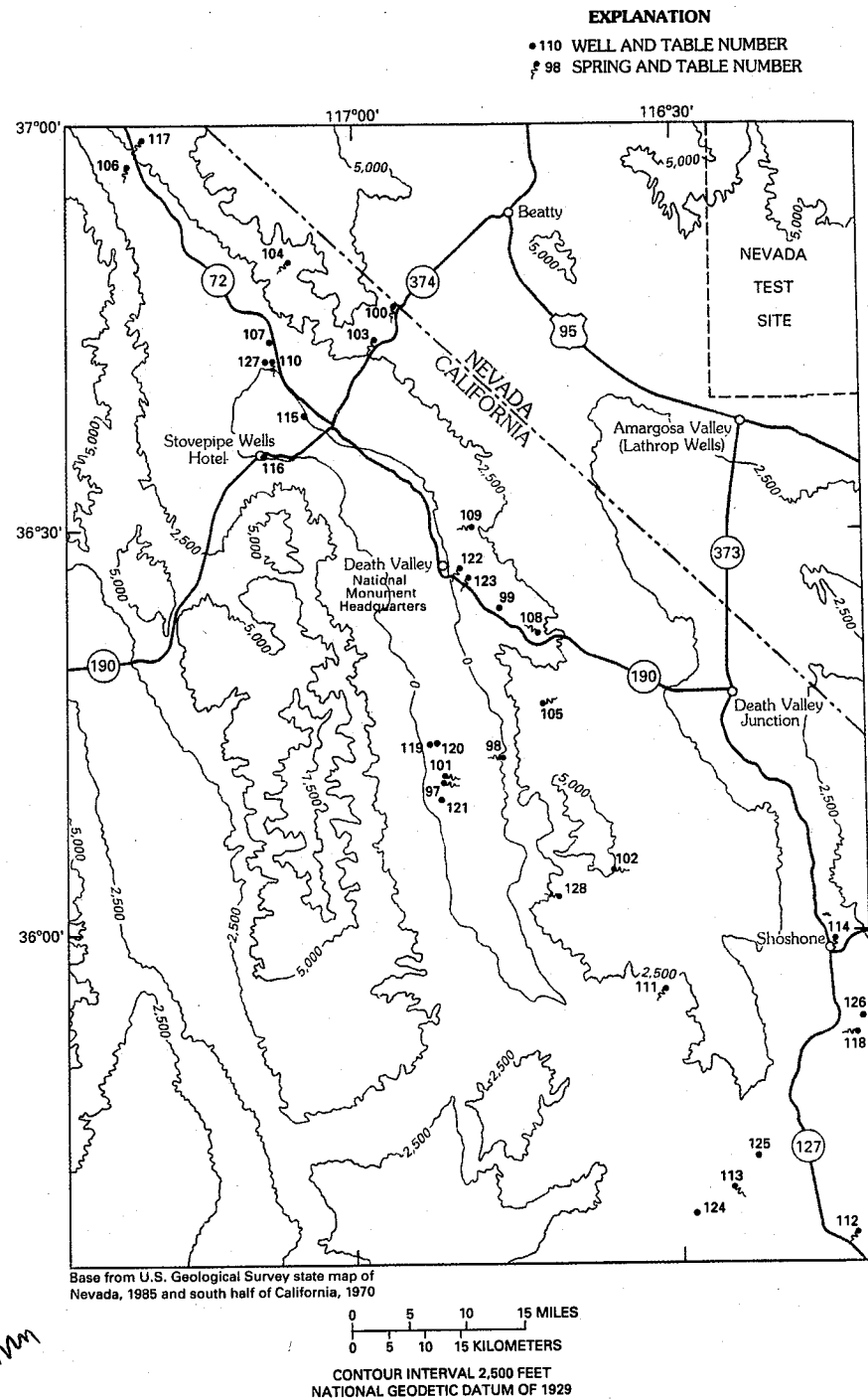
V/L/L/L/L
DBI

Figure 3.--Location of wells and springs in the Death Valley area.

Sampling locations (McKinley et al., 1991)

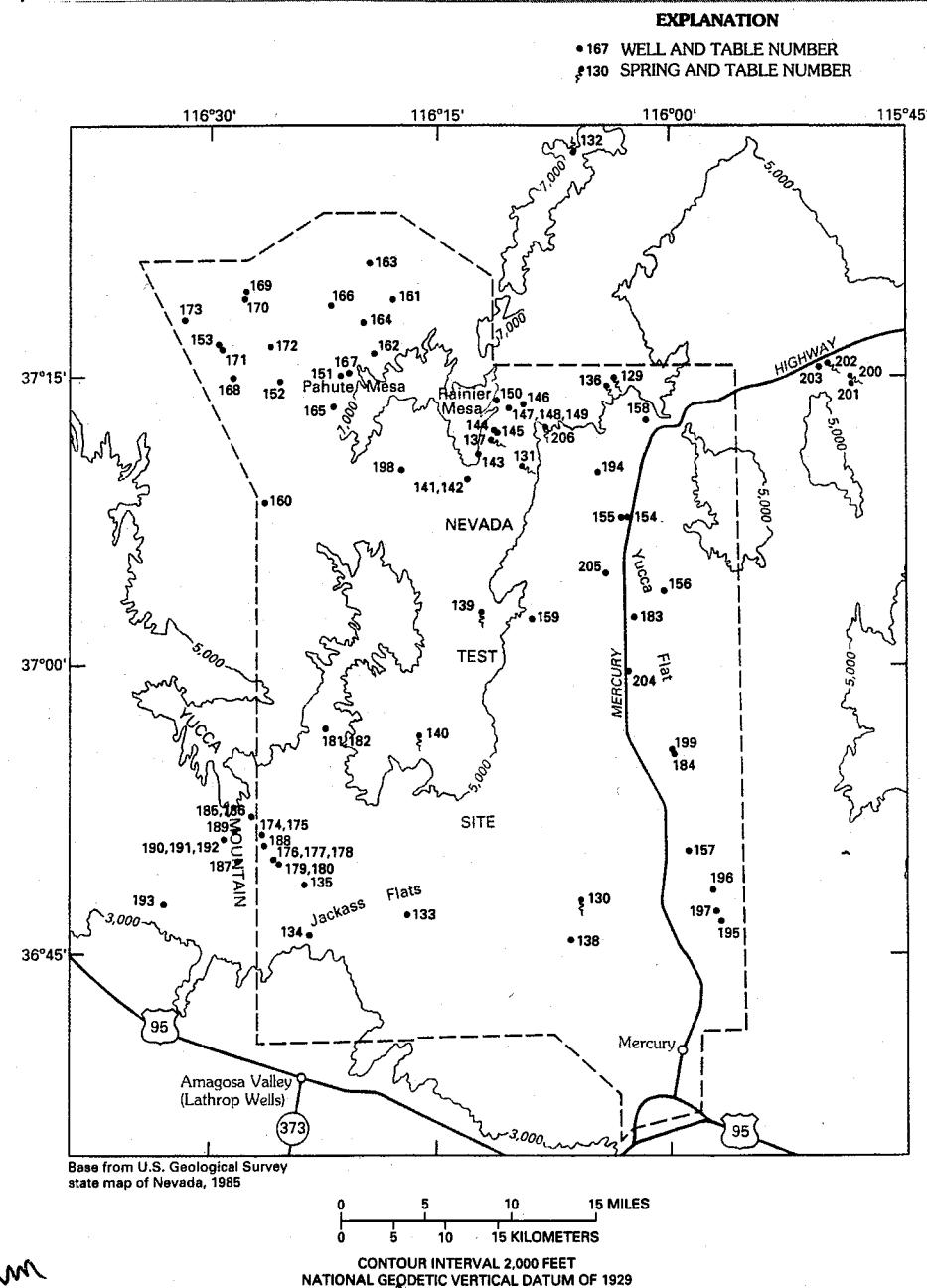
V/L/L/L/L
DBI

Figure 4.--Location of wells and springs in the Nevada Test Site area.

Sampling locations (McKinley et al., 1991)

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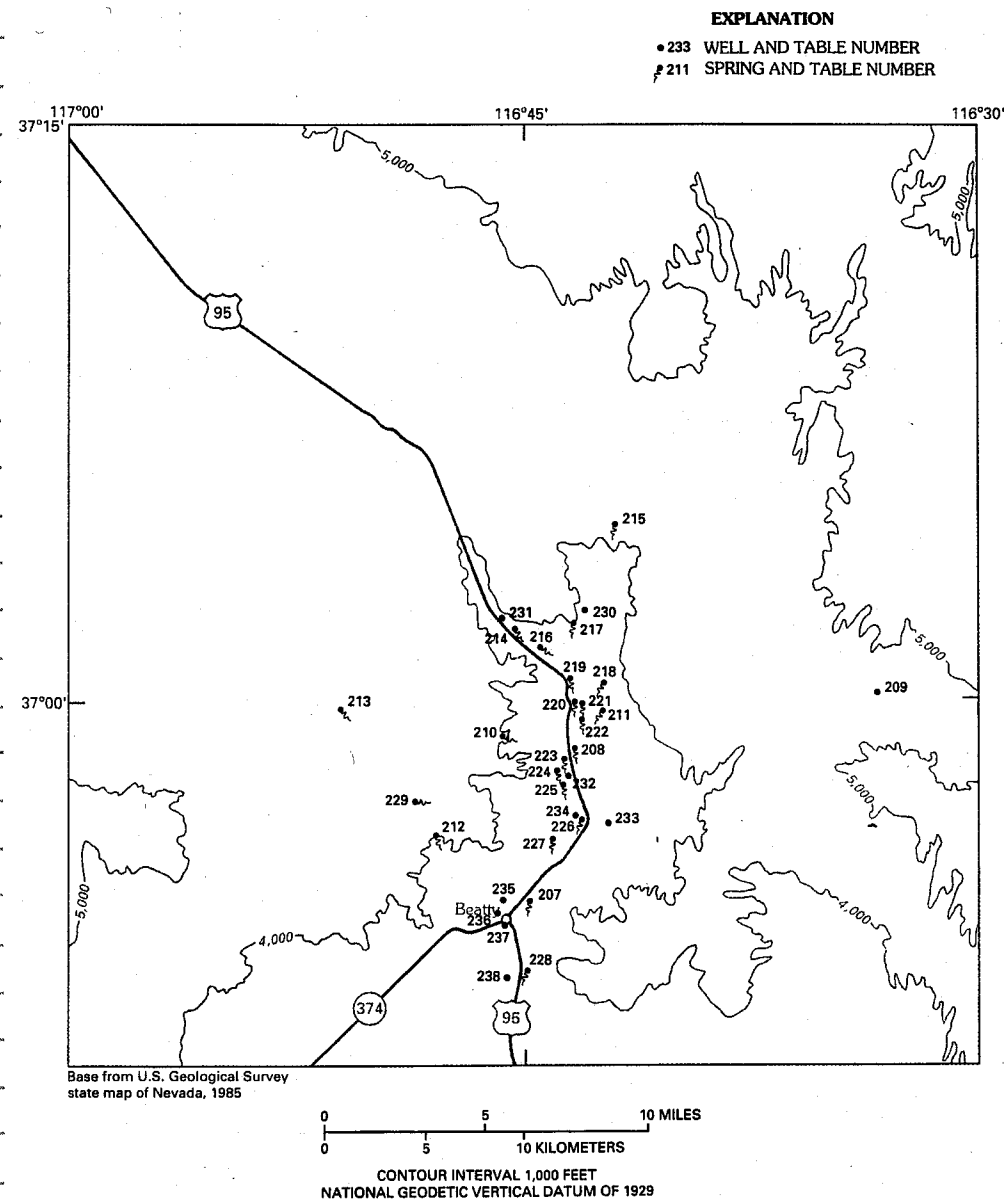


Figure 5.--Location of wells and springs in the Oasis Valley area.

Sampling locations-Mekinky et al. (1991)

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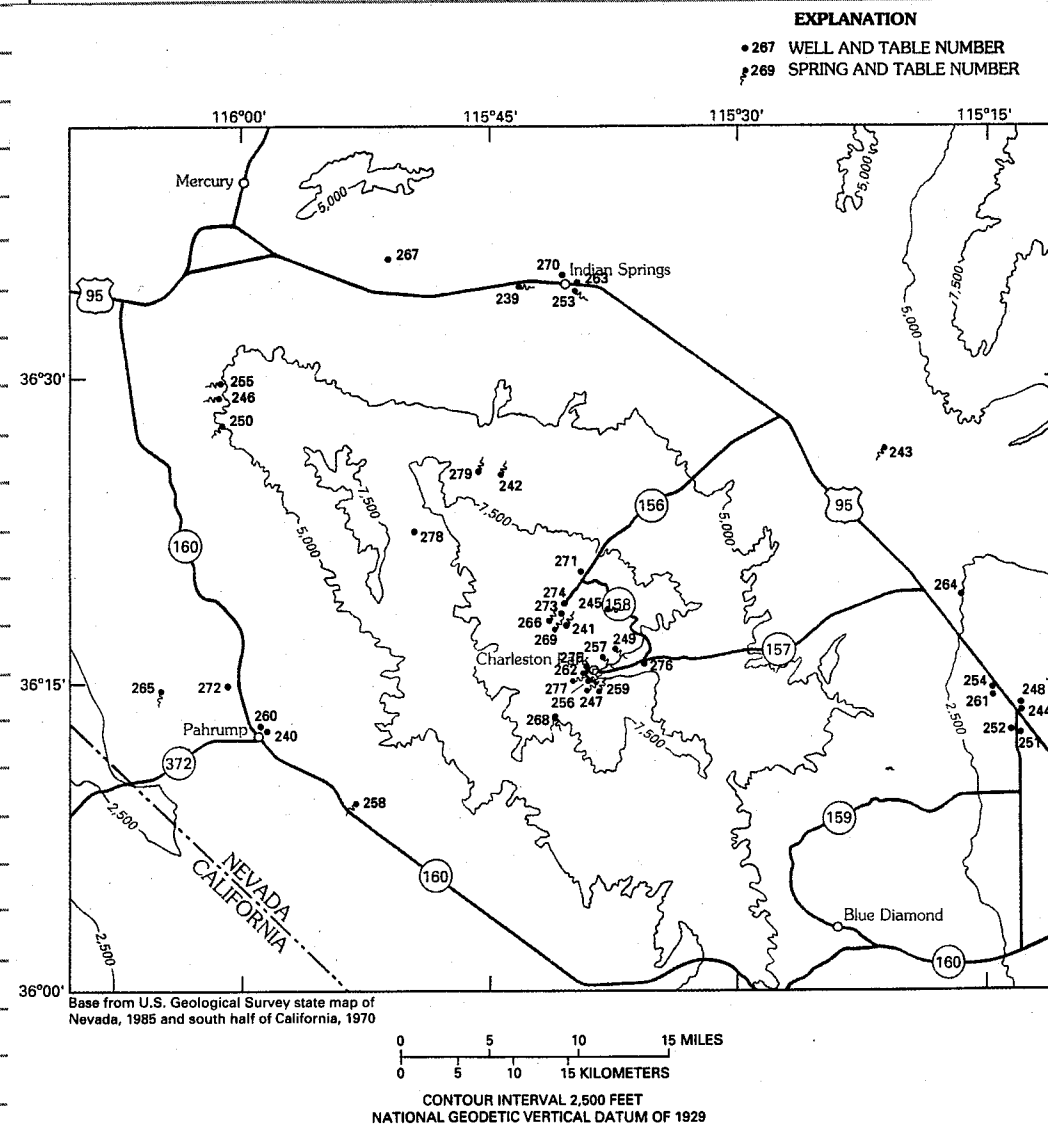


Figure 6.--Location of wells and springs in the Spring Mountains area.

Sampling locations-Mekinky et al. (1991)

McKinley et al. (1991) REFERENCES CITED

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- Moore, J.E., 1961, Records of wells, test holes, and springs in the Nevada Test Site and surrounding area: U.S. Geological Survey Trace Elements Investigations Report 781, 22 p. (NNA.901026.0052)
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References Cited - McKinley et al. (1991)

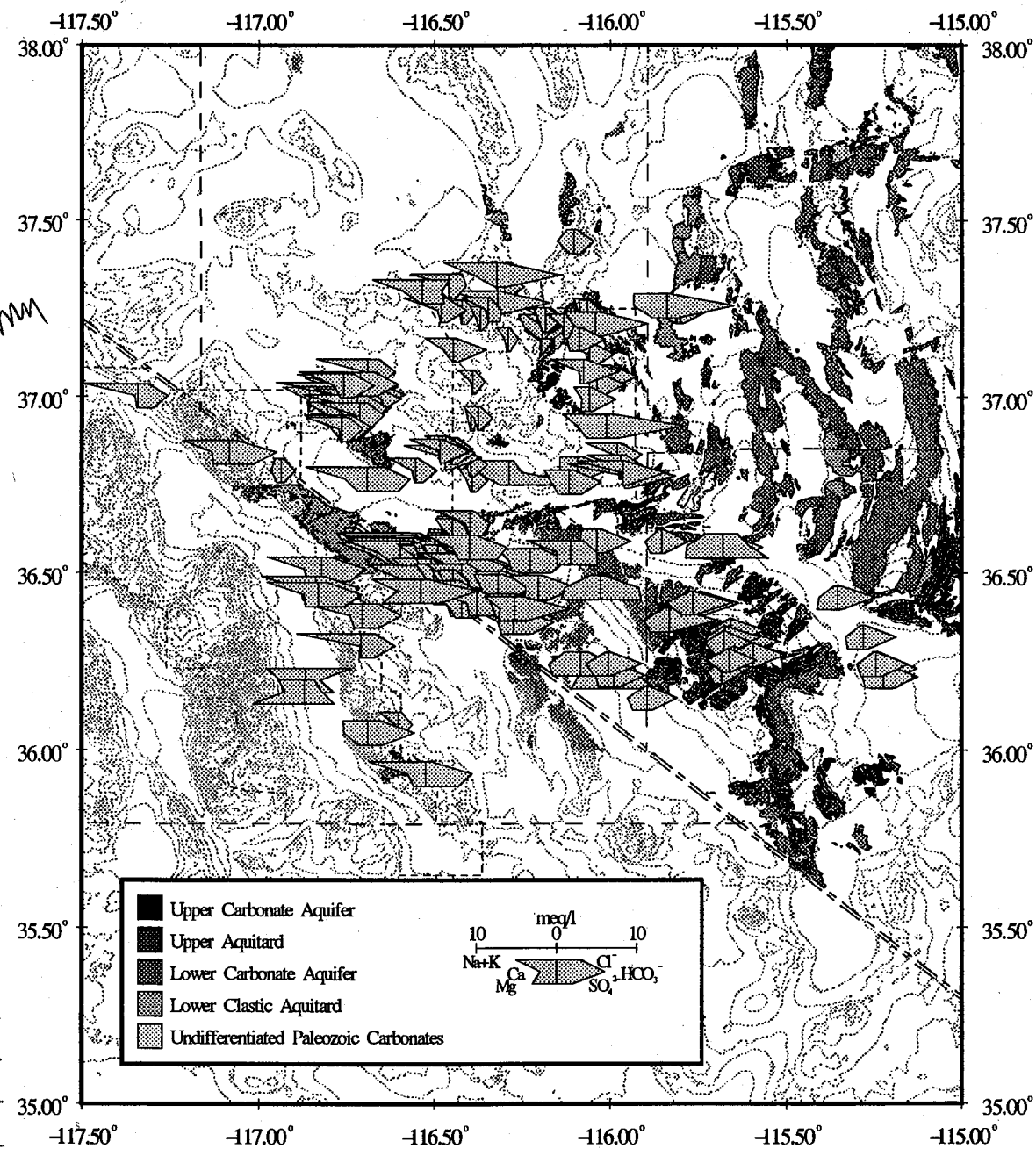
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- Young, R.A., 1972, Water supply for Nuclear Rocket Development Station at the U.S. Atomic Energy Commission's Nevada Test Site: U.S. Geological Survey Water-Supply Paper 1938, 19 p. (NNA.870519.0007)

NOTE: Parenthesized numbers following each cited reference are for U.S. Department of Energy OCRWM Records Management purposes only and should not be used when ordering the publication.

1/16/96
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Stiff diagram map developed by Sandy Nguyen (SwRI, Division 15) using the hydrochemistry data of McKinley et al. (1991) and GIS/ArcInfo coverages (topography, political boundaries) developed in the Tectonics Research Project. S. Nguyen also developed a contouring routine on the CNWRA Silicon Graphics SPARC 10 workstation to investigate trends in chemical data over the Yucca Mountain region.

Coding done using ARC Macro Language (AML) of ArcInfo

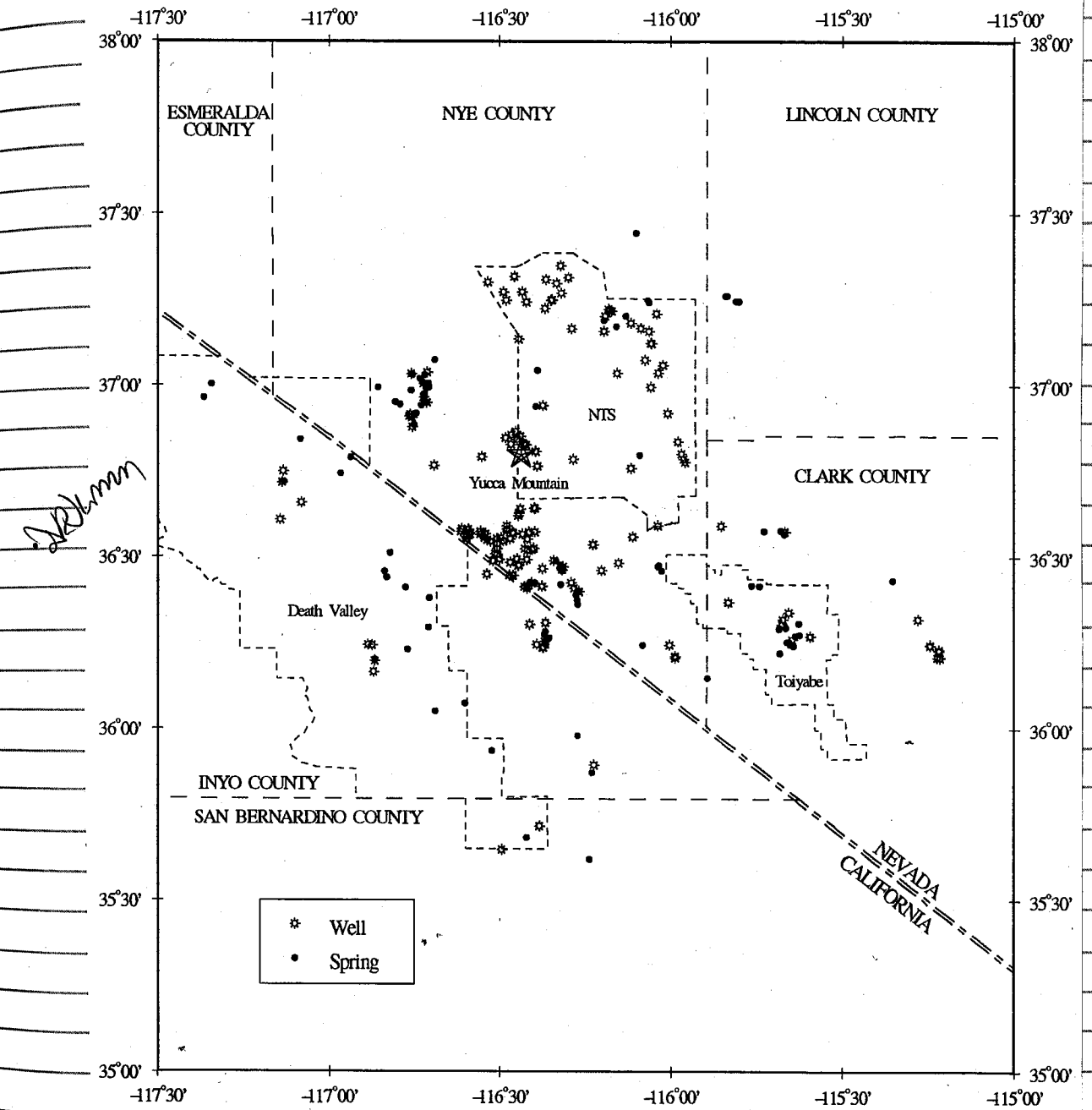


ArcInfo, version 7.0

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Available Water Chemistry Data

McKinley et al. (1991)

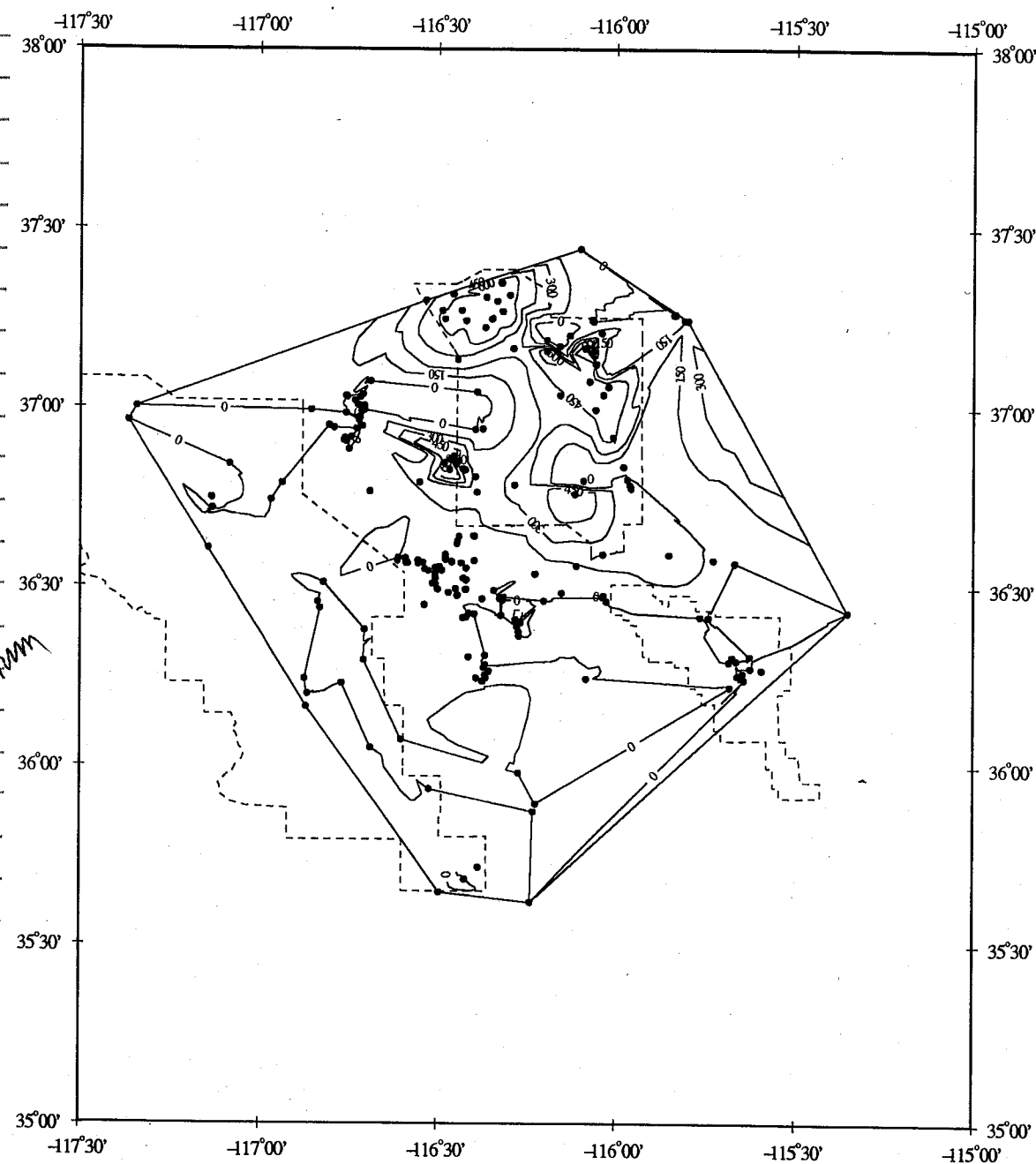


ArcInfo, version 7.0

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Water Depth

0 - 751 m, Contour Interval = 150 m

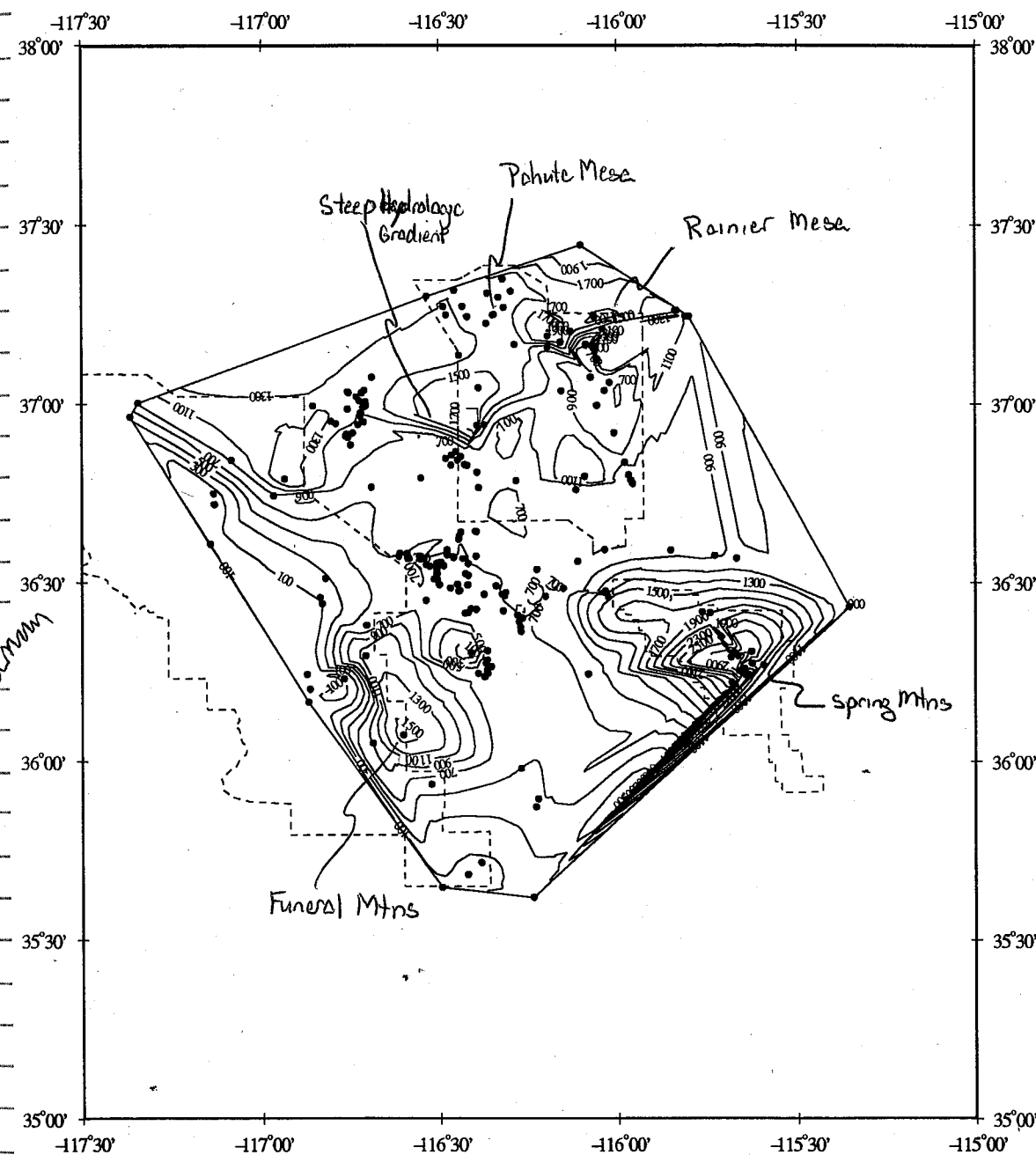


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Water Table Elevation

-100 - 3048 m, Contour Interval = 200 m

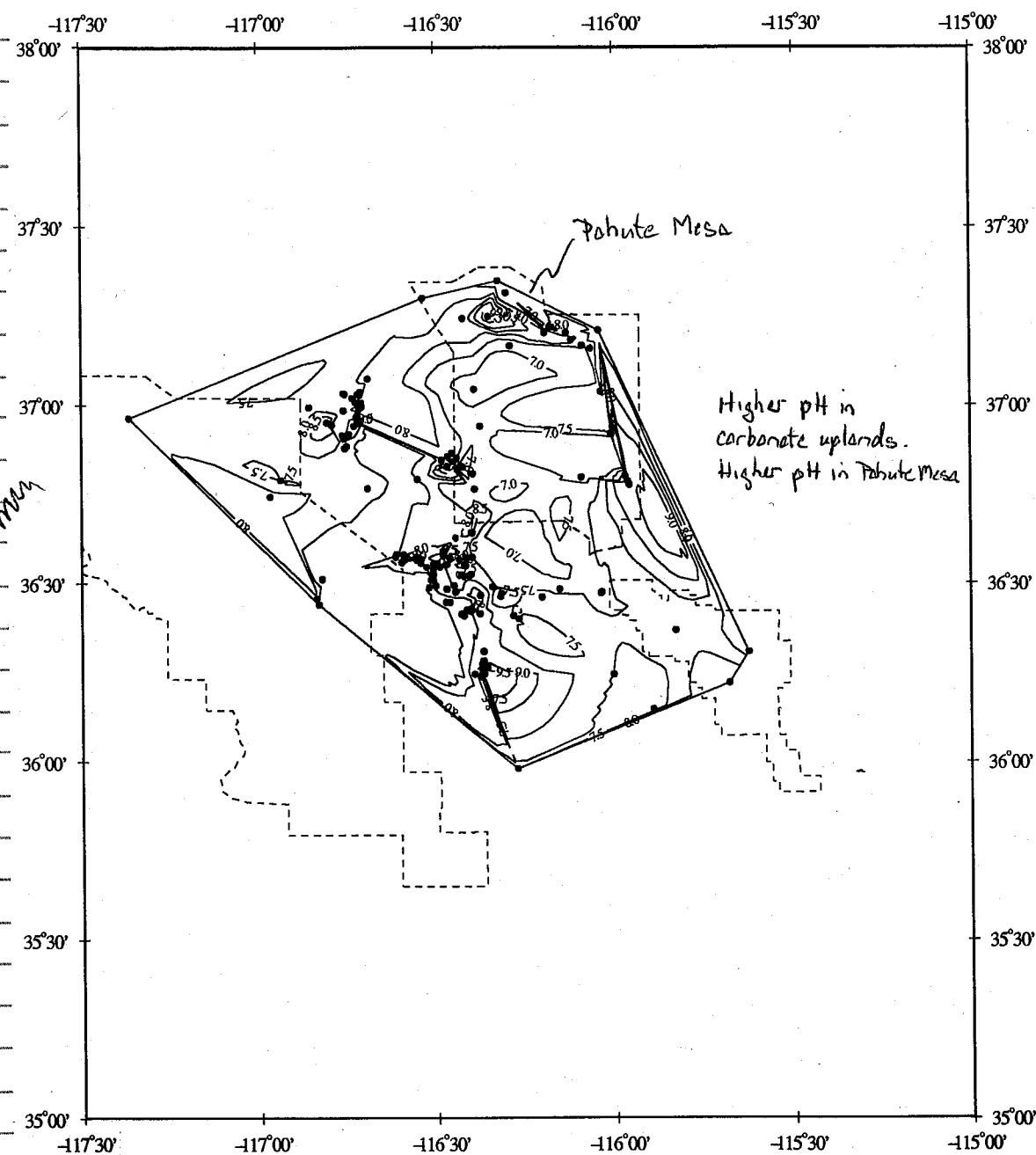


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Field pH

6.5 - 10.0 units, Contour Interval = .5 units

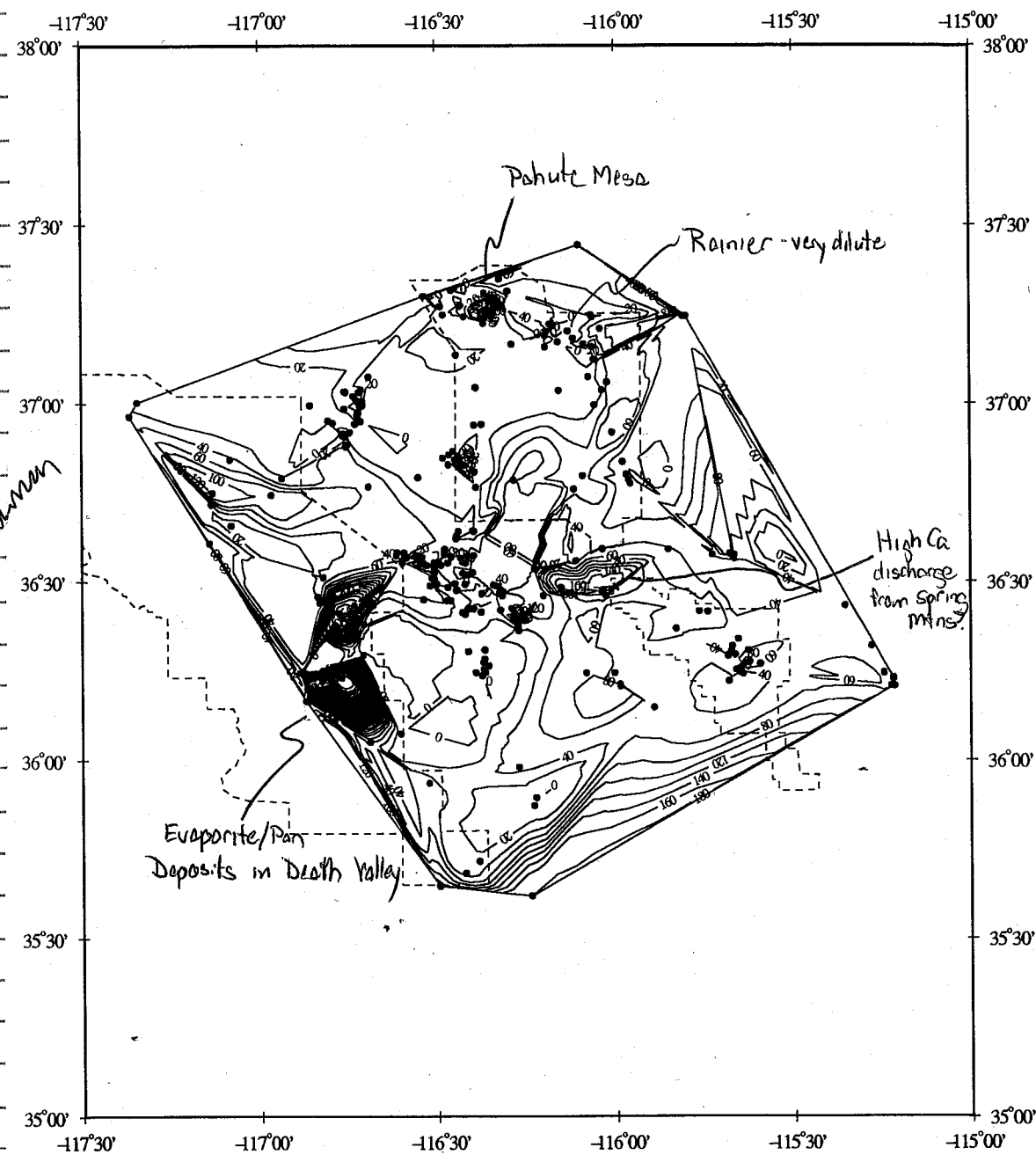


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Calcium

0 - 830 mg/L, Contour Interval = 20 mg/L

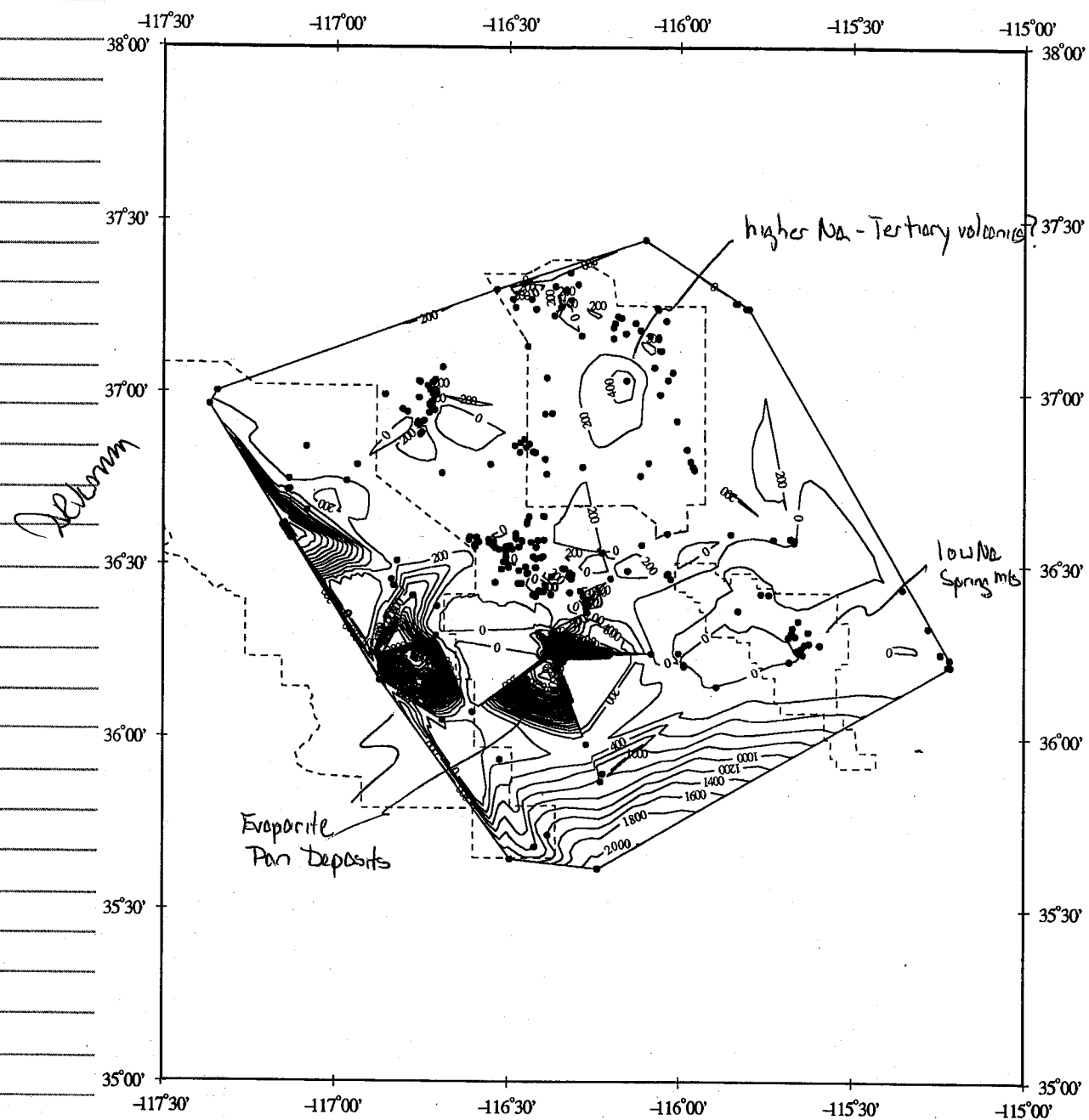


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Sodium

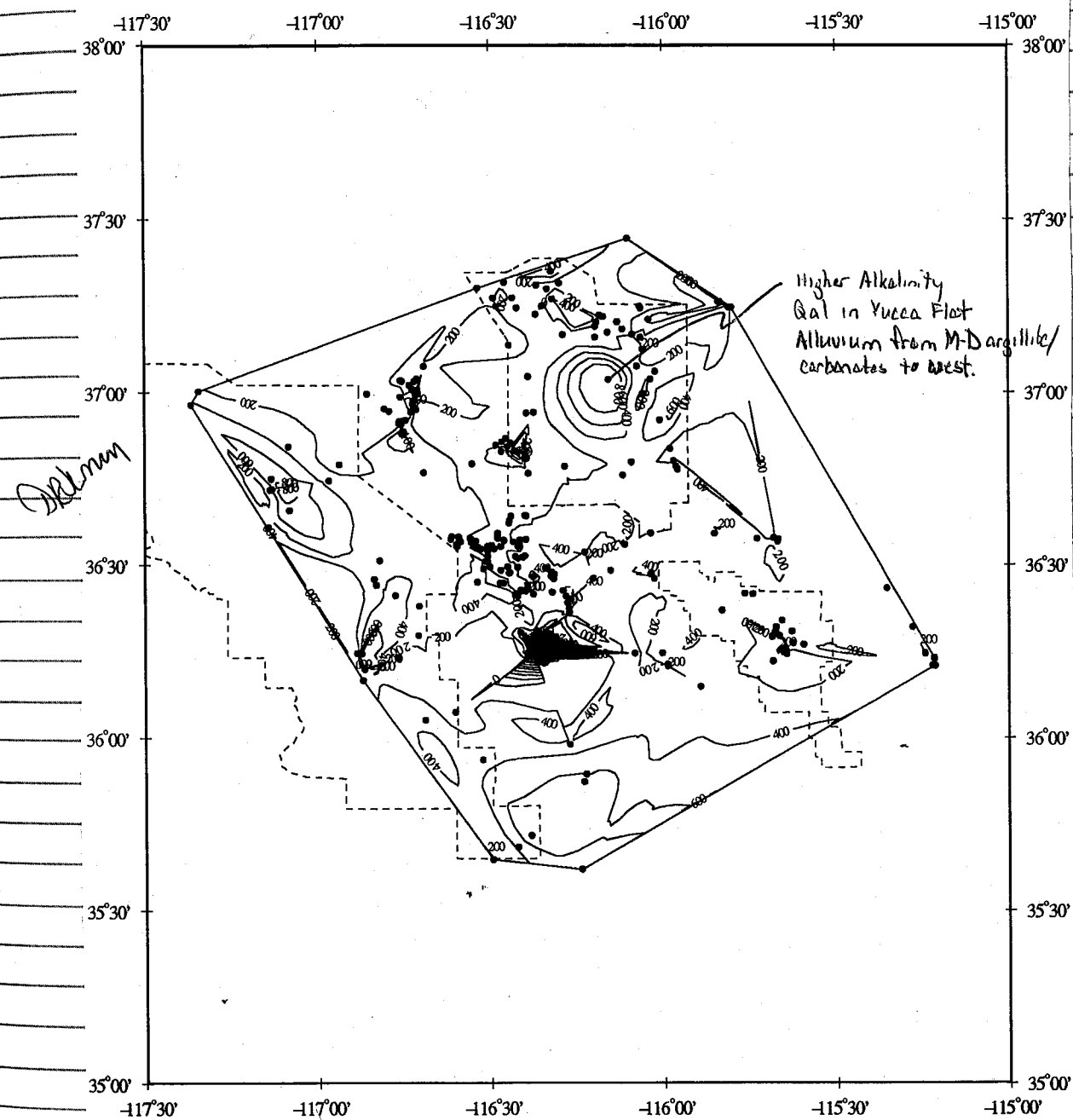
0 - 28000 mg/L, Contour Interval = 200 mg/L



Arc Info, Version 7.0

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DRJAlkalinity as HCO_3

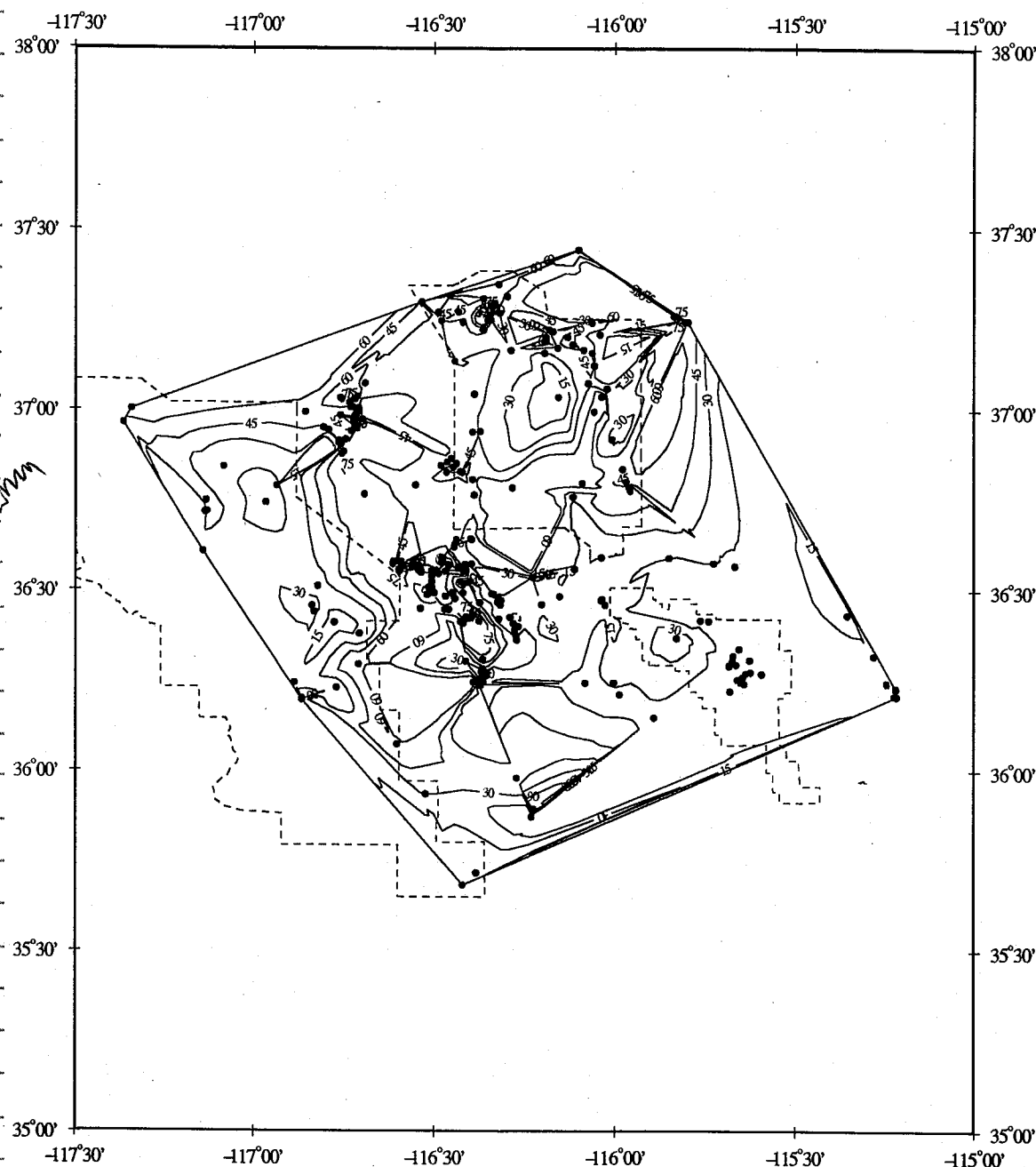
0 - 16000 mg/L, Contour Interval = 200 mg/L



Arc Info, Version 7.0

Silica

0 - 130 mg/L, Contour Interval = 15 mg/L



Arc Info, Version 3.0

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 mineral chemistry data sources and entered them into the ARC/INFO database currently being constructed at CNWRA. For mineral composition, the data source is:

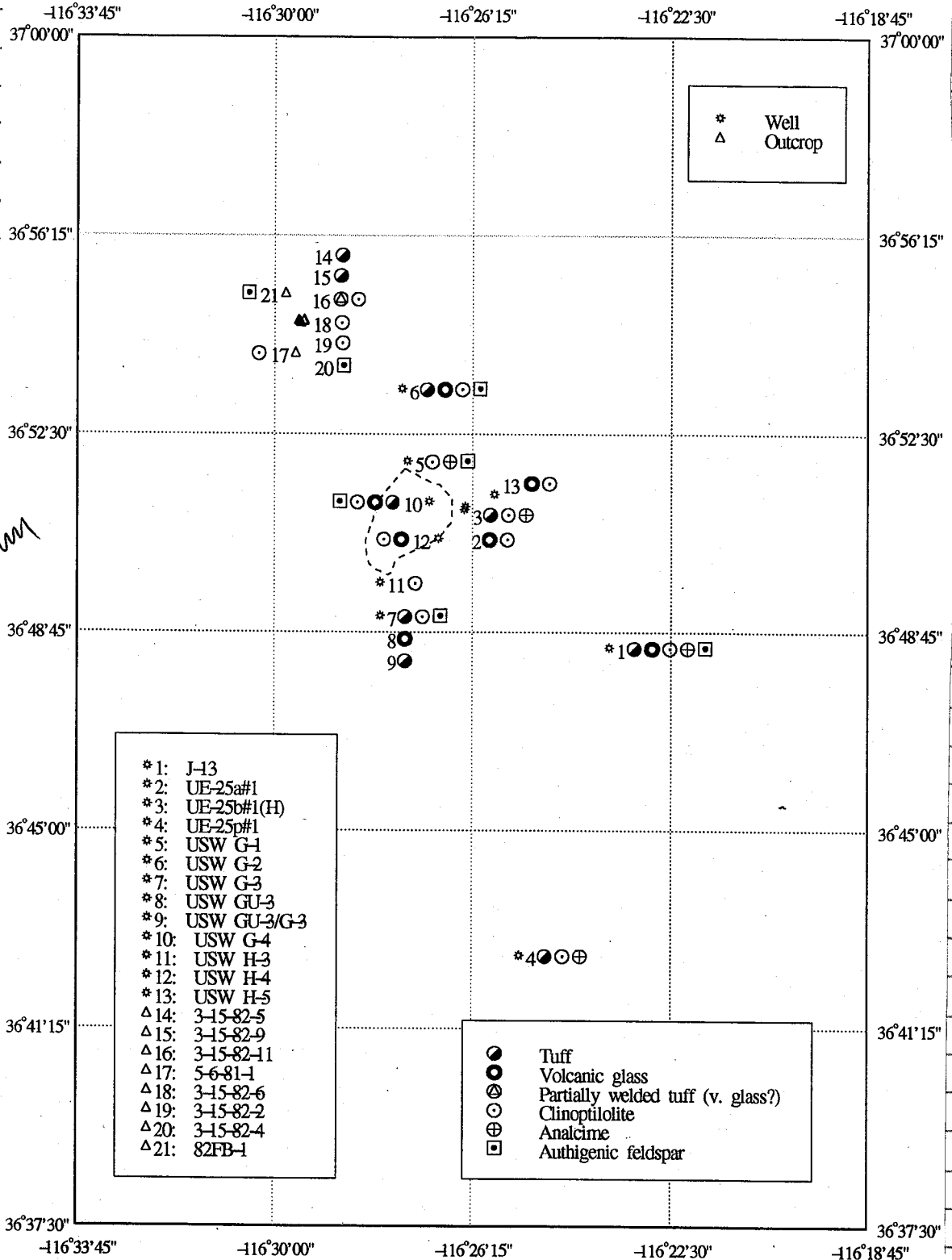
- Broxton, D.E., R.G. Warren, R.C. Hagan, and G. Luedemann. 1986. *Chemistry of Diagenetically Altered Tuffs at a Potential Nuclear Waste Repository, Yucca Mountain, Nye County, Nevada*. LA-10802-MS. Los Alamos, NM: Los Alamos National Laboratory.

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.

Broxton et al. (1986) 1/17/94 DRJ
This report is a Los Alamos report prepared as a compilation of mineral chemistry data collected from drill holes (and a few outcrop samples) at Yucca Mountain. These data were generally collected prior to the implementation of a DOE-approved QA program, but are freely used in this project. The sources referenced in Broxton et al. (1986) should be consulted for determining the quality of the data.

The data included here are originally entered using a Microsoft Excel, Version 4.0 for Windows (IBM PC) spreadsheet. This allows exporting an ASCII-comma delimited format for inclusion in GIS and 3D graphics systems like ArcInfo and EarthVision. In the tables, mineral compositions are expressed in terms of oxide weight percent.

Available Mineral Compositional Data



Page 1

SL	BIT NAME	NOVADA NORTH (COORDINATE)	NOVADA EAST (COORDINATE)	Latitude	Longitude	Data Source	Analysis Lab	Acquirer	Lithology	Use	Elevation	Well-Depth	Water Depth	Pumping Time	Yield	Sampling Method	Filtration	Data	Sp. Cont.	Refr. Act.	Lab. Act.	Temp	Ca	Mg	Na	K	Al(OH3)	CO3	Cl	F	SO4	PO4	Li	Br	TDS	Barium	
1	Amalgam Alkanol OMS Hole	950872	922635	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
2	Amalgam Alkanol OMS Hole	950738	922606	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
3	Amalgam Alkanol OMS Hole	950823	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
4	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
5	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
6	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
7	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
8	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
9	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
10	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
11	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
12	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
13	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
14	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
15	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
16	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
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19	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
20	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
21	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
22	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
23	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
24	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
25	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
26	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
27	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
28	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
29	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
30	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
31	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
32	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
33	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
34	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
35	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
36	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	289
37	Amalgam Alkanol OMS Hole	950720	922607	38.24	118.13	USGS	USGS	OTW	1	UNCONSOLID	729	189	13	-1111	-1111	-1111	-1111	97900	400	-1111	-1111	8.4	28	8.9	7.8	9.4	119	38	22	1.2	1.8	-1111	-1111	0.11	0.11	0.88	2

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Site No.	Site Name	Nevada North (Coordinate)	Nevada East (Coordinate)	Latitude	Longitude	Data Source	Analysis Lab	Analyst	Lithology	Use	Elevation (m)	Well Depth (m)	Water Depth (m)	Permeability (D)	Yield (m ³ /d)	Remedial Method	Fluoride (mg/L)	Date (mm/dd/yy)	No. Cond.	Field pH	Lab pH	Temp. (°C)	Ca (mg/L)	Mg (mg/L)	Na (mg/L)	K (mg/L)	Cl (mg/L)	SO ₄ (mg/L)	CO ₃ (mg/L)	SiO ₂ (mg/L)	NO ₃ (mg/L)	NO ₂ (mg/L)	PO ₄ (mg/L)	Fe (mg/L)	Mn (mg/L)	TDS (mg/L)	Salinity (ppt)
224	Bedrock 11847E-21a	801200	488700	38.48.02	118.43.21	USGS	USGS	GM	-1111	RA	1081	-9999	0	-1111	2	-1111	-1111	7/4/87	1110	7.7	8	21.5	23	2.1	232	8.5	372	158	89	6	60	0	0	0.37	0.21	760	0.4
225	Bedrock 11847E-21b	804400	488700	38.48.06	118.43.20	USGS	USGS	GM	-1111	DOM	1082	-9999	0	-1111	2	-1111	-1111	7/4/87	1180	7.8	8.2	28	26	2.1	246	8.2	396	167	72	9	64	0	0	0.28	0.28	803	0.6
226	Bedrock 11847E-21c	805400	488700	38.48.09	118.43.00	1.2 USGS	USGS	GM	-1111	RA	1081	-9999	0	-1111	2	-1111	-1111	7/4/87	1110	8.1	8.9	21	10	2.3	249	8.8	280	168	68	6	64	0	0	0.33	0.1	721	0.7
227	Bedrock 11847E-21d	787800	488700	38.48.01	118.43.43	1.2 USGS	USGS	TV	-1111	DOM	1081	-9999	0	-1111	2	-1111	-1111	7/4/87	828	8.2	7.9	34	8.7	0.1	112	2.4	178	70	27	2.8	49	0.1	0	0.14	0.03	235	0.4
228	Bedrock 11847E-21e	777100	478700	38.50.06	118.48.00	1.2 USGS	USGS	GM	-1111	DOM/NO	878	-9999	0	-1111	25	-1111	-1111	7/23/87	1210	7.7	8	18.5	27	3.6	254	10	392	184	77	3.8	89	0	0	0.1	0.15	802	0.5
229	Upper Indian Bedrock	801300	488700	38.48.09	118.48.19	1.2 USGS	USGS	TV	-1111	DOM	1280	-9999	0	-1111	-1111	-1111	-1111	7/2/87	281	8.2	7.8	28.8	0	0.4	88	1.7	116	14	14	0.4	44	1.2	0	0.18	0.18	603	0.2
230	Wet 10847E-27a	831200	488900	37.02.16	118.42.42	1.2 USGS	USGS	GM	-1111	DOM	1187	-2	0	-1111	1	-1111	-1111	7/8/87	893	7.7	7.8	10	22	1.5	171	8.1	288	102	65	2.6	62	0.1	0	0.08	0.28	448	1.3
231	Wet 10847E-27b	831100	478200	37.02.00	118.48.50	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
232	Wet 10847E-27c	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	ITOCK	1187	-2	0	-1111	1	-1111	-1111	7/4/87	893	7.7	7.8	10	22	1.5	171	8.1	288	102	65	2.6	62	0.1	0	0.08	0.28	448	1.3
233	Wet 10847E-27d	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
234	Wet 10847E-27e	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
235	Wet 10847E-27f	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
236	Wet 10847E-27g	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
237	Wet 10847E-27h	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
238	Wet 10847E-27i	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
239	Wet 10847E-27j	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
240	Wet 10847E-27k	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
241	Wet 10847E-27l	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
242	Wet 10847E-27m	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
243	Wet 10847E-27n	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
244	Wet 10847E-27o	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
245	Wet 10847E-27p	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
246	Wet 10847E-27q	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
247	Wet 10847E-27r	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
248	Wet 10847E-27s	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
249	Wet 10847E-27t	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
250	Wet 10847E-27u	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
251	Wet 10847E-27v	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
252	Wet 10847E-27w	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
253	Wet 10847E-27x	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
254	Wet 10847E-27y	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
255	Wet 10847E-27z	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
256	Wet 10847E-27aa	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
257	Wet 10847E-27ab	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
258	Wet 10847E-27ac	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2.2	245	8.9	372	167	72	9	64	0	0	0.14	0.03	281	1.7
259	Wet 10847E-27ad	808400	488700	38.48.09	118.43.20	1.2 USGS	USGS	GM	-1111	DOM	1078	-9999	1	-1111	2	-1111	-1111	7/4/87	1180	7.2	8.1	30	23	2													

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PTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH	DEPTH

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SAMPLE	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG	AH	AI	AJ	AK	AL	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW	AX	AY	AZ	BA	BB	BC	BD	BE	BF	BG	BH	BI	BJ	BK	BL	BM	BN	BO	BP	BQ	BR	BS	BT	BU	BV	BW	BX	BY	BZ	CA	CB	CC	CD	CE	CF	CG	CH	CI	CJ	CK	CL	CM	CN	CO	CP	CQ	CR	CS	CT	CU	CV	CW	CX	CY	CZ	DA	DB	DC	DD	DE	DF	DG	DH	DI	DJ	DK	DL	DM	DN	DO	DP	DQ	DR	DS	DT	DU	DV	DW	DX	DY	DZ	EA	EB	EC	ED	EE	EF	EG	EH	EI	EJ	EK	EL	EM	EN	EO	EP	EQ	ER	ES	ET	EU	EV	EW	EX	EY	EZ	FA	FB	FC	FD	FE	FF	FG	FH	FI	FJ	FK	FL	FM	FN	FO	FP	FQ	FR	FS	FT	FU	FV	FW	FX	FY	FZ	GA	GB	GC	GD	GE	GF	GG	GH	GI	GJ	GK	GL	GM	GN	GO	GP	GQ	GR	GS	GT	GU	GV	GW	GX	GY	GZ	HA	HB	HC	HD	HE	HF	HG	HH	HI	HJ	HK	HL	HM	HN	HO	HP	HQ	HR	HS	HT	HU	HV	HW	HX	HY	HZ	IA	IB	IC	ID	IE	IF	IG	IH	II	IJ	IK	IL	IM	IN	IO	IP	IQ	IR	IS	IT	IU	IV	IW	IX	IY	IZ	JA	JB	JC	JD	JE	JF	JG	JH	JI	JJ	JK	JL	JM	JN	JO	JP	JQ	JR	JS	JT	JU	JV	JW	JX	JY	JZ	KA	KB	KC	KD	KE	KF	KG	KH	KI	KJ	KK	KL	KM	KN	KO	KP	KQ	KR	KS	KT	KU	KV	KW	KX	KY	KZ	LA	LB	LC	LD	LE	LF	LG	LH	LI	LJ	LK	LM	LN	LO	LP	LQ	LR	LS	LT	LU	LV	LW	LX	LY	LZ	MA	MB	MC	MD	ME	MF	MG	MH	MI	MJ	MK	ML	MN	MO	MP	MQ	MR	MS	MT	MU	MV	MW	MX	MY	MZ	NA	NB	NC	ND	NE	NF	NG	NH	NI	NJ	NK	NL	NM	NN	NO	NP	NQ	NR	NS	NT	NU	NV	NW	NX	NY	NZ	OA	OB	OC	OD	OE	OF	OG	OH	OI	OJ	OK	OL	OM	ON	OO	OP	OQ	OR	OS	OT	OU	OV	OW	OX	OY	OZ	PA	PB	PC	PD	PE	PF	PG	PH	PI	PJ	PK	PL	PM	PN	PO	PP	PQ	PR	PS	PT	PU	PV	PW	PX	PY	PZ	QA	QB	QC	QD	QE	QF	QG	QH	QI	QJ	QK	QL	QM	QN	QO	QP	QQ	QR	QS	QT	QU	QV	QW	QX	QY	QZ	RA	RB	RC	RD	RE	RF	RG	RH	RI	RJ	RK	RL	RM	RN	RO	RP	RQ	RR	RS	RT	RU	RV	RW	RX	RY	RZ	SA	SB	SC	SD	SE	SF	SG	SH	SI	SJ	SK	SL	SM	SN	SO	SP	SQ	SR	SS	ST	SU	SV	SW	SX	SY	SZ	TA	TB	TC	TD	TE	TF	TG	TH	TI	TJ	TK	TL	TM	TN	TO	TP	TQ	TR	TS	TT	TU	TV	TW	TX	TY	TZ	UA	UB	UC	UD	UE	UF	UG	UH	UI	UJ	UK	UL	UM	UN	UO	UP	UQ	UR	US	UT	UU	UV	UW	UX	UY	UZ	VA	VB	VC	VD	VE	VF	VG	VH	VI	VJ	VK	VL	VM	VN	VO	VP	VQ	VR	VS	VT	VU	VV	VW	VX	VY	VZ	WA	WB	WC	WD	WE	WF	WG	WH	WI	WJ	WK	WL	WM	WN	WO	WP	WQ	WR	WS	WT	WU	WV	WW	WX	WY	WZ	XA	XB	XC	XD	XE	XF	XG	XH	XI	XJ	XK	XL	XM	XN	XO	XP	XQ	XR	XS	XT	XU	XV	XW	XX	XY	XZ	YA	YB	YC	YD	YE	YF	YG	YH	YI	YJ	YK	YL	YM	YN	YO	YP	YQ	YR	YS	YT	YU	YV	YW	YX	YY	YZ	ZA	ZB	ZC	ZD	ZE	ZF	ZG	ZH	ZI	ZJ	ZK	ZL	ZM	ZN	ZO	ZP	ZQ	ZR	ZS	ZT	ZU	ZV	ZW	ZX	ZY	ZZ	Total	Notes

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							HI	HI	J	K	L	M	N	O	P	Q	R	S	T	U	
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	55.8	0	18.4	0	0	0	0	0	0	0	0	0	0	0
2	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.1	0	18.0	0	0	0	0	0	0	0	0	0	0	0
3	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
4	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
5	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
6	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
7	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
8	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
9	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
10	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
11	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
12	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
13	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
14	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
15	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
16	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
17	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
18	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
19	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
20	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
21	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
22	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
23	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
24	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
25	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
26	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
27	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
28	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
29	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
30	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
31	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
32	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
33	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
34	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
35	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
36	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
37	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
38	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
39	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
40	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
41	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
42	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
43	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
44	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
45	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
46	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
47	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
48	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
49	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
50	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
51	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
52	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
53	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
54	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
55	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
56	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
57	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
58	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
59	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
60	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
61	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
62	US-26F11CINOP30-20787	US-26F11H	2678	877.8192	Bradton et al. (1986)	Cinopitella	Electron microprobe	56.0	0	18.0	0	0	0	0	0	0	0	0	0	0	0
63	US-26F11C																				

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Rock/Mineral Chemistry, Braden et al. (1986)

Shannon

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A		B		C		D		E		F		G																			H		I		J		K		L		M		N		O		P		Q		R		S		T		U		V	
SAMPLE	DRILL HOLE NO.	DEPTH (FT)	DEPTH (M)	SOURCE	Rock/Mineral Type	Analytical Method	SiO2	TiO2	Al2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O	P2O5	H2O	Total Oxides	NOTES																																								
USWG-2FSPAR45*2430FT	USWG-2	2430	740.884	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	60.2	0.01	18.9	0	not meas.	not meas.	0	0	0	0.03	15.0	not meas.	not meas.	100.1																																								
USWG-2FSPAR47*4809FT	USWG-2	4809	1464.564	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	55.5	0	20.7	0.01	not meas.	not meas.	0	1.95	0.06	10.7	0.38	not meas.	not meas.	99.0																																								
USWG-2FSPAR49*4809FT	USWG-2	4809	1464.564	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	55.0	0	19.7	0.01	not meas.	not meas.	0	0	0.18	0.32	15.2	not meas.	not meas.	98.0																																								
USWG-2FSPAR49*4838FT	USWG-2	4838	1474.9324	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	56.9	0	16.5	0	not meas.	not meas.	0	0	0.1	0.17	15.1	not meas.	not meas.	98.6																																								
USWG-2FSPAR50*4838FT	USWG-2	4838	1474.9324	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	56.7	0	19.5	0.03	not meas.	not meas.	0	0.36	0	11.7	0.06	not meas.	not meas.	100.4																																								
USWG-2FSPAR51*4838FT	USWG-2	4838	1474.9324	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	56.7	0	19.7	0.04	not meas.	not meas.	0	0.69	0	11.5	0.09	not meas.	not meas.	100.7																																								
USWG-2FSPAR51*4899FT	USWG-2	4899	1736.1408	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	56.6	0.03	18.1	0	not meas.	not meas.	0	0.47	0	11.6	0.02	not meas.	not meas.	99.9																																								
USWG-2FSPAR53*5920FT	USWG-2	5920	1773.538	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	57	0	20.1	0.04	not meas.	not meas.	0	0.84	0.2	11.5	0.02	not meas.	not meas.	99.8																																								
USWG-2FSPAR54*5895FT	USWG-2	5895	1796.796	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	56.5	0	19.5	0.07	not meas.	not meas.	0	0.35	0	11.5	0.07	not meas.	not meas.	101.7																																								
USWG-2FSPAR55*5895FT	USWG-2	5895	1796.796	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	56.7	0	19.5	0	not meas.	not meas.	0	0.46	0.15	11.4	0.04	not meas.	not meas.	99.1																																								
USWG-2FSPAR56*5963FT	USWG-2	5962	1825.3615	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	56.7	0	19.5	0	not meas.	not meas.	0	0.5	0.03	11.4	0.06	not meas.	not meas.	99.2																																								
USWG-2FSPAR56*5963FT	USWG-2	5962	1825.3615	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	56.3	0	19	0	not meas.	not meas.	0	0	0.05	11.9	0.04	not meas.	not meas.	99.2																																								
USWG-3FSPAR58*4708FT	USWG-3	4708	1434.9994	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	53.5	0.03	18	0.08	not meas.	not meas.	0	0.08	1.05	0.42	15.5	not meas.	not meas.	98.6																																								
USWG-4FSPAR59*7738FT	USWG-4	7738	934.5434	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	56.4	0	17.7	0	not meas.	not meas.	0	0.03	0.07	0.03	15.2	not meas.	not meas.	99.3																																								
J-13FSPAR60*2990FT	J-13	2990	908.304	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	56.4	0	17.7	0	not meas.	not meas.	0	0.03	0.05	0.05	16.1	not meas.	not meas.	100.3																																								
J-13FSPAR61*2990FT	J-13	2990	908.304	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	57.2	0	20.1	0	not meas.	not meas.	0	0.58	0	11.8	0.06	not meas.	not meas.	99.8																																								
J-13FSPAR62*2990FT	J-13	2990	908.304	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	57.2	0	19.5	0	not meas.	not meas.	0	0.19	0	12	0.04	not meas.	not meas.	99.0																																								
3-15-81-4FSPAR63	outcrop	0	0	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	56.3	0	19.5	0	not meas.	not meas.	0	0.33	0	12	0.04	not meas.	not meas.	100.3																																								
3-15-81-4FSPAR64	outcrop	0	0	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	57.5	0	17.5	0	not meas.	not meas.	0	0	0	0.23	15.2	not meas.	not meas.	100.5	Outcrop at Prax Pass, N. Yucca Mt., Nonwadded tuff near base of Calico Hills tuff, Nevada State Records, 788500N, 581000E																																							
3-15-81-4FSPAR65	outcrop	0	0	Braden et al. (1990)	Authigenic feldspar	Electron microprobe	57.5	0	17.5	0	not meas.	not meas.	0	0	0	0.17	15.4	not meas.	not meas.	100.6	Outcrop at Prax Pass, N. Yucca Mt., Nonwadded tuff near base of Calico Hills tuff, Nevada State Records, 788500N, 581000E																																							

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An additional, more comprehensive source of water chemistry data is found in the USGS report of Perfect et al. (1995).

Perfect, D.L., C.C. Faunt, W.C. Steinkampf, and A.K. Turner. 1995. *Hydrochemical Data Base for the Death Valley Region, California and Nevada*. USGS Open-File Report 94-305. Denver, CO: U.S. Geological Survey.

JRL

This report includes compressed Lotus 1-2-3 (*.WK1) files with major and minor element analyses compiled over several decades for the region surrounding Yucca Mountain. One contains the raw data for over 4700 wells and springs from USGS and DOE reports and the USGS National Water Information Service (NWIS) database. A second file has been edited to remove duplicates, make chemical data consistent, and calculate charge balance. The "editing" philosophy used by Perfect et al. (1995) is described in the report. These data were not generally collected under a DOE-approved QA program, but are freely used here. The sources referenced in Perfect et al. (1995) should be consulted for determining the quality of the data.

see pgs. 33+34 1/18/96 DRJ

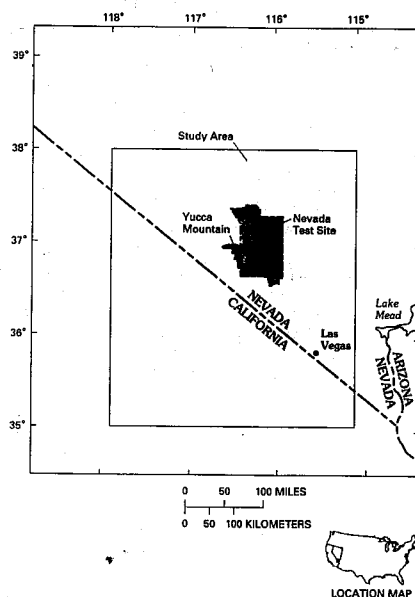
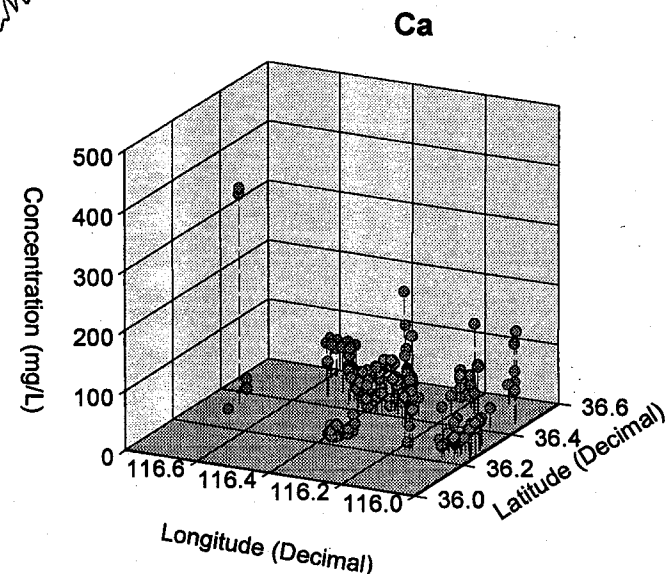
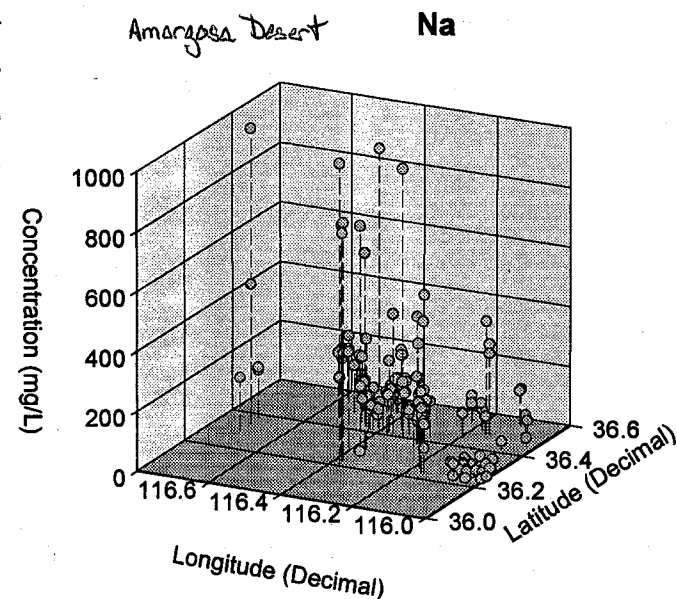


Figure 1. Area of interest.

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Example of major element trends
from Perle et al. (1995)
Amargosa Desert (graphics from Sigma Plot, Version 2.0)



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Table 3. Data sources and codes

Data source code	Data Sources
1	Benson and McKinley, 1985
2	Benson and others, 1983
3	Blankennagel and Weir, 1973
4	Calzia, 1979a
5	Calzia, 1979b
6	Claassen, 1973
7	Claassen, 1983
8	Claassen, H.C., U.S. Geological Survey, unpublished data
9	Cooperative Extension U.S. Department of Agriculture
10	Craig and Robison, 1984
11	Crowley, 1979a
12	Crowley, 1979b
13	Czamecki, J., U.S. Geological Survey, unpublished data
14	Dockter and Server, 1979
15	Dockter, 1979
16	Dudley and Larson, 1976
17	Environmental Protection Agency (EPA), unpublished data
18	Glancy, 1968
19	Hardman and Miller, 1934
20	Hunt and others, 1966
21	Lahoud and others, 1984
22	Malmberg and Eakin, 1962
23	Malmberg, 1967
24	Miller, 1977
25	Moore, 1961
26	U.S. Geological Survey, National Water Data Storage and Retrieval System (WATSTORE)
27	Nichols and Davis, 1979
28	Robinson and Beetem, 1975
29	Rush, 1968
30	Schaefer and others, 1992
31	Schoff and Moore, 1964
32	Thomas and others, 1991
33	Thomas, J. (written communication, 1989)
34	U.S. Energy Research and Development Administration
35	U.S. Geological Survey, National Water Information System (NWIS-1)
36	U.S. Geological Survey, unpublished data
37	Waddell, 1984
38	Walker and Eakin, 1963
39	White, 1979
40	Winograd and Thordarson, 1975
41	Winograd, U.S. Geological Survey, unpublished data
42	Whitfield and others, 1985
43	Whitfield, U.S. Geological Survey, unpublished data
44	Young, 1972

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DRJPerfect et al. (1995)
Original Data Sources

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SUMMARY 9

10 Hydrochemical Data Base for the Death Valley Region, California and Nevada

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Radionuclide Thermodynamic Data

I. Introduction

For the geochemical aspects of HLW disposal, thermodynamic and kinetic data are necessary to model processes such as dissolution of waste forms, precipitation of secondary phases, and retardation of radionuclide transport. There are currently 9 CDMs related to geochemistry, and as identified in Turner and Pickett (1994), most of these CDMs will require some type of thermodynamic data and kinetic rate data to assist in review of the License Application (LA). These include:

- 3.2.3.1 - (FAC) Nature and Rates of Geochemical Processes
- 3.2.3.2 - (FAC) Geochemical Conditions
- 3.2.3.3 - (FAC) Mineral Assemblages
- 3.2.3.4 - (PAC) Groundwater Conditions and the Engineered Barrier System
- 3.2.3.5 - (PAC) Geochemical Processes
- 3.2.3.7 - (PAC) Gaseous Radionuclide Movement

For those CDMs that require confirmatory or independent calculations (Types 4 and 5), accurate state-of-the-art data are needed to produce reliable results. For those CDMs that require checking DOE calculations (Type 3), it is important to confirm that accurate thermodynamic data have been used in the models.

II. Statement of the Problem

Basic thermodynamic and kinetic rate data for gases, solids, and aqueous species are applicable to any system, in addition to Yucca Mountain. These data are typically kept in electronic databases e.g., GEMBOCHS (USDOE, 1993), and are formatted for use with a particular geochemical speciation codes such as EQ3/6, PHREEQE, or MINTEQA2. Many of the thermodynamic databases that are available have been developed to address a wide range of geochemical problems. For this reason, they are commonly quite large (e.g., EQ3/6 has over 1500 aqueous species, gases, and solids) and contain a large number of species that are not directly relevant to waste disposal at Yucca Mountain. In addition, the size of these databases makes them cumbersome to use and slows down geochemical calculations.

The results of geochemical modeling are strongly dependent on the thermodynamic database used. Several different geochemical codes are currently used at CNWRA and NRC (e.g., EQ3/6, PHREEQE, MINTEQA2, GEM). If the databases contain different values, then the results will not be strictly comparable. While there is typically good agreement between different databases on thermodynamic data for common species such as CO_2 and quartz, there is much uncertainty for many of the elements of concern in HLW disposal (Pu, Np, Am, U, Tc); for example, equilibrium constants from different sources may vary by many orders of magnitude. Given these uncertainties, in an effort to develop a complete database, there is the possibility that inappropriate values have been incorporated.

At CNWRA, the EQ3/6 database under development at Lawrence Livermore National Laboratory is the starting point for other radiochemical databases. For example, data for 13 different radioelements have been taken from the EQ3/6 database and added to the MINTEQA2 database currently used in the Sorption Modeling for HLW Performance Assessment Research Project, and the EQ3/6 database is used by the reactive transport codes GEM and MULTIFLOW under development at CNWRA. However, recent scoping calculations (Table 1) performed at CNWRA indicate that for some uranium-silicates, the equilibrium constant (Log K) currently in the EQ3/6 database differ from values calculated using recommended free energies of formation by up to 9 orders of magnitude. This has significant implications for solubility and transport calculations, and also leads to uncertainty about other values in the database.

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Table 1. Thermodynamic data for uranyl silicate minerals and comparison with the EQ3/6 database (Data0.com.r16 release). The difference values are defined as (EQ3/6 value) - (Calculated Values).

Mineral	EQ3/6 Data0.com.r16		New Estimate _{a,b}		Difference	
	ΔG_0 (kJ/mol)	Log K	ΔG_0 (kJ/mol)	Log K	ΔG_0 (kJ/mol)	Log K
Uranophane	-4975	17.289	-6213	8.123	1238	9.166
Soddyite	-3685	0.395	-3706	-3.285	21	3.680
Weeksite	-9043	15.380	-9039	16.081	-4	-0.701

- a. Recent data taken from McKenzie (unpublished) based on Nguyen et al. (1991).
b. Free energies (ΔG_0 in kJ/mol) for aqueous species are: $\text{UO}_2^{2+} = -952.556$; $\text{K}^+ = -282.462$; $\text{Ca}^{2+} = -552.790$; $\text{SiO}_2(\text{aq}) = -833.411$; $\text{H}_2\text{O} = -237.182$. Data for aqueous species are taken from EQ3/6 database (Data0.com.r16 release).

II. Proposed Work

Although it is beyond the intended scope of this activity to undertake the extensive review and critical evaluation of the current literature that is necessary to develop a large thermodynamic database, it should be possible to select a limited set of critical elements such as the actinides, and identify critical species such as the uranium-silicates for closer inspection. Since the EQ3/6 database is already the basis for much of the radionuclide geochemical modeling work done by the DOE and by the CNWRA and NRC, we propose a basic effort to spot check selected thermodynamic data in this database by comparison to other databases, and by checking the original data source where possible. If CNWRA staff can develop acceptable values for selected critical species, then the different geochemical codes used in Research and Technical Assessment will be working from the same baseline and model results will be comparable.

Work would include:

- Identification of critical radioelements such as Np, Am, Pu, U, and Tc for which the CNWRA staff believe thermodynamic data are uncertain.
- Identification of key aqueous species and minerals. Uranium-silicates are of particular interest as solubility-limiting phases in evaluating uranium natural analogs such as Peña Blanca.
- For those identified elements/components of interest, compilation and documentation of free energies of formation, as well as critical data review in a spreadsheet format. This type of approach would provide convenient tabulation of the data, and would accommodate geochemical modeling using either free energies or equilibrium constants that could be calculated from the tabulated data. It may also be possible to compile heat capacity and enthalpy data for extrapolating to elevated temperatures. A similar approach has been used in earlier NRC-sponsored work at Sandia National Laboratories (Phillips et al., 1988).

IV. Anticipated Products

This work was originally envisioned as an ongoing study designed to take advantage of advances in the available thermodynamic data. At the completion of this initial limited study, it is anticipated that there

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would be a spreadsheet containing critically reviewed free energies of formation for a limited number of important elements/components, together with documentation of data sources. These free energies could then be combined according to reaction stoichiometry to develop free energies and equilibrium constants for species and solids important to Research and Technical Assessment needs. This approach would be used to augment the existing EQ3/6 database and provide a standard baseline for geochemical modeling at CNWRA and NRC. The spreadsheet tabulation could be expanded to include other species and solids of interest, and would allow for quick incorporation of new data as they become available.

The final product of this work has been the development of a user-friendly, limited-scale thermodynamic database for Np, Pu, Am, Th, and Tc, with additional work on uranyl silicates (soddyite, weeksite, boltwoodite, and uranophane). The software used for this effort has been Claris Filemaker Pro for Windows, Version 2.1. The database was prepared by Dr. Yiming Pan, working as SwRI temporary staff for CNWRA. Dr. Pan has previously worked for CNWRA as part of the Geochemical Natural Analogues Research Project. Filemaker Pro, Version 2.1 is a commercially available software package used for data compilation and display. No modifications were made to the code as a part of this project, and only the executable is available to CNWRA.

Complete electronic files are included on disks in the envelope at the back of this scientific notebook. A general outline of the data formulation and data sources is included below.

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EQ3/6 database (Data0.com.r16, June 92 release) is the version used in subsequent calculations

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Filemaker Pro has been used to set up 16 types of data display

1) General tabulation of all aqueous species/solids for a given radioelement

2) Detailed tabulation of data with critical comments for a given species/solid for a radioelement

Display Type 1 - General Tabulation - Np solids

Table D Thermodynamic Properties of Neptunium Solid Phases

Species	G_f° (kJ/mol)	H_f° (kJ/mol)	S° (J/mol-K)	Log K°	Reference
Np - 1	0.000	0.000	50.460	-171.2094	[EQ3/6]
Np - 2	0.000	0.000	50.30		[88PHI/HAL]
Np ₂ O ₅ - 1	-2012.956	2092.000	2092.000	-9.5000	[EQ3/6]
Np ₂ O ₅ - 2	-2013.000	-2147.250	163.00		[88PHI/HAL]
NpO ₂ - 1	-1021.800	-1074.065	80.300	7.8026	[EQ3/6]
NpO ₂ - 2	-1021.800	-1074.000	80.30		[88PHI/HAL]
NpO ₂ (OH) - 1	-1128.000	-1224.156	101.000	-4.2364	[EQ3/6]
NpO ₂ (OH) - 2	-1128.000	-1224.100	101.00		[88PHI/HAL]
NpO ₂ (OH) ₂ - 1	-1236.000	-1377.149	118.000	-5.9851	[EQ3/6]
NpO ₂ (OH) ₂ - 2	-1236.000	-1377.010	118.00		[88PHI/HAL]
Np(OH) ₄ - 1	-1447.000	-1620.851	139.000	-0.8103	[EQ3/6]
Np(OH) ₄ - 2	-1447.000	-1621.365	139.00		[88PHI/HAL]
NpO ₃ H ₂ O - 1	-1247.000	-1379.000	146.000		[88PHI/HAL]

Type 1 Display

General Tabulation - Np aqueous species

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Table D Thermodynamic Properties of Neptunium Aqueous Species

Species	G_f° (kJ/mol)	H_f° (kJ/mol)	S° (J/mol-K)	Log K°	Reference
Np ⁺⁺⁺ - 1	-517.100	-527.099	-179.100	-18.2885	[EQ3/6]
Np ⁺⁺⁺ - 2	-517.100	-527.200	-179.10		[88PHI/HAL]
Np ⁺⁺⁺⁺ - 1	-502.900	-555.999	-389.000		[EQ3/6]
Np ⁺⁺⁺⁺ - 2	-502.900	-556.100	-389.10		[88PHI/HAL]
NpO ₂ ⁺ - 1	-915.000	-977.986	-21.000	9.8683	[EQ3/6]
NpO ₂ ⁺ - 2	-915.000	-978.200	-21.00		[88PHI/HAL]
NpO ₂ ⁺⁺ - 1	-795.800	-860.473	-92.000	9.7615	[EQ3/6]
NpO ₂ ⁺⁺ - 2	-795.800	-860.600	-94.00		[88PHI/HAL]
NpO ₂ (OH) (aq) - 1	-1101.379	2092.000	2092.000	-8.9000	[EQ3/6]
NpO ₂ (OH) (aq) - 2	-1101.000	-1220.104	25.00		[88PHI/HAL]
NpO ₂ OH ⁺ - 1	-1003.298	2092.000	2092.000	-5.2000	[EQ3/6]
NpO ₂ OH ⁺ - 2	-1004.000	-1102.990	24.00		[88PHI/HAL]
(NpO ₂) ₂ (OH) ₂ ⁺⁺ - 1	-2029.432	-2092.000	-2092.000	-6.4000	[EQ3/6]
(NpO ₂) ₂ (OH) ₂ ⁺⁺ - 2	-2029.380	-2246.210	-14.00		[88PHI/HAL]
(NpO ₂) ₃ (OH) ₅ ⁺ - 1	-3473.419	-2092.000	-2092.000	-17.5000	[EQ3/6]
(NpO ₂) ₃ (OH) ₅ ⁺ - 2	-3474.000	-3897.550	116.00		[88PHI/HAL]
Np(OH) ₄ (aq) - 1	-1396.828	2092.000	2092.000	-9.6000	[EQ3/6]
Np(OH) ₄ (aq) - 2	-1397.000	-1699.900	75.00		[88PHI/HAL]

Revised Date: January 2, 1996

Table D Thermodynamic Properties of Neptunium Aqueous Species

Species	G_f° (kJ/mol)	H_f° (kJ/mol)	S° (J/mol-K)	Log K°	Reference
NpOH ⁺⁺⁺ - 1	-734.371	2092.000	2092.000	-1.0000	[EQ3/6]
NpOH ⁺⁺⁺ - 2	-734.000	-790.540	-167.00		[88PHI/HAL]
Np(OH) ₂ ⁺⁺ - 1	-961.282	2092.000	2092.000	-2.8000	[EQ3/6]
Np(OH) ₂ ⁺⁺ - 2	-961.000	-1050.400	-44.00		[88PHI/HAL]
Np(OH) ₃ ⁺ - 1	-1181.336	2092.000	2092.000	-5.8000	[EQ3/6]
Np(OH) ₃ ⁺ - 2	-1181.000	-1313.705	44.00		[88PHI/HAL]
Np(OH) ₅ ⁻ - 1	-1607.183	2092.000	2092.000	-14.3000	[EQ3/6]
Np(OH) ₅ ⁻ - 2	-1607.000	-1863.350	96.00		[88PHI/HAL]
NpOH ⁺⁺ - 1	-714.326	2092.000	2092.000	-7.0000	[EQ3/6]
NpOH ⁺⁺ - 2	-714.300	-726.900	-75.00		[88PHI/HAL]
NpO ₂ (CO ₃) ₂ ⁻ - 1	-1931.677	-2183.069	170.000	-6.6576	[EQ3/6]
NpO ₂ (CO ₃) ₂ ⁻ - 2	-1953.800	-2221.700	116.10		[88PHI/HAL]
NpO ₂ CO ₃ (aq)	-1360.000	-1540.000	-36.00		[88PHI/HAL]
NpO ₂ (CO ₃) ₂ ⁻ - 1	-2010.922	-2299.685	110.002	-13.6576	[EQ3/6]
NpO ₂ (CO ₃) ₂ ⁻ - 2	-2009.600	-2298.800	110.00		[88PHI/HAL]
NpO ₂ (CO ₃) ₃ ⁻ - 1	-2547.466	-2977.594	79.998	-22.4864	[EQ3/6]
NpO ₂ (CO ₃) ₃ ⁻ - 2	-2547.000	-2977.700	80.00		[88PHI/HAL]
NpO ₂ (CO ₃) ₃ ⁻ - 1	-2496.191	-2927.110	12.000	-10.5864	[EQ3/6]

Table D Thermodynamic Properties of Neptunium Aqueous Species

Species	G_f° (kJ/mol)	H_f° (kJ/mol)	S° (J/mol-K)	Log K°	Reference
NpO ₂ (CO ₃) ₃ ⁻ - 2	-2505.200	-2927.900	38.10		[88PHI/HAL]
NpO ₂ CO ₃ ⁻ - 1	-1469.241	-1598.752	200.000	-5.7288	[EQ3/6]
NpO ₂ CO ₃ ⁻ - 2	-1470.020	-1599.900	200.00		[88PHI/HAL]
Np(CO ₃) ₅ ⁻ - 1	-3361.434	-3912.931	160.000	-13.3440	[EQ3/6]
Np(CO ₃) ₅ ⁻ - 2	-3361.000	-3912.310	160.00		[88PHI/HAL]
NpO ₂ (OH) ₂ ⁻ - 1	-1262		40	-22.4	[89LEM/GAR]

Display Type II - Detailed Tabulation Np-solid

Table D (Cont'd)

Species	NpO ₂ - 1
del G_f° (kJ/mol)	-1021.800
del H_f° (kJ/mol)	-1074.065
S° (J/mol-K)	80.300
Log K°	7.8026
Reaction	Np ⁺⁺⁺⁺ + 2H ₂ O = NpO ₂ + 4H ⁺
Reference	[EQ3/6]

Data Assessment

1. The data are from review evaluations. The data source is from [84LEM].
2. The log K° value in [EQ3/6] is for dissolution of NpO₂.
3. Using del G_f° [Np⁺⁺⁺⁺] = -502.900 kJ/mol and del G_f° [H₂O] = -237.18 kJ/mol both from EQ3/6, we then have del G_f° = -44.538 kJ/mol and del G_f° = -1021.798 kJ/mol.

Back-calculating ΔG_f° in the data assessment comments provides assurance that the log K used in EQ3/6 (Data.com.r16) is consistent with free energy given in original data source

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Table D (Cont'd)

Species	Np ⁺⁺⁺ - 1
G _f ^o (kJ/mol)	-517.100
H _f ^o (kJ/mol)	-527.099
S ^o (J/mol-K)	-179.100
Log K ^o	-18.2885
Reaction	Np ⁺⁺⁺⁺ + 0.5H ₂ O = Np ⁺⁺⁺ + 0.25O ₂ + H ⁺

Reference [EQ3/6]

Data Assessment

1. The data are from review evaluations. The data source is from [84LEM].
2. The log K^o value in [EQ3/6] is for dissolution of Np⁺⁺⁺.
3. Using del G_f^o [Np⁺⁺⁺⁺] = -502.9 kJ/mol and del G_f^o [H₂O] = -237.18 kJ/mol both from EQ3/6, we then have del G_r^o = 104.391 kJ/mol and del G_f^o = -517.098 kJ/mol.

Original Data Sources

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Reorganization of CNWRA. Research transferred to
20-5708-871 - KT1 Radionuclide Transport
effective 1/20/96 (DB)

4/12/96 49
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DB

Some modifications have been made to the comprehensive water chemistry database of Perfect et al. (1995).

Perfect, D.L., C.C. Faunt, W.C. Steinkampf, and A.K. Turner. 1995. *Hydrochemical Data Base for the Death Valley Region, California and Nevada*. USGS Open-File Report 94-305. Denver, CO: U.S. Geological Survey.

The Lotus 1-2-3 file DATAEDIT.WK1 file of Perfect et al. (1995) has been converted to an Excel 4.0 for Windows file (*.XLS). As mentioned earlier, the second file has been edited by Perfect et al. (1995) to remove duplicates, make chemical data consistent, and calculate charge balance. The "editing" philosophy used by Perfect et al. (1995) is described in the report.

The edited file consists of some 3733 water chemistry analyses. Most of the analyses are replicated samples collected at different times from springs and wells in the Yucca Mountain region. Complete major and minor element concentrations are commonly reported, but in some instances only trace contaminants such as Cd, Cu, and Zn were reported for a given analyses. All concentrations are reported in mg/L, and -99998 indicates no reported value.

Once entered in Excel, the data files have been modified using spreadsheet formulas in several ways:

1) A column was added and Arc ID# were assigned to each analysis. The analyses were first ordered by increasing latitude from south to north, and numbered sequentially from 1-3733. These ID#'s should be maintained in subsequent analyses.

2) Sampling locations are reported in terms of latitude and longitude (degrees, minutes, seconds). For incorporation into existing ArcInfo coverages, additional columns have been developed that convert locations first to decimal degrees (degrees + (minutes/60) + (seconds/3600)), and then projected to UTM coordinates. The UTM projection conversion is based on UTM Zone 18, with a central meridian of -117°, and using the Clarke 1866 ellipsoid. The formulas used in the conversion were taken from:

Snyder, J. 1987. *Map Projections, A Working Manual*. USGS Professional Paper 1395. Washington, DC: U.S. Geological Survey.

and checked against examples given in Snyder (1987) (see below).

3) Analyses for each element are checked for positive concentrations (to account for the -99998, not reported), converted to molality (m_i), and total groundwater ionic strength was calculated such that:

$$I = 0.5(\sum m_i z_i^2)$$

This requires adding two rows. The first added row identifies the assumed aqueous species. In most cases, this was assumed to be the unspciated cation or anion (e.g., Ca^{++} , Cl^-), but in some cases, particularly for anions, other species were assumed such as SO_4^{-2} , PO_4^{-3} , and $\text{VO}_2(\text{OH})_3^{-2}$. The second added row contains the gram formula weight for each of the assumed species.

Confirmatory calculations to follow

Added
Columns

Comparison exact
to 1 meters

UTM conversion formulas from Snyder (1987)

$I.S. \text{ major} = \text{Ionic strength major} + \text{minor elements: } Ca^{++} \text{ to } SiO_2(aq)$
 $I.S. \text{ trace} = \text{Ionic strength trace elements: } As \text{ to } Hg$
 $I.S. \text{ total} = \text{Ionic strength (major)} + I.S. (\text{trace})$

Broken into three columns due to Excel 4.0 limits on formula length

Added columns.

DO

UIN
transformation

CCS	PO4	NO3	F	S02	As	Ba	Be	B	Br	C	Ca	Co	Cu	Fe	TOTAL Fe	Pb	Mn	Mo	N	Na	Ag	Sr	V	Zn	Li	So4-2	I
CO2-3	PO4-3	NO3-	F-	S02(g)	H4SiO4	Ba2+	Be++	B	BrO3(g)	Ca++	Co++	Cu++	Cu++	Fe++		Pb++	Mn++	Mo	N	Na	Ag	Sr++	V	Zn++	Li	So4-2	I
60.201	94.937	62	18	69.08	139.82713	107.827	61.83202	112.111	51.8691	55.3592	63.546	55.847	207.2	54.8305	58.89	107.6892	87.822	153.88322	6.841	142.8976	128.90447						
498988.00	0.00184854	498988.00	498988.00	43.00	498988.00	498988.00	498988.00	10.80	498988.00	498988.00	498988.00	498988.00	498988.00	0.07	498988.00	498988.00	0.03	498988.00	498988.00	498988.00	498988.00	0.89	498988.00	498988.00	0.03	498988.00	0.38
498989.00	0	498989.00	7.10	28.00	498988.00	498988.00	498988.00	11.00	498988.00	498988.00	498988.00	498988.00	498988.00	0.02	498988.00	498988.00	0.60	498988.00	498988.00	498988.00	498988.00	2.30	498988.00	498988.00	0.10	498988.00	0.36
498990.00	0	498990.00	4.70	28.00	498989.00	498989.00	498989.00	1.80	498988.00	498988.00	498988.00	498988.00	498988.00	0.08	498988.00	498988.00	0.49	498988.00	498988.00	498988.00	498988.00	11.00	498988.00	498988.00	0.55	498988.00	0.21
498991.00	0	498991.00	7.80	15.00	498989.00	498989.00	498989.00	0.36	498988.00	498988.00	498988.00	498988.00	498988.00	0.03	498988.00	498988.00	0.01	498988.00	498988.00	498988.00	498988.00	0.83	498988.00	498988.00	0.08	498988.00	0.07
498992.00	0	498992.00	498992.00	46.00	498989.00	498989.00	498989.00	498989.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00
498993.00	0.00	498993.00	498993.00	56.00	498989.00	498989.00	498989.00	498989.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00
498994.00	0.00	498994.00	498994.00	1.20	498989.00	498989.00	498989.00	15.00	498988.00	498988.00	498988.00	498988.00	498988.00	0.03	498988.00	498988.00	0.07	498988.00	498988.00	498988.00	498988.00	1.80	498988.00	498988.00	4.70	498988.00	0.16
498995.00	0.00	498995.00	498995.00	75.00	498989.00	498989.00	498989.00	3.10	498988.00	498988.00	498988.00	498988.00	498988.00	0.02	498988.00	498988.00	0.14	498988.00	498988.00	498988.00	498988.00	1.80	498988.00	498988.00	0.37	498988.00	0.05
498996.00	0	498996.00	1.00	17.00	498989.00	498989.00	498989.00	1.40	498988.00	498988.00	498988.00	498988.00	498988.00	0.02	498988.00	498988.00	0.07	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00	498988.00
498997.00	0	498997.00	498997.00	65.00	498989.00	498989.00	498989.00	0.09	498988.00	498988.00	498988.00	498988.00	498988.00	0.13	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
498998.00	D103691.135	498988.00	0.80	15.00	498988.00	498988.00	498988.00	0.09	498988.00	498988.00	498988.00	498988.00	498988.00	0.09	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
498999.00	0.00	498999.00	498999.00	59.00	498988.00	498988.00	498988.00	0.20	498988.00	498988.00	498988.00	498988.00	498988.00	0.20	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499000.00	0.00	498999.00	498999.00	1.00	498989.00	498989.00	498989.00	0.20	498988.00	498988.00	498988.00	498988.00	498988.00	0.20	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499001.00	0.00	498999.00	498999.00	2.00	498989.00	498989.00	498989.00	0.25	498988.00	498988.00	498988.00	498988.00	498988.00	0.25	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499002.00	0.00	498999.00	498999.00	2.10	498989.00	498989.00	498989.00	0.20	498988.00	498988.00	498988.00	498988.00	498988.00	0.20	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499003.00	12.00	498999.00	498999.00	19.00	498989.00	498989.00	498989.00	0.20	498988.00	498988.00	498988.00	498988.00	498988.00	0.20	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499004.00	498988.00	498999.00	498999.00	41.00	498988.00	498988.00	498988.00	0.25	498988.00	498988.00	498988.00	498988.00	498988.00	0.25	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499005.00	498988.00	498999.00	498999.00	55.00	498988.00	498988.00	498988.00	0.25	498988.00	498988.00	498988.00	498988.00	498988.00	0.25	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499006.00	0.00	498989.00	17.00	0.80	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499007.00	0.00	498989.00	498989.00	1.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499008.00	498988.00	498989.00	498988.00	2.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499009.00	498988.00	498989.00	498988.00	2.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499010.00	498988.00	498989.00	498988.00	2.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499011.00	0.00	498989.00	498988.00	17.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499012.00	0.00	498989.00	498988.00	17.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499013.00	0.00	498989.00	498988.00	17.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499014.00	0.00	498989.00	498988.00	17.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499015.00	0.00	498989.00	498988.00	17.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499016.00	0.00	498989.00	498988.00	17.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499017.00	0.00	498989.00	498988.00	17.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499018.00	0.00	498989.00	498988.00	17.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499019.00	0.00	498989.00	498988.00	17.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	498988.00	0.31	498988.00	498988.00	0.02	498988.00	0.03
499020.00	0.00	498989.00	498988.00	17.00	498989.00	498989.00	498989.00	0.21	498988.00	498988.00	498988.00	498988.00	498988.00	0.21	498988.00	498988.00	0.00	498988.00	498988.00	498988.00	4						

$I.S. \text{ major} = \text{Ionic strength major} + \text{minor elements: } Ca^{++} \text{ to } SiO_2(aq)$
 $I.S. \text{ trace} = \text{Ionic strength trace elements: } As \text{ to } Hg$
 $I.S. \text{ total} = \text{Ionic strength (major)} + I.S. (\text{trace})$

Added columns.

DO

UIN
transformation

Confirmatory I.S. calculations for Arc ID# 1

$$I = 0.5 * \left[\left(\frac{15}{4000} \right) * 10^{-3} + \left(\frac{2.8}{2431} * 10^{-3} + \frac{2}{2} \right) + \left(\frac{1650}{22.44} * 10^{-3} \right. \right]$$

[illegible]

$$\begin{bmatrix} \frac{1}{183} * 0.2 \\ \frac{1}{359} * 0.4 \\ \frac{1}{55} * 0.7 \\ \frac{1}{83} * 1.2 \end{bmatrix} + \begin{bmatrix} \frac{0.7}{55} * 7^2 \\ \frac{0.3}{83} * 17^2 \\ \frac{0.3}{54} * 27^2 \\ \frac{0.3}{84} * 37^2 \end{bmatrix} + \begin{bmatrix} \frac{0.6}{83} * 2^2 \\ \frac{0.6}{83} * 6^2 \\ \frac{0.6}{83} * 12^2 \\ \frac{0.6}{84} * 12^2 \end{bmatrix} + \begin{bmatrix} \frac{0.38}{126} * 84^2 \\ \frac{0.38}{126} * 84^2 \\ \frac{0.38}{126} * 84^2 \\ \frac{0.38}{126} * 84^2 \end{bmatrix}$$

$$= 0.077345$$
$$= 7.7345 \times 10^{-2}$$

vs.

spreadsheet $77345 \times 10^{-2} \text{ m}$

agreement in rounding error.

6/21/96
DR

Two FORTRAN 77 programs were developed to help in the interpretation of the water chemistry compilation of Perfect et al. (1995). Source codes are included below.

The first program is entitled MINTMK and is designed to go line by line through the Perfect et al. (1995) database and read the reported values column by column and assign them to the appropriate value. These must be read in the order in which they are entered in Perfect et al. (1995). The major elements pH, Ca, Mg, Na, K, HCO_3^- , CO_3^{2-} , SO_4^{2-} , Cl, F, and $\text{SiO}_2(\text{aq})$ are then written to create an input file appropriately formatted for MINTEQA2, Version 3.11. In the MINTEQA2 file, the intermediate output option is specified, the pH and temperature are fixed at the measured values, Eh is unspecified, and all mineral precipitation is suppressed.

The second program, called MNTFIL is designed to read a MINTEQA2 output file (Intermediate level) line-by-line searching for key phrases. The first phrase "Part 1 of Output File" indicates the start of each file, and then the words 'co2 (g)', 'calcite', and 'cristobalite' are searched for. Once these key words are found, the value for log P(CO_2), and the saturation indices for calcite and cristobalite are written to a comma-delimited ASCII file. If key words are not found, the letters n.d. (not determined) are entered in the ASCII file. The ArcID# as discussed above is used to tie these values to the original dataset for plotting in GIS format.

It should be noted that these programs can be relatively easily modified to write other variables to the MINTEQA2 input files or search for additional phrases in the MINTEQA2 output file.

For testing these programs, the dataset of Perfect et al. (1995) was edited according to the following criteria:

- 1) Ca++ is reported (positive values only)
- 2) Either CO_3^{2-} and/or HCO_3^- are reported (positive values only)
- 2) pH is reported (values between 1 and 14)
- 3) The water analysis is charged balanced as described and reported by Perfect et al. (1995)

This resulted in a dataset of about 1448 entries from the original 3733. The ArcID# assigned above maintains the relationship to the original Perfect et al. (1995) database.

6/21/96
DR

PROGRAM MINTMK Pg.1

```

C 45678901234567890123456789012345678901234567890123456789012
C The following program is a feeble attempt to read hydrochemical
C input files and prepare files suitable for input into MINTEQA2
C Version 3.11. This program was prepared by D.R. Turner for the
C Center For Nuclear Waste Regulatory Analyses in San Antonio, TX
C for the Radionuclide Transport KTI 20-5708-871. Many of the
C necessary parameters/flags are hard-wired and cannot currently be
C modified by the user during the run session. (05/31/96)

```

```

C CHARACTER Name*40,Siteid*15,Arcid*4,Balanc*2,DatSrc*10,Lab*8,
C + Aqufer*20,Lithol*20,SmpSrc*10,Commnt*60,Filin*12,Filout*12
C INTEGER Lat,Long,Date,Time
C REAL Latdec,Londec,UTMNor,UTMEst,Temp,Alk,Hard,Cond,pH,Ca,Mg,
C + Na,K,Cl,SO4,HCO3,CO3,PO4,NO3,F,SiO2,As,Ba,Be,Boron,Cd,Cr,Co,Cu,
C + Fe,TotFe,Pb,Mn,Mo,Ni,Ag,Sr,V,Zn,Li,Se,Iodine,Br,TotN,Hg,DisOrg,
C + DOC,TDS,ISMaj,ISTrac,ISTot,Alt,Weldep,Watdep,Watlev,HGue,CaGue,
C + MgGue,NaGue,KGue,ClGue,SO4Gue,CO3Gue,PO4Gue,NO3Gue,FGue,SiGue,
C + Totcrb

```

```

C Prompt the user for the names of the input file containing the
C hydrochemical data, and the MINTEQA2 filename to be created.

```

```

C PRINT*, 'Enter the name of the Comma-Delimited ASCII file
C + containing the water chemistry data?'
C READ(*,11) Filin
C FORMAT(A12)
C PRINT*, 'Enter the name of MINTEQA2 file to be created (8.3)?'
C READ(*,12) Filout
C FORMAT(A12)

```

```

C Open the water chemistry file and the MINTEQA2 input file

```

```

C OPEN(Unit=8, File=Filin, Status='Old', Access='Sequential',
C + Form='Formatted', Action='Read')
C OPEN(Unit=9, File=Filout, Status='Unknown', Access='Append',
C + Form='Formatted', Position='Append')

```

```

C 45678901234567890123456789012345678901234567890123456789012
C Reading the data out of the original water chemistry file. The order
C in which column input will be read is reasonably standard, and is
C based on the analysis tables of Perfect et al. (1995). Site Name,
C SiteID,ArcID(CNWRA added),Lat,LatDec,UTMNor(CNWRA added),Long,LonDec,
C UTMEst(CNWRA added),Date,Time,Temp,Alk,Hard,Cond,pH,Ca,Mg,Na,K,Cl,
C SO4,HCO3,CO3,PO4,NO3,F,SiO2,As,Ba,Be,Boron,Cd,Cr,Co,Cu,Fe,TotFe,Pb,
C Mn,Mo,Ni,Ag,Sr,V,Zn,Li,Se,Iodine,Br,TotN,Hg,DisOrg,DOC,TDS,ISMaj,
C ISTrac,ISTot,Balanc,DatSrc,Lab,Aqufer,Lithol,SmpSrc,Commnt,Alt,
C Weldep,Watdep,Watlev.

```

```

C READ(*,end=31)Name,SiteID,ArcID,Lat,LatDec,UTMNor,Long,LonDec,
C + UTMEst,Date,Time,Temp,Alk,Hard,Cond,pH,Ca,Mg,Na,K,Cl,SO4,HCO3,
C + CO3,PO4,NO3,F,SiO2,As,Ba,Be,Boron,Cd,Cr,Co,Cu,Fe,TotFe,Pb,Mn,
C + Mo,Ni,Ag,Sr,V,Zn,Li,Se,Iodine,Br,TotN,Hg,DisOrg,DOC,TDS,ISMaj,
C + ISTrac,ISTot,Balanc,DatSrc,Lab,Aqufer,Lithol,SmpSrc,Commnt,
C + Alt,Weldep,Watdep,Watlev

```

```

C Write the selected data to the MINTEQA2 Output File

```

```

C Write two Title Lines for MINTEQA2
C WRITE(9,40)Name,SiteID,ArcID
C FORMAT(A35,' ','SiteID=',A15,' ','ArcID=',A4)
C WRITE(9,42)UTMNor,UTMEst,Date,Time
C FORMAT('UTM='F9.1,'North',' ',1x,F8.1,'East',' ',1x,
C + 'Date=',I6,' ',1x,'Time=',I4)

```

```

C Write Temperature-Concentration Units. If Temp>0, use logged temp. If
C no temperature is reported, a value of -99998 is typically entered in
C database (Perfect et al., 1995), and a temp of 25.00 degrees C is
C assumed for the geochemical speciation and entered in the MINTEQA2
C input file. Concentration units are assumed to be in the reported
C units of mg/L. Regardless of input concentration units, MINTEQA2

```


c output, is in molal.

```
c
  IF(Temp.gt.0)THEN
    WRITE(9,43)Temp
    FORMAT(F5.2,1X,'MG/L 0.000 0.00000E-01')
  ELSE
    WRITE(9,44)
    FORMAT('25.00 MG/L 0.000 0.00000E-01')
  ENDIF
```

c Lines 4 & 9 of MINTEQA2 output contain flags that are hardwired.
c Because there are no sweep options, writing to a Lotus-file, or
c Sorption Models, lines 5,6,7,8, & 10 of the MINTEQA2 files contain
c no line entry.

```
c
  WRITE(9,45)
  FORMAT('0 0 1 0 3 0 0 0 1 1 0 0 0')
  WRITE(9,46)
  FORMAT('0 0 0')
```

c For each major element, write the 3-digit MINTEQA2 ID number, the
c reported concentration (in mg/L), an initial activity guess
c (log molal), a "y" flag for improved activity guess, and the text
c identifier from the MINTEQA2 databases.

```
c
  IF(pH.gt.0)THEN
    HGue=-1*pH
    WRITE(9,47)HGue
    FORMAT(' 330 0.000E-01 ',F6.2,' y',20X,'/H+1')
```

```
  ENDIF
  IF(Ca.gt.0)THEN
    CaGue=DLOG10((Ca/40.078)*1e-3)
    WRITE(9,48)Ca,CaGue
    FORMAT(' 150 ',E9.3,2X,F6.2,' y',20X,'/Ca+2')
```

```
  ENDIF
  IF(Mg.gt.0)THEN
    MgGue=DLOG10((Mg/24.305)*1e-3)
    WRITE(9,49)Mg,MgGue
    FORMAT(' 460 ',E9.3,2X,F6.2,' y',20X,'/Mg+2')
```

```
  ENDIF
  IF(Na.gt.0)THEN
    NaGue=DLOG10((Na/22.98977)*1e-3)
    WRITE(9,50)Na,NaGue
    FORMAT(' 500 ',E9.3,2X,F6.2,' y',20X,'/Na+1')
```

```
  ENDIF
  IF(K.gt.0)THEN
    KGue=DLOG10((K/39.0983)*1e-3)
    WRITE(9,51)K,KGue
    FORMAT(' 410 ',E9.3,2X,F6.2,' y',20X,'/K+1')
```

```
  ENDIF
  IF(Cl.gt.0)THEN
    ClGue=DLOG10((Cl/35.4527)*1e-3)
    WRITE(9,52)Cl,ClGue
    FORMAT(' 180 ',E9.3,2X,F6.2,' y',20X,'/Cl-1')
```

```
  ENDIF
  IF(SO4.gt.0)THEN
    SO4Gue=DLOG10((SO4/96.0636)*1e-3)
    WRITE(9,53)SO4,SO4Gue
    FORMAT(' 732 ',E9.3,2X,F6.2,' y',20X,'/SO4-2')
```

```
  ENDIF
  IF(HCO3.gt.0.and.CO3.le.0)THEN
    CO3Gue=DLOG10((HCO3/61.01714)*1e-3)
    TotCrb=HCO3*(61.01714/60.0092)
    WRITE(9,54)TotCrb,CO3Gue
```

```
  ENDIF
  IF(HCO3.gt.0.and.CO3.gt.0)THEN
    CO3Gue=DLOG10(((HCO3/61.01714)+(CO3/60.0092))*1e-3)
    TotCrb=CO3+(HCO3*(61.01714/60.0092))
    WRITE(9,54)TotCrb,CO3Gue
```

```
  ENDIF
  IF(HCO3.le.0.and.CO3.gt.0)THEN
    CO3Gue=DLOG10((CO3/60.0092)*1e-3)
    WRITE(9,54)CO3,CO3Gue
    FORMAT(' 140 ',E9.3,2X,F6.2,' y',20X,'/CO3-2')
```

```
  ENDIF
  IF(PO4.gt.0)THEN
    PO4Gue=DLOG10((PO4/94.971362)*1e-3)
```

Convert HCO₃⁻
to CO₃²⁻ which
is the base
component used
in MINTEQA2

54

```
  WRITE(9,55)PO4,PO4Gue
  FORMAT(' 580 ',E9.3,2X,F6.2,' y',20X,'/PO4-2')
```

```
  ENDIF
  IF(NO3.gt.0)THEN
    NO3Gue=DLOG10((NO3/62.00494)*1e-3)
    WRITE(9,56)NO3,NO3Gue
    FORMAT(' 492 ',E9.3,2X,F6.2,' y',20X,'/NO3-1')
```

```
  ENDIF
  IF(F.gt.0)THEN
    FGue=DLOG10((F/18.998403)*1e-3)
    WRITE(9,57)F,FGue
    FORMAT(' 270 ',E9.3,2X,F6.2,' y',20X,'/F-1')
```

```
  ENDIF
  IF(SiO2.gt.0)THEN
    SiO2=SiO2*(60.0843/96.11486)
    SiGue=DLOG10((SiO2/60.0843)*1e-3)
    WRITE(9,58)SiO2,SiGue
    FORMAT(' 770 ',E9.3,2X,F6.2,' y',20X,'/H4SiO4')
```

```
  ENDIF
  c
  c Insert Blank Line
  c
```

```
  WRITE(9,59)
  FORMAT(' ')
```

c Fixed pH

```
  WRITE(9,60)
  FORMAT(' 3 1')
  WRITE(9,61)pH
  FORMAT(' 330 ',F7.4,' 0.0000',19X,'/H+1')
```

c Insert Blank Lines

```
  c
  WRITE(9,62)
  FORMAT(' ', ' ')
  WRITE(9,63)
  FORMAT(' ', ' ')
```

GOTO 30

CONTINUE

```
c 45678901234567890123456789012345678901234567890123456789012
  STOP
  END
```

Program MINTEMK designed to read lotus chemistry files of
Puffer et al (1995)

SITE NAME	AFC D#	LATITUDE	LAT DEG	UTMin(n)	LONGITUDE	LONG DEG	UTM(east)	DATE	TIME	TEMP	ALK	HARDNESS	COND	pH	Ca ++	Mg ++	Na+	K	Cl	SO4-
Assumed Precipitation Species, Stream Molecular Weight,															40.078	22.8977	38.0983	35.4527	88.0142	
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
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CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
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CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
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CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
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CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.04306	337.6865	1164521	-116.756	522264	780017	88988	24.3	320	54	7195	7.6	18	18	1600	330	1800	300
CO-1 NENE SEC 01 T1 N4Z SEC 00-1-1	98888	350347	35.																	

[illegible]

TOTAL N		DO	TDS	I.S. (mg/l)	I.S. (Total)	BALANCE	DE#	LAB	AQUIFER	LITHOLOGY	SAMPLE SOURCE	COMMENTS	ALTITUDE	WELL DEPTH	WATER DEPTH	WL ALT
mg	ppm															
mg++																
200.50																
0.05	-99999	-99999	4140	7.73E-02	2.10E-05	7.73E-02	8	14	USGS	SAND	WELL	DOCKTER, R.D. COVOTE DRY LAKE, CA	-99999	235	-99999	-99999
0.07	-99999	-99999	4480	8.29E-02	8.35E-05	8.29E-02	9	14	USGS	SAND	WELL	DOCKTER, R.D. COVOTE DRY LAKE, CA	-99999	455	-99999	-99999
0.14	-99999	-99999	7520	1.24E-01	2.89E-04	1.24E-01	8	5	USGS	CLAY, SANDY	WELL	CALZIN, SODA DRY LAKE, CA	-99999	75	-99999	-99999
0.18	-99999	-99999	670	1.27E-02	2.71E-05	1.27E-02	8	5	USGS	SAND	WELL	CALZIN, SODA DRY LAKE, CA	-99999	400	-99999	-99999
0.12	-99999	-99999	8770	1.89E-01	3.84E-04	1.89E-01	8	15	USGS	SAND	WELL	DOCKTER, R.D. CUDEBACK DRY LAKE, CA	-99999	75	-99999	-99999
2.3	-99999	-99999	3410	6.02E-02	1.00E-04	6.02E-02	9	15	USGS	GRAVEL	WELL	DOCKTER, R.D. CUDEBACK DRY LAKE, CA	-99999	400	-99999	-99999
4.3	-99999	-99999	1180	2.22E-02	6.44E-05	2.22E-02	8	15	USGS	SAND	WELL	DOCKTER, R.D. CUDEBACK DRY LAKE, CA	-99999	-99999	-99999	-99999
1.8	-99999	-99999	215	4.37E-03	1.78E-05	4.39E-03	8	4	USGS	CLAY, SANDY, SILTY	WELL	CALZIN, J.P. VAMPAH VALLEY, CA	-99999	335	-99999	-99999
-99999	-99999	-99999	-99999	7.09E-03	0.00E+00	7.09E-03	8	18	CA DWR	X	WELL	TABLE 14,	-99999	-99999	-99999	-99999
-99999	-99999	-99999	-99999	8.10E-03	0.00E+00	8.10E-03	8	18	CA DWR	X	WELL	TABLE 14,	-99999	-99999	-99999	-99999
-99999	-99999	-99999	-99999	5.89E-03	0.00E+00	5.89E-03	9	18	CA DWR	X	WELL	TABLE 14,	-99999	-99999	-99999	-99999
-99999	-99999	-99999	-99999	1.59E-02	0.00E+00	1.59E-02	9	33	X	X	X	X	-99999	-99999	-99999	-99999
-99999	-99999	-99999	-99999	1.10E-02	0.00E+00	1.10E-02	9	18	CA DWR	X	WELL	TABLE 14,	-99999	-99999	-99999	-99999
-99999	-99999	-99999	-99999	9.29E-03	0.00E+00	9.29E-03	9	18	CA DWR	X	WELL	TABLE 14,	-99999	-99999	-99999	-99999

constant $pH = 7.4$

$$/H+1$$

units in mg/L
reported T = 25.5°C

0.0000
measured pit

$-3.52 \text{ y} / \text{H4SiO4}$
concentrations in mg/L (measured)


Program Minthink results reading
Dataedit.* Files of Perfect et al. (1995)
Monteqad input files at logged Temp (C),
mg/L input, constant pH at reported value.

Perfect at 21.01945) water chemistry as comma-delimited ASCII files

[illegible]

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APKmm



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      1.490      3.100E-01
      2.326E-04      4.700E-06
      2.455E-04      5.610      4.700E-06
      2.892E-04      3.570      1.630E-01
      1.000E-06      3.500      0.000E-01

Charge Balance: UNSPECIFIED

Sum of CATIONS= 1.169E-01 Sum of ANIONS = 1.182E-01
PERCENT DIFFERENCE = 6.767E-01 (ANIONS - CATIONS)/ANIONS * 100

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:
SO4 2-      Log activity guess: 3.49
H2O         Log activity guess: 3.49
H2O         Log activity guess: 3.77
H2O         Log activity guess: 3.77
H2O         Log activity guess: 3.77
H2O         Log activity guess: 0.00
H2O         Log activity guess: 0.00

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Type II - OTHER SPECIES IN SOLUTION OR ADSORBED									
TD	NAME	CALC. VAL. IN SOLUTION		ACTIVITY		LOS ACTIVITY		GMAW	
330	H+1	576720	116 - 2	7.715E-27	2.178E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
456	H+2	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
500	Na+1	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
510	Ca	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
520	Ca+1	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
530	Ca+2	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
540	Ca+3	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
550	Ca+4	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
560	Ca+5	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
570	Ca+6	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
580	Ca+7	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
590	Ca+8	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
600	Ca+9	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
610	Ca+10	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
620	Ca+11	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
630	Ca+12	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
640	Ca+13	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
650	Ca+14	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
660	Ca+15	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
670	Ca+16	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
680	Ca+17	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
690	Ca+18	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
700	Ca+19	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
710	Ca+20	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
720	Ca+21	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
730	Ca+22	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
740	Ca+23	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
750	Ca+24	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
760	Ca+25	150140	ca303	2.085E-26	1.641E-25	4.497E-27	5.699E-25	4.937E-27	6.162E-25
770	H4SiO4			1.698E-04	1.745E-04			3.750E-05	1.028E-04

330720	hs04 -	2.610E-10	2.07E-10	-9.69992	0.76222
330720	hs104 -	1.192E-06	9.39E-07	-6.07993	0.76223
330720	hs104 -2	4.39E-07	1.33E-07	-15.71946	0.76224
410720	hs04				0.76225

H₂-2
 Na-1
 K-1
 Cl-1
 SO₄-2
 MC

[illegible]

EQUILIBRATED MASS DISTRIBUTION									
No.	DISPERSED				SEMI-SEPARATED				
	MOLALS	PERCENT	MOLALS	PERCENT	MOLALS	PERCENT	MOLALS	PERCENT	
4	1.89E-04	100	0	0.00E-01	0	0.00E-01	0	0.00E-01	
	2.89E-03	100	0	0.00E-01	0	0.00E-01	0	0.00E-01	
	7.84E-04	100	0	0.00E-01	0	0.00E-01	0	0.00E-01	
	1.90E-04	100	0	0.00E-01	0	0.00E-01	0	0.00E-01	
	1.90E-04	100	0	0.00E-01	0	0.00E-01	0	0.00E-01	
	5.10E-02	100	0	0.00E-01	0	0.00E-01	0	0.00E-01	
	3.11E-03	100	0	0.00E-01	0	0.00E-01	0	0.00E-01	
	3.11E-03	100	0	0.00E-01	0	0.00E-01	0	0.00E-01	
	3.75E-04	100	0	0.00E-01	0	0.00E-01	0	0.00E-01	
	3.12E-03	100	0	0.00E-01	0	0.00E-01	0	0.00E-01	
	3.12E-03	100	0	0.00E-01	0	0.00E-01	0	0.00E-01	

the Balance: SECIATED

OF CATIONS = 7.021E-02 mol of ANIONS 6.698E-02

[illegible][illegible]

83.4	PERCENT BOUND IN SPECIES #	460	My-2
1.7	PERCENT BOUND IN SPECIES #460140	spod + aq	
2.4	PERCENT BOUND IN SPECIES #4601401	mpb + aq	
1.6	PERCENT BOUND IN SPECIES #4602700	mf +	
10.9	PERCENT BOUND IN SPECIES #4603200	mg + aq	
98.7	PERCENT BOUND IN SPECIES #	500	Nh+1
98.7	PERCENT BOUND IN SPECIES #	410	K+1
1.3	PERCENT BOUND IN SPECIES #410200	ksd +	
100.0	PERCENT BOUND IN SPECIES #	180	Cl-1
	PERCENT BOUND IN SPECIES #	772	SO4-2

SPECIES (not included in male balance)	WITH FEMALE ACTIVITY			
	CALC. NO.	LOG. NO.	HEAT. LOG.	NO. BAL.
1. 3. WFE 105	2,397	2,191	8,400	0.000
2. 3. WFE 106	2,398	2,191	8,400	0.000
3. 3. WFE 107	2,399	2,191	8,400	0.000
4. 3. WFE 108	2,400	2,191	8,400	0.000
5. 3. WFE 109	2,401	2,191	8,400	0.000
6. 3. WFE 110	2,402	2,191	8,400	0.000
7. 3. WFE 111	2,403	2,191	8,400	0.000
8. 3. WFE 112	2,404	2,191	8,400	0.000
9. 3. WFE 113	2,405	2,191	8,400	0.000
10. 3. WFE 114	2,406	2,191	8,400	0.000
11. 3. WFE 115	2,407	2,191	8,400	0.000
12. 3. WFE 116	2,408	2,191	8,400	0.000
13. 3. WFE 117	2,409	2,191	8,400	0.000
14. 3. WFE 118	2,410	2,191	8,400	0.000
15. 3. WFE 119	2,411	2,191	8,400	0.000
16. 3. WFE 120	2,412	2,191	8,400	0.000
17. 3. WFE 121	2,413	2,191	8,400	0.000
18. 3. WFE 122	2,414	2,191	8,400	0.000
19. 3. WFE 123	2,415	2,191	8,400	0.000
20. 3. WFE 124	2,416	2,191	8,400	0.000
21. 3. WFE 125	2,417	2,191	8,400	0.000
22. 3. WFE 126	2,418	2,191	8,400	0.000
23. 3. WFE 127	2,419	2,191	8,400	0.000
24. 3. WFE 128	2,420	2,191	8,400	0.000
25. 3. WFE 129	2,421	2,191	8,400	0.000
26. 3. WFE 130	2,422	2,191	8,400	0.000
27. 3. WFE 131	2,423	2,191	8,400	0.000
28. 3. WFE 132	2,424	2,191	8,400	0.000
29. 3. WFE 133	2,425	2,191	8,400	0.000
30. 3. WFE 134	2,426	2,191	8,400	0.000
31. 3. WFE 135	2,427	2,191	8,400	0.000
32. 3. WFE 136	2,428	2,191	8,400	0.000
33. 3. WFE 137	2,429	2,191	8,400	0.000
34. 3. WFE 138	2,430	2,191	8,400	0.000
35. 3. WFE 139	2,431	2,191	8,400	0.000
36. 3. WFE 140	2,432	2,191	8,400	0.000
37. 3. WFE 141	2,433	2,191	8,400	0.000
38. 3. WFE 142	2,434	2,191	8,400	0.000
39. 3. WFE 143	2,435	2,191	8,400	0.000
40. 3. WFE 144	2,436	2,191	8,400	0.000
41. 3. WFE 145	2,437	2,191	8,400	0.000
42. 3. WFE 146	2,438	2,191	8,400	0.000
43. 3. WFE 147	2,439	2,191	8,400	0.000
44. 3. WFE 148	2,440	2,191	8,400	0.000
45. 3. WFE 149	2,441	2,191	8,400	0.000
46. 3. WFE 150	2,442	2,191	8,400	0.000
47. 3. WFE 151	2,443	2,191	8,400	0.000
48. 3. WFE 152	2,444	2,191	8,400	0.000
49. 3. WFE 153	2,445	2,191	8,400	0.000
50. 3. WFE 154	2,446	2,191	8,400	0.000
51. 3. WFE 155	2,447	2,191	8,400	0.000
52. 3. WFE 156	2,448	2,191	8,400	0.000
53. 3. WFE 157	2,449	2,191	8,400	0.000
54. 3. WFE 158	2,450	2,191	8,400	0.000
55. 3. WFE 159	2,451	2,191	8,400	0.000
56. 3. WFE 160	2,452	2,191	8,400	0.000
57. 3. WFE 161	2,453	2,191	8,400	0.000
58. 3. WFE 162	2,454	2,191	8,400	0.000
59. 3. WFE 163	2,455	2,191	8,400	0.000
60. 3. WFE 164	2,456	2,191	8,400	0.000
61. 3. WFE 165	2,457	2,191	8,400	0.000
62. 3. WFE 166	2,458	2,191	8,400	0.000
63. 3. WFE 167	2,459	2,191	8,400	0.000
64. 3. WFE 168	2,460	2,191	8,400	0.000
65. 3. WFE 169	2,461	2,191	8,400	0.000
66. 3. WFE 170	2,462	2,191	8,400	0.000
67. 3. WFE 171	2,463	2,191	8,400	0.000
68. 3. WFE 172	2,464	2,191	8,400	0.000
69. 3. WFE 173	2,465	2,191	8,400	0.000
70. 3. WFE 174	2,466	2,191	8,400	0.000
71. 3. WFE 175	2,467	2,191	8,400	0.000
72. 3. WFE 176	2,468	2,191	8,400	0.000
73. 3. WFE 177	2,469	2,191	8,400	0.000
74. 3. WFE 178	2,470	2,191	8,400	0.000
75. 3. WFE 179	2,471	2,191	8,400	0.000
76. 3. WFE 180	2,472	2,191	8,400	0.000
77. 3. WFE 181	2,473	2,191	8,400	0.000
78. 3. WFE 182	2,474	2,191	8,400	0.000
79. 3. WFE 183	2,475	2,191	8,400	0.000
80. 3. WFE 184	2,476	2,191	8,400	0.000
81. 3. WFE 185	2,477	2,191	8,400	0.000
82. 3. WFE 186	2,478	2,191	8,400	0.000
83. 3. WFE 187	2,479	2,191	8,400	0.000
84. 3. WFE 188	2,480	2,191	8,400	0.000
85. 3. WFE 189	2,481	2,191	8,400	0.000
86. 3. WFE 190	2,482	2,191	8,400	0.000
87. 3. WFE 191	2,483	2,191	8,400	0.000
88. 3. WFE 192	2,484	2,191	8,400	0.000
89. 3. WFE 193	2,485	2,191	8,400	0.000
90. 3. WFE 194	2,486	2,191	8,400	0.000
91. 3. WFE 195	2,487	2,191	8,400	0.000
92. 3. WFE 196	2,488	2,191	8,400	0.000
93. 3. WFE 197	2,489	2,191	8,400	0.000
94. 3. WFE 198	2,490	2,191	8,400	0.000
95. 3. WFE 199	2,491	2,191	8,400	0.000
96. 3. WFE 200	2,492	2,191	8,400	0.000
97. 3. WFE 201	2,493	2,191	8,400	0.000
98. 3. WFE 202	2,494	2,191	8,400	0.000
99. 3. WFE 203	2,495	2,191	8,400	0.000
100. 3. WFE 204	2,496	2,191	8,400	0.000
101. 3. WFE 205	2,497	2,191	8,400	0.000
102. 3. WFE 206	2,498	2,191	8,400	0.000
103. 3. WFE 207	2,499	2,191	8,400	0.000
104. 3. WFE 208	2,500	2,191	8,400	0.000
105. 3. WFE 209	2,501	2,191	8,400	0.000
106. 3. WFE 210	2,502	2,191	8,400	0.000
107. 3. WFE 211	2,503	2,191	8,400	0.000
108. 3. WFE 212	2,504	2,191	8,400	0.000
109. 3. WFE 213	2,505	2,191	8,400	0.000
110. 3. WFE 214	2,506	2,191	8,400	0.000
111. 3. WFE 215	2,507	2,191	8,400	0.000
112. 3. WFE 216	2,508	2,191	8,400	0.000
113. 3. WFE 217	2,509	2,191	8,400	0.000
114. 3. WFE 218	2,510	2,191	8,400	0.000
115. 3. WFE 219	2,511	2,191	8,400	0.000
116. 3. WFE 220	2,512	2,191	8,400	0.000
117. 3. WFE 221	2,513	2,191	8,400	0.000
118. 3. WFE 222	2,514	2,191	8,400	0.000
119. 3. WFE 223	2,515	2,191	8,400	0.000
120. 3. WFE 224	2,516	2,191	8,400	0.000
121. 3. WFE 225	2,517	2,191	8,400	0.000
122. 3. WFE 226	2,518	2,191	8,400	0.000
123. 3. WFE 227	2,519	2,191	8,400	0.000
124. 3. WFE 228	2,520	2,191	8,400	0.000
125. 3. WFE 229	2,521	2,191	8,400	0.000
126. 3. WFE 230	2,522	2,191	8,400	0.000
127. 3. WFE 231	2,523	2,191	8,400	0.000
128. 3. WFE 232	2,524	2,191	8,400	0.000
129. 3. WFE 233	2,525	2,191	8,400	0.000
130. 3. WFE 234	2,526	2,191	8,400	0.000
131. 3. WFE 235	2,527	2,191	8,400	0.000
132. 3. WFE 236	2,528	2,191	8,400	0.000
133. 3. WFE 237	2,529	2,191	8,400	0.000
134. 3. WFE 238	2,530	2,191	8,400	0.000
135. 3. WFE 239	2,531	2,191	8,400	0.000
136. 3. WFE 240	2,532	2,191	8,400	0.000
137. 3. WFE 241	2,533	2,191	8,400	0.000
138. 3. WFE 242	2,534	2,191	8,400	0.000
139. 3. WFE 243	2,535	2,191	8,400	0.000
140. 3. WFE 244	2,536	2,191	8,400	0.000
141. 3. WFE 245	2,537	2,191	8,400	0.000
142. 3. WFE 246	2,538	2,191	8,400	0.000
143. 3. WFE 247	2,539	2,191	8,400	0.000
144. 3. WFE 248	2,540	2,191	8,400	0.000
145. 3. WFE 249	2,541	2,191	8,400	0.000
146. 3. WFE 250	2,542	2,191	8,400	0.000
147. 3. WFE 251	2,543	2,191	8,400	0.000
148. 3. WFE 252	2,544	2,191	8,400	0.000
149. 3. WFE 253	2,545	2,191	8,400	0.000
150. 3. WFE 254	2,546	2,191	8,400	0.000
151. 3. WFE 255	2,547	2,191	8,400	0.000
152. 3. WFE 256	2,548	2,191	8,400	0.000
153. 3. WFE 257	2,549	2,191	8,400	0.000
154. 3. WFE 258	2,550	2,191	8,400	0.000
155. 3. WFE 259	2,551	2,191	8,400	0.000
156. 3. WFE 260	2,552	2,191	8,400	0.000
157. 3. WFE 261	2,553	2,191	8,400	0.000
158. 3. WFE 262	2,554	2,191	8,400	0.000
159. 3. WFE 263	2,555	2,191	8,400	0.000
160. 3. WFE 264	2,556	2,191	8,400	0.000
161. 3. WFE 265	2,557	2,191	8,400	0.000
162. 3. WFE 266	2,558	2,191	8,400	0.000
163. 3. WFE 267	2,559	2,191	8,400	0.000
164. 3. WFE 268	2,560	2,191	8,400	0.000
165. 3. WFE 269	2,561	2,191	8,400	0.000
166. 3. WFE 270	2,562	2,191	8,400	0.000
167. 3. WFE 271	2,563	2,191	8,400	0.000
168. 3. WFE 272	2,564	2,191	8,400	0.000
169. 3. WFE 273	2,565	2,191	8,400	0.000
170. 3. WFE 274	2,566	2,191	8,400	0.000
171. 3. WFE 275	2,567	2,191	8,400	0.000
172. 3. WFE 276	2,568	2,191	8,400	0.000
173. 3. WFE 277	2,569	2,191	8,400	0.000
174. 3. WFE 278	2,570	2,191	8,400	0.000
175. 3. WFE 279	2,571	2,191	8,400	0.000
176. 3. WFE 280	2,572	2,191	8,400	0.000
177. 3. WFE 281	2,573	2,191	8,400	0.000
178. 3. WFE 282	2,574	2,191	8,400	0.000
179. 3. WFE 283	2,575	2,191	8,400	0.000
180. 3. WFE 284	2,576	2,191	8,400	0.000
181. 3. WFE 285	2,577	2,191	8,400	0.000
182. 3. WFE 286	2,578	2,191	8,400	0.000
183. 3. WFE 287	2,579	2,191	8,400	0.000
184. 3. WFE 288	2,580	2,191	8,400	0.000
185. 3. WFE 289	2,581	2,191	8,400	0.000
186. 3. WFE 290	2,582	2,191	8,400	0.000
187. 3. WFE 291	2,583	2,191	8,400	0.000
188. 3. WFE 292	2,584	2,191	8,400	0.000
189. 3. WFE 293	2,585	2,191	8,400	0.000
190. 3. WFE 294	2,586	2,191	8,400	0.000
191. 3. WFE 295	2,587	2,191	8,400	0.000
192. 3. WFE 296	2,588	2,191	8,400	0.000
193. 3. WFE 297	2,589	2,191	8,400	0.000
194. 3. WFE 298	2,590	2,191	8,400	0.000
195. 3. WFE 299	2,591	2,191	8,400	0.000
196. 3. WFE 300	2,592	2,191	8,400	0.000
197. 3. WFE 301	2,593	2,191	8,400	0.000
198. 3. WFE 302	2,594	2,191	8,400	0.000
199. 3. WFE 303	2,595	2,191	8,400	0.000
200. 3. WFE 304	2,596	2,191	8,400	0.000
201. 3. WFE 305				

[illegible]

PERCENT BOUND IN SPECIES #	460	Mg-2		829
PERCENT BOUND IN SPECIES #460101		magnoc3 +		207171
PERCENT BOUND IN SPECIES #460102		magnoc4 +		221515
PERCENT BOUND IN SPECIES #460720		magnoc4q		501501
				546464
				615151
				654654
				501501
PERCENT BOUND IN SPECIES #	500	N+1		504654
PERCENT BOUND IN SPECIES #500720		naso4 -		801501
				201501
				246464
				306464
				356464
				406464
				456464
				506464
PERCENT BOUND IN SPECIES #	410	K-1		201501
PERCENT BOUND IN SPECIES #410720		k4o4 -		306464
				356464
				406464
				456464
				506464
PERCENT BOUND IN SPECIES #	100	C1-1		201501
				251501
				301501
				351501
				401501
				451501
PERCENT BOUND IN SPECIES #	710	SOL-2		801501

PERCENT BOUND IN SPECIES #300140 no03 -
PERCENT BOUND IN SPECIES #3001401 h200d mq

8151502	8151503	8151504	8151505	8151506	8151507	8151508	8151509	8151510	8151511	8151512	8151513	8151514	8151515	8151516	8151517	8151518	8151519	8151520	8151521	8151522	8151523	8151524	8151525	8151526	8151527	8151528	8151529	8151530	8151531	8151532	8151533	8151534	8151535	8151536	8151537	8151538	8151539	8151540	8151541	8151542	8151543	8151544	8151545	8151546	8151547	8151548	8151549	8151550	8151551	8151552	8151553	8151554	8151555	8151556	8151557	8151558	8151559	8151560	8151561	8151562	8151563	8151564	8151565	8151566	8151567	8151568	8151569	8151570	8151571	8151572	8151573	8151574	8151575	8151576	8151577	8151578	8151579	8151580	8151581	8151582	8151583	8151584	8151585	8151586	8151587	8151588	8151589	8151590	8151591	8151592	8151593	8151594	8151595	8151596	8151597	8151598	8151599	8151600	8151601	8151602	8151603	8151604	8151605	8151606	8151607	8151608	8151609	8151610	8151611	8151612	8151613	8151614	8151615	8151616	8151617	8151618	8151619	8151620	8151621	8151622	8151623	8151624	8151625	8151626	8151627	8151628	8151629	8151630	8151631	8151632	8151633	8151634	8151635	8151636	8151637	8151638	8151639	8151640	8151641	8151642	8151643	8151644	8151645	8151646	8151647	8151648	8151649	8151650	8151651	8151652	8151653	8151654	8151655	8151656	8151657	8151658	8151659	8151660	8151661	8151662	8151663	8151664	8151665	8151666	8151667	8151668	8151669	8151670	8151671	8151672	8151673	8151674	8151675	8151676	8151677	8151678	8151679	8151680	8151681	8151682	8151683	8151684	8151685	8151686	8151687	8151688	8151689	8151690	8151691	8151692	8151693	8151694	8151695	8151696	8151697	8151698	8151699	8151700	8151701	8151702	8151703	8151704	8151705	8151706	8151707	8151708	8151709	8151710	8151711	8151712	8151713	8151714	8151715	8151716	8151717	8151718	8151719	8151720	8151721	8151722	8151723	8151724	8151725	8151726	8151727	8151728	8151729	8151730	8151731	8151732	8151733	8151734	8151735	8151736	8151737	8151738	8151739	8151740	8151741	8151742	8151743	8151744	8151745	8151746	8151747	8151748	8151749	8151750	8151751	8151752	8151753	8151754	8151755	8151756	8151757	8151758	8151759	8151760	8151761	8151762	8151763	8151764	8151765	8151766	8151767	8151768	8151769	8151770	8151771	8151772	8151773	8151774	8151775	8151776	8151777	8151778	8151779	8151780	8151781	8151782	8151783	8151784	8151785	8151786	8151787	8151788	8151789	8151790	8151791	8151792	8151793	8151794	8151795	8151796	8151797	8151798	8151799	8151800	8151801	8151802	8151803	8151804	8151805	8151806	8151807	8151808	8151809	8151810	8151811	8151812	8151813	8151814	8151815	8151816	8151817	8151818	8151819	8151820	8151821	8151822	8151823	8151824	8151825	8151826	8151827	8151828	8151829	8151830	8151831	8151832	8151833	8151834	8151835	8151836	8151837	8151838	8151839	8151840	8151841	81																																																													
ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene	ethylene

NAME	DISSEMINATED		SORIZED		RECEIVED	
	MAILING PERCENT	NO. OF	MAILING PERCENT	NO. OF	MAILING PERCENT	NO. OF
ALBERTA	2.3	111	0.0	0	0.0	0
ALABAMA	2.3	111	0.0	0	0.0	0
ALASKA	6.6	319	0.0	0	0.0	0
ARIZONA	6.6	319	0.0	0	0.0	0
ARKANSAS	5.3	242	0.0	0	0.0	0
CALIFORNIA	5.3	242	0.0	0	0.0	0
COLORADO	5.3	242	0.0	0	0.0	0
CONNECTICUT	6.6	319	0.0	0	0.0	0
DELAWARE	6.6	319	0.0	0	0.0	0
FLORIDA	6.6	319	0.0	0	0.0	0
GEORGIA	6.6	319	0.0	0	0.0	0
HAWAII	6.6	319	0.0	0	0.0	0
ILLINOIS	6.6	319	0.0	0	0.0	0
INDIANA	6.6	319	0.0	0	0.0	0
IOWA	6.6	319	0.0	0	0.0	0
KANSAS	6.6	319	0.0	0	0.0	0
KENTUCKY	6.6	319	0.0	0	0.0	0
LOUISIANA	6.6	319	0.0	0	0.0	0
MAINE	6.6	319	0.0	0	0.0	0
MARYLAND	6.6	319	0.0	0	0.0	0
MASSACHUSETTS	6.6	319	0.0	0	0.0	0
MICHIGAN	6.6	319	0.0	0	0.0	0
MINNESOTA	6.6	319	0.0	0	0.0	0
MISSISSIPPI	6.6	319	0.0	0	0.0	0
MISSOURI	6.6	319	0.0	0	0.0	0
MONTANA	6.6	319	0.0	0	0.0	0
NEBRASKA	6.6	319	0.0	0	0.0	0
NEVADA	6.6	319	0.0	0	0.0	0
NEW HAMPSHIRE	6.6	319	0.0	0	0.0	0
NEW JERSEY	6.6	319	0.0	0	0.0	0
NEW MEXICO	6.6	319	0.0	0	0.0	0
NEW YORK	6.6	319	0.0	0	0.0	0
NORTH CAROLINA	6.6	319	0.0	0	0.0	0
NORTH DAKOTA	6.6	319	0.0	0	0.0	0
OHIO	6.6	319	0.0	0	0.0	0
OKLAHOMA	6.6	319	0.0	0	0.0	0
OREGON	6.6	319	0.0	0	0.0	0
PENNSYLVANIA	6.6	319	0.0	0	0.0	0
RHODE ISLAND	6.6	319	0.0	0	0.0	0
SOUTH CAROLINA	6.6	319	0.0	0	0.0	0
SOUTH DAKOTA	6.6	319	0.0	0	0.0	0
TENNESSEE	6.6	319	0.0	0	0.0	0
TEXAS	6.6	319	0.0	0	0.0	0
UTAH	6.6	319	0.0	0	0.0	0
Vermont	6.6	319	0.0	0	0.0	0
VIRGINIA	6.6	319	0.0	0	0.0	0
WASHINGTON	6.6	319	0.0	0	0.0	0
WEST VIRGINIA	6.6	319	0.0	0	0.0	0
WISCONSIN	6.6	319	0.0	0	0.0	0
WYOMING	6.6	319	0.0	0	0.0	0

ID		NAME	
1590141	ce03	1590141	ce03
1590142	ce04	1590142	ce04
1590143	ce05	1590143	ce05
1590144	ce06	1590144	ce06
1590145	ce07	1590145	ce07
1590146	ce08	1590146	ce08
1590147	ce09	1590147	ce09
1590148	ce10	1590148	ce10
1590149	ce11	1590149	ce11
1590150	ce12	1590150	ce12
1590151	ce13	1590151	ce13
1590152	ce14	1590152	ce14
1590153	ce15	1590153	ce15
1590154	ce16	1590154	ce16
1590155	ce17	1590155	ce17
1590156	ce18	1590156	ce18
1590157	ce19	1590157	ce19
1590158	ce20	1590158	ce20
1590159	ce21	1590159	ce21
1590160	ce22	1590160	ce22
1590161	ce23	1590161	ce23
1590162	ce24	1590162	ce24
1590163	ce25	1590163	ce25
1590164	ce26	1590164	ce26
1590165	ce27	1590165	ce27
1590166	ce28	1590166	ce28
1590167	ce29	1590167	ce29
1590168	ce30	1590168	ce30
1590169	ce31	1590169	ce31
1590170	ce32	1590170	ce32
1590171	ce33	1590171	ce33
1590172	ce34	1590172	ce34
1590173	ce35	1590173	ce35
1590174	ce36	1590174	ce36
1590175	ce37	1590175	ce37
1590176	ce38	1590176	ce38
1590177	ce39	1590177	ce39
1590178	ce40	1590178	ce40
1590179	ce41	1590179	ce41
1590180	ce42	1590180	ce42
1590181	ce43	1590181	ce43
1590182	ce44	1590182	ce44
1590183	ce45	1590183	ce45
1590184	ce46	1590184	ce46
1590185	ce47	1590185	ce47
1590186	ce48	1590186	ce48
1590187	ce49	1590187	ce49
1590188	ce50	1590188	ce50
1590189	ce51	1590189	ce51
1590190	ce52	1590190	ce52
1590191	ce53	1590191	ce53
1590192	ce54	1590192	ce54
1590193	ce55	1590193	ce55
1590194	ce56	1590194	ce56
1590195	ce57	1590195	ce57
1590196	ce58	1590196	ce58
1590197	ce59	1590197	ce59
1590198	ce60	1590198	ce60
1590199	ce61	1590199	ce61
1590200	ce62	1590200	ce62
1590201	ce63	1590201	ce63
1590202	ce64	1590202	ce64
1590203	ce65	1590203	ce65
1590204	ce66	1590204	ce66
1590205	ce67	1590205	ce67
1590206	ce68	1590206	ce68
1590207	ce69	1590207	ce69
1590208	ce70	1590208	ce70
1590209	ce71	1590209	ce71
1590210	ce72	1590210	ce72
1590211	ce73	1590211	ce73
1590212	ce74	1590212	ce74
1590213	ce75	1590213	ce75
1590214	ce76	1590214	ce76
1590215	ce77	1590215	ce77
1590216	ce78	1590216	ce78
1590217	ce79	1590217	ce79
1590218	ce80	1590218	ce80
1590219	ce81	1590219	ce81
1590220	ce82	1590220	ce82

Type III - SPECIFIC

10 200

on represents total inorganic carbon.
large imbalance exceeds 30t
where the solids specified as ALLOWED
coefficients is: Davies equation

[illegible]

94-1	0.103
1.87E-04	0.78965
-3.54110	0.103
90E-04	-3.72054
	1.01830

need by MINIFIL

PC	INTERDAY	73-10	DATE	OF	VAL
CO-1-NESENE	SECTD	11/10/82	00-1-2		
UIN-33005	0067H	022234	0067H		
8215002	w-olastone	-3.699			
8215003	w-olastant	-4.551			
<p>Temperature (C): 35.50 Units of Concentration: M/L & Ionic strength to be computed Do not automatically terminate if Precipitation is allowed only for The maximum number of iterations The method used to compute activity Interference output: life</p>					
330	0.000E 01	-7.90			

PC	PRINT002	V3.10	DATE OF CAL	1979
IMPROVED ACTIVITIES				
SUM OF CATIONS = 7.231E-02				
PERCENT DIFFERENCE = 1.22				
TOTAL				
ITER F-1				
NAME				
TOTAL				
3.754E				

770 HAS104
270 F.1
3.643E-0
1.669E-0

7/1/96
JRB

ID	NAME	WGT	PERCENT	NO. OF	PERCENT	NO. OF	PERCENT	NO. OF
100	WATER	1.0000	100.0	0.0000	0.0	0.0000	0.0	0.0
101	CO2	1.0000	100.0	0.0000	0.0	0.0000	0.0	0.0
102	CO2	1.0000	100.0	0.0000	0.0	0.0000	0.0	0.0
103	CO2	1.0000	100.0	0.0000	0.0	0.0000	0.0	0.0
104	CO2	1.0000	100.0	0.0000	0.0	0.0000	0.0	0.0
105	CO2	1.0000	100.0	0.0000	0.0	0.0000	0.0	0.0
106	CO2	1.0000	100.0	0.0000	0.0	0.0000	0.0	0.0
107	CO2	1.0000	100.0	0.0000	0.0	0.0000	0.0	0.0
108	CO2	1.0000	100.0	0.0000	0.0	0.0000	0.0	0.0
109	CO2	1.0000	100.0	0.0000	0.0	0.0000	0.0	0.0
110	CO2	1.0000	100.0	0.0000	0.0	0.0000	0.0	0.0

Example MINTEQA2 output files for 1st three records in QAddata.XLS file shown on pg. 58, this volume. Data taken from Perfect et al. (1995) (see pocket disk in back pocket)

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PROGRAM MNTFIL

Pg. 1 of 2

456789012345678901234567890123456789012345678901234567890123456789012
The following program is a feeble attempt to read MINTEQA2 output files and extract information regarding mineral saturations (S.I.). This program was prepared by D.R. Turner for the CNWRA in San Antonio, TX for the Radionuclide Transport KTI (20-5708-871). Many of the necessary parameters/flags are hard-wired and cannot currently be modified by the user during the run session.

IMPLICIT NONE
CHARACTER Line*80, Name*35, ArcID*10, Filin*12, Filout*12, CO2*6,
+ CcSI*7, CrsbSI*7
INTEGER I, Flag

Prompt the user for the names of the MINTEQA2 output file and the Filename to be created.

PRINT*, 'Enter the name of MINTEQA2 output file to be searched'
READ(*, 11) Filin
FORMAT(A12)
PRINT*, 'Enter the name of output file to be created (8.3)'
READ(*, 12) Filout
FORMAT(A12)

Open the MINTEQA2 output file being read and the output file being created.

OPEN(Unit=8, File=Filin, Status='Old', Access='Sequential',
+ Form='Formatted', Action='Read')
OPEN(Unit=9, File=Filout, Status='Unknown', Access='Sequential',
+ Form='Formatted', Position='Append')

456789012345678901234567890123456789012345678901234567890123456789012
This program will read the MINTEQA2 output file line-by-line, checking for the phrase "Part One of Output File indicating the start of a different chemical analysis. The site ID from Perfect et al. (1995) is read, and then a line-by-line search is initiated for the word "calcite". Once "calcite" is located, the saturation index is read into the output file. The process is then repeated for the next water sample.

Write headers

WRITE(9, 20)
FORMAT('12x, 'Site Name', 13x, '1x, 'ArcID', 6x, 'P(CO2)',
+ 3x, 'SI(Cc)', 1x, 'SI(Crsb)')

Set Flag and Start Reading MINTEQA2 output file

Flag=0
READ(8, 40, end=31) Line
FORMAT(A80)

Look for start of speciation file

IF(Line(32:52).eq.'PART 1 of OUTPUT FILE') THEN

After first pass through the read loop, write Name, CO2, CcSI, CrsbSI to output file

IF(Line(32:52).eq.'PART 1 of OUTPUT FILE'.and.Flag.gt.0) THEN
WRITE(9, 60) Name, ArcID, CO2, CcSI, CrsbSI
FORMAT('12x, A35, '1x, A10, '1x, A7, '1x, A7, '1x, A7)
ENDIF

Set Initial Values for CO2, CcSI, CrsbSI

CO2='n.d.'
CcSI='n.d.'
CrsbSI='n.d.'

Skip Lines to find Title

do 50 I=1, 3
read(8, 45, end=31) Line

} Set initially at n.d., will be overwritten if saturation index is reported

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[Handwritten signature]

Program Mntfil Output

Extracted S.I. from MINTEQA2 Output
files, speciation of water chemistry from
Perfect et al. (1995)

- n.d. means not determined. No $\text{SiO}_2(\text{aq})$ analysis reported in Perfect et al. (1995)

Compare results from 1st 3 records w/ MINTEQA2 output files record on pp. 60-62 this volume. All values match.

Additional coverages and data sources that are currently being used in ArcView include:

- YMP Boundaries: (e.g., NTS boundaries, ESF outline, Controlled Access Boundary) - USDOE
- State/County: Nevada Bureau of Mines
- Geologic coverage: Frizzell, V.A., Jr., and J. Shulters. 1990. *Geologic Map of the Nevada Test Site, Southern Nevada*. Map I-2046. Miscellaneous Investigations, U.S. Geol. Survey.
Geologic (DR) 7/22/96
Additional coverages that are to be converted from Arc/Info to ArcView format include 10x20 (1:250,000) sheets from the Geologic Atlas of California as described in:

D'Agnese, F.A., C.C. Faunt, and A.K. Turner. 1995. *Preliminary Digital Geologic Maps of the Mariposa, Kingman, Trona, and Death Valley Sheets, California*. Open File Report 94-318, U.S. Geological Survey. Denver, DO.
- Landsat Imagery: TM bands, purchased from EOSAT by CNWRA.
- Hypsography: Topography from USGS Digital Elevation Models.

These coverages were initially prepared for use in Arc/Info, Version 6.1, and have been converted to ArcView, Version 2.0b coverages at CNWRA using the SHAPE command in Arc/Info

Additional Background information on available Arc/Info coverages includes:

- Much of the available geospatial data is focused on the nine 7.5 minute quadrangle area about Yucca Mountain Nevada. Both raster and vector datasets are included. Geospatial data is organized in a hierarchical file system, with abbreviated names (for a discussion of file nomenclature and file naming constraints, see file "aafile.std" on this CDROM).

A complete, recursive listing of the file tree on this CDROM is beyond the scope of this document. An abbreviated file list is included here to illustrate the major divisions and types of data included in this distribution. This file tree list has been extensively pruned to aid illustration and discussion. Root level categories are: DEMS, FAULTS, HYDRO, HYPISO, ROADS, and SLAR.

DEMS subdirectory/workspace contains Digital Terrain Elevation Data and shaded reliefs for two resolutions of raster data: (a) Goldfield and Death Valley 1x2 degree (1:250,000 scale) domains of California and Nevada, at 3 arc seconds resolution (subdirectory/workspace "dvgr3sec"), and (b) nine 7.5 minute quadrangles (1:24,000 scale) about Yucca Mountain Nevada, at 30 meter resolution (subdirectory/workspace "ymlocal").

FAULTS subdirectory/workspace contains CNWRA digital tracings of faults published on the maps of Dohrenwend and many others (1991 thorough 1993), Frizzel et al. (1990), Jennings (1992), Nakata et al. (1982), and O'Neill et al. (1992). These fault maps were digitized from paper map copies using ARC/Info. The resolution of these fault traces vary, depending upon the scale of the original maps. Thus, not all maps are applicable at all scales. The original maps should be consulted to obtain an indication of the degree of resolution that can be demanded from each of these maps. Simple (x,y) raw line data is available in the **RAWLIN** subdirectory/workspace for use by applications software other than

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ARC/Info (basically output from the ARC/Info UNGENERATE command output).

HYDRO subdirectory/workspace contains hydrographic vectors (streams) for nine 7.5 minute quadrangles (1:24,000 scale) about Yucca Mountain Nevada. These data were purchased from the USGS in DLG (digital line graph) format, and converted into formats suitable for use in ARC/Info. Simple (x,y) raw line data is available in the RAWLIN subdirectory/workspace for use by applications software other than ARC/Info (UNGENERATE output).

HYPISO subdirectory/workspace contains hypsographic vectors (topographic contours) for nine 7.5 minute quadrangles (1:24,000 scale) about Yucca Mountain Nevada. These data were purchased from the USGS in DLG format, and converted into formats suitable for use in ARC/Info. Simple (x,y) raw line data is available in the RAWLIN subdirectory/workspace for use by applications software other than ARC/Info (UNGENERATE output).

ROADS subdirectory/workspace contains Road and Trail vectors for nine 7.5 minute quadrangles (1:24,000 scale) about Yucca Mountain Nevada. These data were purchased from the USGS in DLG format, and converted into formats suitable for use in ARC/Info. Simple (x,y) raw line data is available in the RAWLIN subdirectory/workspace for use by applications software other than ARC/Info (UNGENERATE output).

SLAR subdirectory/workspace contains Synthetic Aperture Radar/Side Looking Airborne Radar (SAR/SLAR) imagery for the middle third of both Goldfield and Death Valley 1x2 degree quadrangles (1:250,000 scale). These data were purchased from the USGS, formatted as 8-bit unsigned binary files. The file format was similar to Planetary Data Systems (PDS) format used by Jet Propulsion Laboratory. See appendix 2.0 for more detail. The ground pixel resolution of this data is 12 meters. Each pixel is an indication of X-Band (8.0 to 12.0 gigahertz) radar backscatter, and was received renormalized into the 0-255 integer range. Original files have been modified slightly so that ARC/Info users can display this SLAR data in a first order map registered space using the MAPWARP and IMAGE commands of ARCPLOT. Non-ARC/Info users must be able to read unsigned, 8-bit integer binary files (referred to as Band Interleaved by Line (BIL) files in some remote sensing image processing software). Map registration of SLAR imagery varies from very good near the Yucca Mountain site (few tens of meters) to poor at the north-south extremes of the SLAR scans (few hundreds of meters). SLAR imagery was acquired by the USGS contractor in some unknown scanner space, and reprojection into a true map space is probably impossible (scanner distortions are unknown). On this CDROM, SLAR imagery has been registered to UTM map space using a first order linear transformation, most accurate around Yucca Mountain Nevada.

last updated, 02-feb-95. R.Martin.

Blum

1/9/97
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Notebook closed due to closing of Radioclide
Transport KTI (20-5708-871). Final deliverables
transmitted to NRC.

I have reviewed
this notebook and
find it in general
compliance with
QA-001. There is
sufficient information for
another qualified
person to
conduct the activities.

E.C. De

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ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK #: 157A

Document Date:	01/20/1996
Availability:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, Texas 78228
Contact:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 78228-5166 Attn.: Director of Administration 210.522.5054
Data Sensitivity:	<input type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
Date Generated:	1996 through 1997
Operating System: (including version number)	Windows
Application Used: (including version number)	
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	5 - 3 1/2 disks
File Types: (.exe, .bat, .zip, etc.)	exe, xls
Remarks: (computer runs, etc.)	Media contains: H ₂ O chemistry raw data; limited thermodynamic data evaluation; ionic strength calculations.