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**Civilian Radioactive Waste Management System
Management & Operating Contractor**

**Data Qualification Report: Composition of J-13 Well Water
for Use on the Yucca Mountain Project, Revision 0**

TDR-NBS-HS-000003 REV 00

June 15, 2000

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TDR-NBS-HS-000003 REV 00B

June 15, 2000

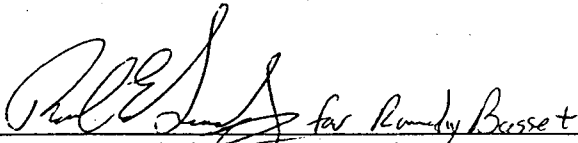
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EXECUTIVE SUMMARY

This data qualification report uses technical assessment according to Attachment 2 of AP-SIII.2Q, Rev. 0, ICN 2, *Qualification of Unqualified Data and the Documentation of Rationale for Accepted Data*, to qualify hydrochemical data from the well J-13. This report was prepared in accordance with Data Qualification Plan TDP-NBS-HS-000096 (Revision 0) and requires Assistant Manager of Project Execution (AMOPE) approval because the subject data are Principal Factor-related.

The data which are the subject of this report are contained in a report by Harrar, et al. (1990) which evaluated chemical analysis data measured on samples collected from the J-13 well up to that date. That report evaluated those data and developed a set of means and standard deviations for the major and minor constituents in water from that well, and it is those data that are the subject of this Data Qualification Report. The Data Tracking Numbers (DTNs) addressed by this report include two tables from a report by Harrar et al. (1990), and certain manipulations of those data. The qualification of each of these DTNs is discussed.

Harrar et al. (1990) performed the same types of evaluations of the subject data as are specified in AP-SIII.2Q, Rev. 0, ICN 2. The report documents the results of those evaluations and contains a data set which includes mean values and standard deviations calculated from the data the authors considered to meet the requirements of the Nevada Nuclear Waste Storage Investigations project (precursor to the YMP, prior to formal adoption of YMP QA program). The mean values of the major constituents of J-13 well water make up the data set that is actually used in the AMRs that cite the subject DTNs.

Based on a review of the Harrar et al. (1990) report, a data set derived from that report and containing only the mean values of the major constituents is considered qualified for use for testing and modeling interactions of water with materials. The new DTN (MO0006J13WTRCM.000) has been extracted from the original unqualified DTN (LL980711104242.054). AMRs and other documents should cite the new DTN.

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ACRONYMS AND ABBREVIATIONS

AMOE	Assistant Manager Office of Project Execution
AMR	Analysis/Model Report
ATDT	Automated Technical Data Tracking (System)
CRWMS M&O	Civilian Radioactive Waste Management System Management and Operations (Contractor)
DTN	Data Tracking Number
QA	Quality Assurance
QAPP	Quality Assurance Program Plan (USGS)
SNL	Sandia National Laboratories
USGS	U.S. Geological Survey
YMP	Yucca Mountain Site Characterization Project
WIPP	Waste Isolation Pilot Plant

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1. INTRODUCTION

1.1 PURPOSE

The data evaluated in this qualification report have been cited in analysis and model reports (AMRs) in support of the Site Recommendation in determining the suitability of the Yucca Mountain Site for a repository for high level nuclear waste. The AMRs use these hydrochemical data as a basis for modeling the chemical interactions between groundwater and engineered materials, including waste forms, packages and materials in the engineered barrier system. J-13 water is also used as a reactant in experiments performed to collect data on corrosion of waste packages and repository materials, on solubility of radionuclides, on waste form leach rates, and in simulations of the mobility of radionuclides in groundwater, among other applications. J-13 water serves effectively as a reference or surrogate water composition across the program. Establishing a qualified data set describing the composition of J-13 will help ensure commonality among the various studies. This Data Qualification Report evaluates the Final Report by Harrar et al. (1990), which contains the unqualified data, based on their critical evaluation and assessment of validity of the use of J-13 water (DTN: LL980711104242.054). The unqualified data considered in this report were cited in the following AMRs:

- AMR E0040, In-Drift Microbial Communities, ANL-EBS-MD-000038
- AMR E0100, Physical and Chemical Process Model, ANL-EBS-MD-000033
- AMR E0105, In Drift Precipitates/Salts Analysis, ANL-EBS-MD-000045
- AMR F0085, Pure Phase Solubility Limits: LANL, ANL-EBS-MD-000017
- AMR F0095, Summary of Dissolved Concentration Limits, ANL-WIS-MD-000010
- AMR F0130, Summary of In-Package Chemistry for Waste Forms, ANL-EBS-MD-000050
- AMR F0155, Cladding Degradation - Summary and Abstraction, ANL-WIS-MD-000007
- AMR W0070, Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier, ANL-EBS-MD-000001

Some of these AMRs use DTNs that are derived from the mean values from Table 4.1 in the Harrar et al. (1990) report.

1.2 SCOPE

This report evaluates a data set identified in Data Qualification Plan TDP-NBS-HS-000096 (Revision 0). The Data Qualification Plan identifies three data tracking numbers (DTNs) containing two tables of chemical analyses (Harrar et al., 1990, Tables 4.1 and 4.2) and tables of data derived from those tables. The DTNs are:

- LL980711104242.054 Report of the Committee to Review the Use of J-13 Well Water in Nevada Nuclear Waste Storage Investigations, Tables 4.1 and 4.2 from Harrar et al. (1990)
- LL000203605924.124 Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier, Mole equivalents of mean wt. % in Harrar et al. (1990)
- MO9909SPA00J13.006 J-13 Water Compositions Used in MING Calculations, Table 4.1 Means from Harrar et al. (1990) with assumed dissolved organic carbon abundance from DTN MO9909SEPDOC08.005

Tables 4.1 and 4.2 in Harrar et al., (1990) contain a compilation of major and minor constituent data for water drawn from well J-13 and a set of associated means and standard deviations. Only the major ion, pH and alkalinity mean values are used in the AMRs citing the DTNs.

1.3 DATA QUALIFICATION TEAM

The Responsible Manager for this data qualification task is Robert F. Wernheuer.

The Chairperson for this data qualification team is Terry Steinborn: Dr. Steinborn has a BA (1968) in Chemistry with emphasis on inorganic and radiochemistry, and an MS (1972) and Ph.D. (1976) in Geology with emphasis in geochemistry and volcanology. He has 24 years of experience, most of it in activities related to nuclear and hazardous waste environmental issues. He served on the Department of Energy - Headquarters Independent Review Team for the Waste Isolation Pilot Plant (WIPP), and worked with Sandia National Laboratories (SNL) on WIPP, the Greater Confinement Disposal Program, and SNL Site Environmental Restoration. He has had no involvement with the collection or processing of any YMP data.

Qualification Team Members include:

R. L. Bassett: Dr. Bassett has a Ph.D. in Geochemistry from Stanford University, and MS and BS Degrees in Geology (Geochemistry Emphasis) from Texas Technological University and Baylor University. He has 23 years experience in aqueous and isotopic geochemistry and hydrogeology. He has worked on projects or had funded research related to the nuclear waste site characterization in the Palo Duro Basin, Nuclear Regulatory Commission-funded field site investigations for unsaturated zone geochemical characterization and modeling, National Academy of Science Panel on Low Level Radioactive Waste, Hanford Expert Panel, Geochemistry Session Organizer for Waste Management Conferences, research projects on field tracer tests, isotopic fingerprinting, geochemical and transport modeling. He is a professor at the University of Arizona, Department of Hydrology and Water Resources, teaching geochemistry, isotopic chemistry and radioactive waste classes. He has had no involvement with the collection or processing of any YMP data.

Robert W. Bonisolli: Mr. Bonisolli has a BS in Marine Engineering from Massachusetts Maritime Academy (1981) and 19 years experience in nuclear power plant construction and operational support. Within the YMP, Mr. Bonisolli has conducted independent assessments such as the "Independent Assessment of the Office of Civilian Radioactive Waste Management

(OCRWM)/M&O Procurement Practices." Mr. Bonisolli has had no involvement with the collection or processing of these data.

1.4 BACKGROUND

The quality issues associated with the data in the cited DTNs include:

- Collection of data prior to implementation of the YMP-approved U.S. Geological Survey (USGS) Quality Assurance Program Plan (QAPP)
- Qualification of a study that attempted to determine the validity of the use of J-13 water as a reference material performed before recent Quality Assurance (QA) requirements and procedures were in place.

The cited DTNs contain a summary of analytical data and a set of mean and standard deviations of major and minor constituents in water from one well at the Nevada Test Site (NTS), designated UE-25 J-13, referred to in this report as J-13. The source data from which the subject DTNs were derived are unqualified data collected by the USGS and several national laboratories (Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Argonne National Laboratory and Hanford Engineering Development Laboratory). The data in the DTNs are drawn from Tables 4.1 and 4.2 of Harrar et al. (1990), which performed a critical evaluation of the source data for well J-13 available at that time and calculated means and standard deviations from those source data. Harrar et al. (1990) evaluated the source data by examining the location relative to the repository block, the stability of the water chemistry over time, and a comparison of J-13 water composition to other area wells. They also reported model calculations performed comparing the J-13 composition to expected composition resulting from interaction between rainwater and the Topopah Spring Tuff, which makes up the aquifer from which J-13 water is drawn. That report also discussed the effects of water chemistry variations on calculated behavior of waste package components.

The Harrar et al. (1990) report did not evaluate the sample collection or laboratory analysis procedures employed in developing the source data. All other evaluations made in that report led to the conclusion that J-13 well water is a valid composition for use in testing and modeling geochemical interactions between groundwater and materials associated with the Yucca Mountain repository. They found that J-13 samples water from the same stratigraphic horizon as the proposed repository and that the major constituents in J-13 water have displayed little variation over time and over various sampling and analysis events.

2. QUALIFICATION METHODS

The qualification method of *technical assessment* is used. Technical assessments have been applied to determine the appropriateness and adequacy of the data evaluation performed and reported by Harrar et al. (1990). The report has been critically reviewed to determine if the evaluation process used and the documentation presented are appropriate and adequate to allow the means of the major chemical constituents presented in that report to be qualified for use.

Technical assessments were conducted by subject matter experts in accordance with the requirements of procedure AP-SIII.2Q Attachment 2.

2.1 EVALUATION CRITERIA

The criteria considered in evaluating the qualification status of the means of the constituents in the J-13 well water presented by Harrar et al. (1990) are identified below. These criteria were selected to incorporate the considerations in procedure AP-SIII.2Q Attachment 2 and the applicable qualification process attributes listed in procedure AP-SIII.2Q Attachment 3.

1. Are qualifications of personnel or organizations generating the data comparable to qualification requirements of personnel generating similar data under the approved 10 CFR 60, Subpart G program?
2. To what extent do the data demonstrate properties of interest?
3. For what prior applications have the data been used?
4. What are the results of prior reviews of the data?

2.2 RECOMMENDATION CRITERIA

The following recommendation criteria are considered in determining whether the status of the data should be changed to qualified.

1. The data evaluation performed by Harrar et al. (1990) is appropriate and adequate.
2. The data adequately represent the properties of interest.
3. The data are appropriate for the intended uses.

A finding that the data are qualified for use means that the J-13 water composition (major constituents) presented as a mean of a number of source observations, can be used for all applications where J-13 water is deemed by users to be appropriate.

3. EVALUATION RESULTS

The evaluation results are reported in subsections corresponding to the evaluation criteria described in Section 2.1.

3.1 QUALIFICATIONS OF PERSONNEL

Biographical information presented in Appendix 2 of Harrar et al. (1990) indicates that the authors of that report have suitable qualifications to perform the evaluation of the source data and to generate the set of means from those source data.

Jackson E. Harrar was the chairman of the evaluation committee and the principal author of the report. Dr. Harrar has a B.S. in Chemistry from Purdue University and a Ph.D. in Analytical Chemistry from the University of Washington. At the time of the evaluation, he was Section Leader for Inorganic Analysis in the Chemistry and Materials Science Department at Lawrence Livermore National Laboratory. He has experience and expertise in electroanalytical chemistry,

solution chemistry, field and laboratory water analysis, chemical instrumentation and nuclear materials analysis.

James F. Carley was a member of the evaluation committee and a co-author of the report. Dr. Carley has undergraduate and Ph.D. degrees in Chemical Engineering from Cornell University. At the time of the evaluation, he was a staff scientist in the Polymers Section of the Chemistry and Materials Science Department at Lawrence Livermore National Laboratory. He has experience and expertise in polymer processing, oil-shale research, statistics, quality assurance and experimental design. He is a registered engineer (by exam) in California and Colorado.

William F. Isherwood was a member of the evaluation committee and a co-author of the report. Dr. Isherwood has an A.B. in Mathematics from Princeton University, and M.S. in Geophysics from the University of Utah, and a Ph.D. in Geological Sciences from the University of Colorado. At the time of the evaluation, he was a member of the Earth Sciences Department at Lawrence Livermore National Laboratory and was Project Leader for the Livermore Site Ground Water Project. He has experience and expertise in geophysics, particularly in geothermal resource geophysics including reservoir modeling and environmental studies.

Ellen Raber was a member of the evaluation committee and a co-author of the report. Ms. Raber has a B.A. in Geology from Lafayette College and a M.S. in Geochemistry from the University of Massachusetts. At the time of the evaluation, she was Group Leader for Applied Technology in the Special Projects Division at Lawrence Livermore National Laboratory. She has experience and expertise in the use of hydrogeological, geophysical and geochemical measurements in field site assessment. She has worked on projects in geothermal energy development, environmental geochemistry and radionuclide migration.

These qualifications meet or exceed the qualifications for similar activities in the YMP.

3.2 DEMONSTRATION OF PROPERTIES OF INTEREST

The data contained in Table 4.1 of Harrar et al. (1990) include all of the major constituents of interest, including major ions, pH and alkalinity, for waste package, engineered barrier and radionuclide migration testing and modeling for the YMP. Harrar et al. (1990) found that the water from J-13 was a reasonable surrogate for water expected to enter the repository after closure, with certain stipulations. Well J-13 is completed in the same lithostratigraphic unit as the host rock of the repository, although at the J-13 well location the unit is saturated (below the water table). While this is different from the unsaturated repository setting, it is not possible to draw the large amounts of water needed for chemical and geochemical laboratory testing from an unsaturated rock mass. Well J-13 is located several miles to the east of the proposed repository site, but this is necessary for the target horizon to be saturated. Users of these data must consider the possible consequences of the differences between the proposed repository host rock and the saturated rock into which J-13 is completed, and that even though the majority of J-13 water is derived from the Topopah Spring member, as much as 20 % could be derived from lower horizons.

Some of the data considered by Harrar et al. (1990) were collected by the USGS prior to program approval of their Quality Assurance Program Plan (QAPP). The USGS has had a set of sample

collection and laboratory analysis procedures for hydrochemical data collection since at least the early 1960s, and these procedures have changed in only minor ways since that time to reflect improvements in technology.

Data obtained prior to approval of the USGS YMP QAPP in May 1989 are unqualified. In general, data collected by the USGS after May 1989 are considered qualified. After May 1989, USGS *Hydrologic Procedures* became the approved implementation procedures for USGS data collection activities. The USGS began developing and implementing these procedures as early as 1983 but they were not formally adopted by the survey until 1986.

Descriptions of the collection and analytical methodologies can be found in published USGS literature. Between 1967 and 1985, USGS *Techniques of Water Resources Investigations* are cited as the source for hydrochemical sampling and analytical protocols. Major ion data were also collected by other agencies and provided to and published by the USGS. These agencies include the Nevada Department of Conservation and Natural Resources, U.S. Bureau of Reclamation, and University of Nevada Desert Research Institute.

The USGS procedures in effect from 1960 to the present indicate an evolution and elaboration of the methodology for water sample collection. This methodology includes ensuring the cleanliness of the sample containers, filtering of the samples, acidification to preclude precipitation of metals, tightly sealed caps and stoppers for sample bottles, and timeliness of conducting analysis of the obtained samples.

The hydrochemical data collected by the USGS are adequate for YMP use because of the use of officially established procedures for sample collection and laboratory chemical analysis. Harrar et al. (1990) determined that data collected by the National Laboratories were similar enough to the USGS data to include in the DTN considered in this DQR.

3.3 PRIOR APPLICATIONS

Water from the J-13 well has been used since the beginning of investigations related to nuclear waste storage at Yucca Mountain for a variety of experimental studies, and its composition has been used as a primary reactant in geochemical modeling calculations. In addition to the AMRs listed in Section 1.1, the water has been used over many years for experimental work covering engineered materials corrosion, leaching and mobility of radionuclides, and many other areas. One set of these studies, behavior of components of the waste package system, was investigated as part of the Harrar et al. (1990) evaluation.

3.4 RESULTS OF PRIOR REVIEWS

Harrar et al. (1990) reviewed the available data and produced the tables that comprise these DTNs. That review determined that the data were appropriate for use as a program-wide groundwater composition. The Harrar et al. (1990) review compiled means and standard deviations for the major chemical characteristics. As that report points out, these were calculated using the assumption that their source data all represented single analyses. In fact, Harrar et al. (1990) recognized that many of their source analyses were in fact averages of more than one individual chemical analysis. Because they did not have information as to how many analyses

were represented in each of their input analyses, they were left with no choice but to calculate the mean and standard deviation on the basis of equal weight for each of their source analyses. Harrar et al. (1990) observed that this would not have a significant effect on the means, since all of their source data were quite similar, but that their calculated standard deviations may be much larger than would have been the case if all individual analyses were used instead of the averages available to them. The standard deviations in Tables 4.1 and 4.2 of Harrar et al. (1990) do not accurately characterize the variance in J-13 water chemical composition.

However, chemical interactions between rainwater and the Topopah rock were modeled as part of that evaluation, and it was found that the J-13 well water was not in complete equilibrium with the host rock. More recent studies (CRWMS-M&O, 1997, CRWMS-M&O, 2000) have shown that the pH and carbonate species data do not reflect equilibrium with the rest of the water chemistry. While this does not mean that J-13 water should not be used for experimental studies where a water similar in composition to probable repository seepage water is desired, it does mean that modeling chemical reactions with this water composition requires that the water chemistry (particularly carbonate species and pH) be adjusted to reflect probable *in situ* conditions. The Harrar et al. (1990) report mentions that field pH measurements appeared to range between 6.9 and 7.1, with laboratory measurements yielding higher values. The deviation in carbonate and pH from laboratory analyses may be due to loss of dissolved CO₂ during sample collection and handling, causing the samples measured in the laboratory to be out of equilibrium with the *in situ* atmosphere.

4. EVALUATION CONCLUSIONS

1. Was the critical evaluation of the source data performed by Harrar et al. (1990) appropriate and adequate?

The evaluation reported in Harrar et al. (1990) examined the appropriateness of J-13 water as a surrogate for repository water. That evaluation looked at geography, stratigraphy and stability as the primary grounds for its recommendation. It did not look at the quality of individual analyses. The consistency of the analyses, coupled with the other findings of the report comprise an appropriate and adequate evaluation of data available at that time.

2. Do the data adequately represent the properties of interest?

The means presented in Table 4.1 of Harrar et al. (1990) adequately represent the major chemical constituents and characteristics of J-13 water. These characteristics are the ones necessary for geochemical modeling and for experimental geochemical studies.

3. Are the data appropriate for the intended uses?

The water composition data are appropriate for geochemical modeling, although the user needs to be aware that J-13 water, as characterized by the data presented by Harrar et al. (1990) is not in equilibrium with the atmosphere. This disequilibrium requires that an adjustment be made in the composition, usually in pH or carbonate (or some combination of both) to make sure that the composition used as a starting point in geochemical modeling studies is appropriate. J-13 water can be used directly as a surrogate for repository water in experimental studies. The standard

deviations reported by Harrar et al. (1990) should not be used to characterize variance in J-13 chemical composition, although they may have some use as upper limits.

5. RECOMMENDATIONS

Based on the Technical Assessment reported here, the qualification team recommends that the following DTN be qualified for inclusion in technical products in support of the Site Recommendation for generalized uses as described in this report. Table 1 presents the data recommended for qualification and for use as a surrogate groundwater composition for geochemical modeling studies involving groundwater.

DTN MO0006J13WTRCM.000 should be qualified as a source of mean data for major constituents of J-13 well water, including Na, Si, Ca, K, Mg, pH, F, Cl, NO₃, SO₄ and alkalinity. Minor element data considered by Harrar et al. (1990) and given in Table 4.2 of that report are too inconsistent to include as qualified. These constituents should be the subject of future study to establish a more complete surrogate groundwater composition. Geochemical modeling studies may require that assumptions appropriate to the application be made for the minor and trace element abundances.

The following recommendations apply to the DTNs covered by this DQR:

- LL980711104242.054 *Report of the Committee to Review the Use of J-13 Well Water in Nevada Nuclear Waste Storage Investigations*, Tables 4.1 and 4.2 from Harrar et al. (1990)

This DTN remains unqualified. All prior and future users of J-13 mean major constituent composition data should use the new DTN: MO0006J13WTRCM.000, which contains Table 1, above. These data were extracted from DTN LL980711104242.054.

- LL000203605924.124 *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier*, Mean major constituent compositions from Harrar et al. (1990) and the calculate milliequivalents of those major constituents

This DTN should be classified as *qualified*. This DTN was calculated by dividing the major constituent means in Harrar et al. Table 4.1, which are equivalent to the new DTN listed above, by the appropriate atomic weights, which are accepted data available in handbooks and multiplying by the charges of the ionic species, which are accepted data - fact.

- MO9909SPA00J13.006 *J-13 Water Compositions Used in MING Calculations*, Harrar et al. (1990) Table 4.1 mean values with assumed dissolved organic carbon abundance data from DTN MO9909SEPDOC08.005

AMR authors citing DTN MO9909SPA00J13.006 for major constituent composition data from J13 should cite DTN MO0006J13WTRCM.000. AMR authors using dissolved organic carbon abundance data from J13 should not cite DTN MO9909SEPDOC00.005. These data should be discussed in the Assumptions section of the AMR.

6. REFERENCES

CRWMS-M&O, 1997, Degraded Mode Criticality Analysis Of Immobilized Plutonium Waste Forms In A Geologic Repository. A00000000-01717-5705-00014, Revision 01, ACC:MOL.19970723.0058.

CRWMS-M&O, 2000, In-Drift Precipitates/Salts Analysis. ANL-EBS-MD-000045. ACC: Pending.

Harrar, J.E., Carley, J. F., W. F. Isherwood, and E. Raber, 1990, Report of the Committee to Review the Use of J-13 Well Water in Nevada Nuclear Waste Storage Investigations. UCID-21967, Livermore, California, TIC: 209096.

Table 1-1. Recommended Mean Values of Major Constituents in J-13 Well Water

Constituent	Mean Value (mg/L)	Std. Dev.
Na	45.8	2.29
Si	28.5	1.85
Ca	13.0	0.99
K	5.04	0.61
Mg	2.01	0.21
pH	7.41 ^{a,b}	0.44
Alkalinity (as HCO ₃ ⁻) ^c	128.9	8.6
F ⁻	2.18	0.29
Cl ⁻	7.14	0.61
NO ₃ ⁻	8.78	1.03
SO ₄ ²⁻	18.4	1.03

a - Standard units

b - This pH value may not represent down-hole conditions. Users must adjust to suit the application

c - Assumes alkalinity is determined by titration and that the total acid consumed is represented as HCO₃⁻.