Center for Nu_ear Waste Regulatory Analyses

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Subject: NRC High-Level Radioactive Waste Research at CNWRA (CNWRA 94-02S) Page 154

Dear Dr. Randall:

Page 154 of the Research Program Semi-Annual Report containing references for the Field Volcanism chapter (Chapter 9) was inadvertently left out. A copy of the missing page is enclosed.

After NRC approval, we shall include this page in the reprinting of the bound report that we will mail to our NRC approved distribution list.

Please contact me if you have any questions regarding this matter.

Sincerely yours,

Budhi Sagar
Technical Director

Enclosures
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NRC HIGH-LEVEL RADIOACTIVE WASTE RESEARCH AT CNWRA JULY—DECEMBER 1994

Prepared for

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Number	Name	Date Issued
CNWRA 90-01Q	First Quarterly Research Report for 1990 January 1–March 30	May 1990
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CNWRA 90-03Q	Third Quarterly Research Report for 1990 July 1–September 30	November 1990
NUREG/CR-5817 Volume 1 CNWRA 90-01A	Report on Research Activities for Calendar Year 1990	December 1991
CNWRA 91-01Q	First Quarterly Research Report for 1991 January 1–March 30	May 1991
CNWRA 91-02Q	Second Quarterly Research Report for 1991 April 1–June 30	August 1991
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PREFACE

The Center for Nuclear Waste Regulatory Analyses (CNWRA), a Federally Funded Research and Development Center (FFRDC), conducts research on behalf of the Nuclear Regulatory Commission (NRC). The NRC-funded research at the CNWRA is focused on activities related to the NRC responsibilities defined under the Nuclear Waste Policy Act (NWPA), as amended. Progress for the period of July 1, 1994 to December 31, 1994 on nine of twelve research projects that are currently active is described in this report. Three research projects not reported here are the Thermohydrology, Subregional Hydrogeologic Flow and Transport Processes, and High-Level Waste Near-Field Processes and Variations. The final report for the Thermohydrology Research Project has been prepared and submitted for peer review. The Subregional Hydrogeologic Flow and Transport Processes and High-Level Waste Near-Field Processes and Variations Research Projects were initiated in December 1994 and February 1995, respectively, and have not progressed sufficiently for inclusion in this report. For a brief summary of the work performed during the reporting period, the reader is referred to the Executive Summary.

In addition to disseminating research results through publications in appropriate open literature (e.g., CNWRA topical reports, NRC documents, and journals) and at technical meetings, workshops, and symposia, the CNWRA produces these research reports twice yearly. A list of previous reports in this series is on page iii.

Each chapter in this semi-annual report summarizes the progress made in a particular research project and is authored by the researchers in that project. Since readers of this report may be interested only in a particular topic, each chapter is self-contained and can be read without reference to other chapters. Coverage in the semi-annual reports is limited to only the key aspects of progress made; greater detail is provided in topical reports that are produced during the course of the research or at its conclusion, as appropriate. The editor of this report ensures that each chapter is reviewed for its technical and programmatic content and that some uniformity as to the depth of descriptions is maintained across the various chapters.

The NRC evaluates its research needs continually as the research progresses. The research needs are based on user needs identified jointly by the NRC Offices of Nuclear Material Safety and Safeguards (NMSS) and Nuclear Regulatory Research (RES). Generally, the NMSS is the user in the sense that its staff applies the research results to strengthen its reviews of the submittals by the U.S. Department of Energy (DOE), including the License Application (LA) for the first High-Level Nuclear Waste (HLW) Repository. In their turn, the user needs are based on Key Technical Uncertainties (KTUs) identified during the process of developing strategies and methods for determining compliance with the applicable regulations—in this case, 10 CFR Part 60. Thus, the research is directed toward evaluation of the KTUs.

ACKNOWLEDGMENTS

This report was prepared to document work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) for the Nuclear Regulatory Commission (NRC) under Contract NRC-02-93-005. The activities reported herein were performed on behalf of the NRC Office of Nuclear Regulatory Research (RES), Division of Regulatory Applications (DRA). The report is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the NRC.

Active support from several people during the production of this report is thankfully acknowledged. First and foremost, this report is possible only because of the wholehearted cooperation from the principal investigators and researchers within each project who kept to the tight schedule of the editor. Technical reviewers—A.C. Bagtzoglou, A.R. DeWispelare, D.A. Ferrill, A.B. Gureghian, B.E. Hill, W.M. Murphy, P.K. Nair, J.L. Russell, and D.R.Turner—provided substantive comments that materially improved the quality of the report. Programmatic reviews were performed by P.C. Mackin, W.C. Patrick, and the editor. Able secretarial support was provided by E.F. Cantu, B.L. Garcia, C. Garcia, L.F. Gutierrez, M.A. Gruhlke, L.G. Hearon, A. Ramos, R.A. Sanchez, and A.Woods. The overall support from E.F. Cantu and R.A. Sanchez in producing this document using FrameMaker is especially appreciated. R.L. Marshall's assistance in sorting out the graphic files for FrameMaker was a valuable contribution.

Southwest Research Institute (SwRI) Publications Services staff provided illustration, editorial, format adherence, printing, and binding support.

Finally, the valued interaction with NRC project officers G.F. Birchard, L.A. Kovach, M.B. McNeil, T.J. Nicholson, J. Philip, and J.D. Randall is gratefully acknowledged.

QUALITY OF DATA

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

ANALYSES AND CODES: Scientific/engineering computer codes used in analyses contained in this report are: UDEC and ABAQUS (Chapter 2), PORFLOW (Chapter 4), FITEQL and MINTEQA2 (Chapter 5), VTOUGH (Chapter 6), and ARC/INFO Geographic Information System (GIS) (Chapters 8 through 10). The computer codes UDEC, PORFLOW, FITEQL, and MINTEQA2 are presently controlled under the CNWRA Software Configuration Procedure TOP-018. The ABAQUS and ARC/INFO are commercial software, and only their object codes are available to the CNWRA.

1 EXECUTIVE SUMMARY

1.1 INTRODUCTION

Progress from July 1 to December 31, 1994, on nine of twelve research projects underway at the Center for Nuclear Waste Regulatory Analyses (CNWRA) is discussed in this report. One of the three research projects not reported, namely Thermohydrology, has been completed with its final report (Green et al., 1995) submitted for external peer review. The Subregional Hydrogeologic Flow and Transport Processes and High-Level Waste Near-Field Processes and Variations Projects were initiated in December 1994 and February 1995, respectively, and have not progressed sufficiently for reporting in this report. The Integrated Waste Package Experiments Research Project is planned for completion during the next reporting period.

All research projects at the CNWRA are sponsored by the Nuclear Regulatory Commission (NRC) to fulfill its mandate under the Nuclear Waste Policy Act (NWPA), as amended. To understand the role of NRC-funded research, it is important to recognize that the NRC regulatory responsibilities are distinct from those of the U.S. Department of Energy (DOE), which is responsible for siting, constructing, and operating a repository for the permanent disposal of high-level waste (HLW). The DOE has undertaken the development and implementation of a broad range of techniques and methods to obtain information and to produce analyses necessary to determine site suitability, design the engineered portions of the repository, and complete a license application for review by the NRC. In fulfilling its responsibilities for assuring the radiological health and safety of the public, the NRC conducts confirmatory and exploratory (also referred to as anticipatory) research to

- Develop the licensing tools and technical bases necessary to judge the adequacy of the DOE license application
- Ensure a sufficient independent understanding of the basic physical processes taking place at the proposed geologic repository site
- Maintain an independent, but limited, confirmatory research capability to be used in evaluating DOE prelicensing and license application submittals

Figure 1-1 depicts the basic relationship between the NRC research program and licensing needs. Regulations applicable to the licensing of a HLW repository (primarily 10 CFR Part 60) are translated into regulatory requirements, each of which must be met before the NRC staff can recommend the issuance of a license. Strategies and methods for determining if DOE demonstration of compliance with the regulatory requirements is acceptable are currently being developed and documented in the NRC License Application Review Plan (LARP). Key technical uncertainties (KTUs) are defined based on the risk to compliance determination. Evaluation and reduction of those aspects of the KTUs that are the NRC responsibility are the primary objectives of the research undertaken by the NRC. Each chapter of this report outlines the specific KTUs being addressed by the research described in that chapter.

Each research project discussed herein is being conducted in accordance with approved research project plans, which were developed consistent with an associated NRC statement of work. These plans are the vehicle for establishing the objectives, technical approach, justification, and funding for each of

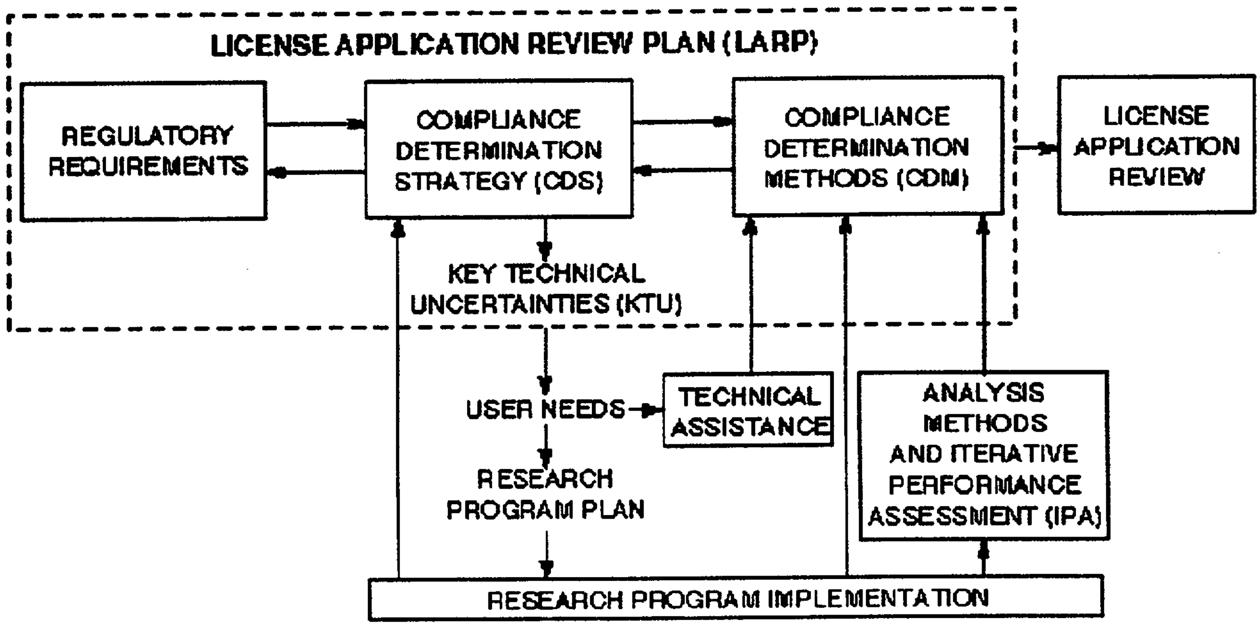

Figure 1. Relationship of the NRC HLW Research Program to licensing needs

the studies. They also describe the interrelationships among the various projects, which provide a sound basis for integrating research results across disciplines. Because the plans primarily address planning and management matters, they are not discussed further in this report.

This executive summary covers, in capsule form, the progress of each research project over the past 6 mo. The executive summary is followed by Chapters 2 through 10, representing each of the nine currently active research projects. Project objectives and a report of research activities and results to date, as appropriate, are given in each chapter. The progress toward fulfillment of identified research needs and the development of particular regulatory products are addressed in cases where such progress has been significant. In addition, commentary is provided on anticipated progress for each project in the ensuing 6-mo period.

1.2 ROCK MECHANICS

Long-term deterioration of emplacement drifts and potentially enhanced near-field fluid flow resulting from coupled processes are among the important concerns for safe high-level nuclear waste (HLW) disposal. Repetitive seismic loads and thermal loads generated by decay of the emplaced waste are among the factors that could potentially cause rock degradation or change near-field flow patterns due to joint normal and shear deformations. Evidence in the literature indicates that the most likely significant effect of earthquakes on hydrology is changes in fracture permeability.

A key technical uncertainty (KTU) that could pose a high risk of noncompliance with the performance objectives of 10 CFR Part 60 has been described in the License Application Review Plan (LARP). This KTU has the ability to predict the long-term effects of repetitive seismic load and high temperatures on the degradation of emplacement drifts. These long-term effects may have implications on the performance of the Engineered Barrier Systems (EBS), retrievability of waste, and long-term waste isolation, especially if some of the openings to the HLW repository are left unfilled at closure. The objective of the Rock Mechanics Research Project is to develop techniques that could be used to predict the response of the near-field rock mass at the proposed repository at the Yucca Mountain (YM) site when it is subjected to repetitive seismic loads and high-temperature conditions. The knowledge gained through laboratory, field, and theoretical analyses in this project has supported the development and implementation of portions of the License Application Review Plan (LARP) and prelicensing activities, including reviews of Exploratory Studies Facility (ESF) design packages. The results of ongoing activities in Tasks 4 and 9 are reported herein.

Task 4 activities during this reporting period included assembly and dynamic experiments of a small-scale model of jointed rock mass. This scale model consisted of approximately 670 cast simulated-rock ingots aligned within a testing frame at 45 degrees to the horizontal. In the center of the simulated rock mass was a 15.2-cm circular tunnel. The simulated-rock ingots were fabricated with appropriate physical and surface (interface) roughness properties to simulate those of naturally jointed Apache Leap welded tuff with a scale of 1/15. However, the density of the simulant material did not strictly follow the similitude requirements due to the need for this material to remain brittle and exhibit surface wear properties approximately similar to those of the prototype material. This physical distortion is judged not to have much effect on the validity of the experimental results for use in verifying of computer codes in predicting rock-mass responses to repetitive dynamic loads and in obtaining a better understanding of rock mass dynamic behavior around underground openings. The ingredients included in the rock-simulant material are Type I Portland cement, barite, water, bentonite, DARACEM-100 (plasticizer), vinsol resin (air entrainment), and Ivory Liquid Soap. Test procedures were based on what can be called an "incremental fragility level" philosophy. Test runs were started at a very low peak excitation displacement level, and this amplitude was incrementally increased as the runs progressed. The excitation displacement input signal was derived from an accelerogram measured at the Guerrero array for the September 1985 Mexico City earthquake using a 1/15-scale. The data acquisition system was centered with a 486 (66 MHz) personal computer and consisted of 50 data channels. The sampling rate for each channel was 2,800 data points/second for a duration of 10 seconds for each run. The measurements for the dynamic scale model experiments included ingot deformation (strain), accelerations, interface (joint) normal and shear displacements, variations of cable loads that provided the initial stress boundary condition for the scale model, and opening convergencies. Significant amounts of data were collected for the dynamic scale model experiments and are being analyzed.

The third phase of Task 9, the **DE**velopment of **CO**upled models and their **VAL**idation against **EX**periments (DECOVALEX), is nearing completion. The numerical modeling of the Big-Ben Experiment (TC3) using the finite element code ABAQUS has been completed. This work involved analyzing the coupled thermal-hydrologic-mechanical (THM) behavior of a partially saturated bentonitic buffer material surrounding a heater system within a simulated rock (concrete). Simulated fractures were also present in the system so that water could be injected into the partially saturated buffer. The purposes of the test were to evaluate the water uptake within the buffer as well as to determine the degree of moisture-induced swelling and expansion under heated conditions and water injection. The experiment involved many complex coupled processes, some of which could not be modeled with the ABAQUS code (Version 5.3) used by the Center for Nuclear Waste Regulatory Analyses (CNWRA). One such process was the heat and moisture flow within the vapor. Even so, the CNWRA results using ABAQUS appear to agree, for the most part, with the experimental measurements as well as with numerical results from other codes. One exception to this agreement is in the higher temperature regions of the buffer adjacent to the heater in which the CNWRA results did not account for the drying within the bentonite. Also, with regard to the mechanical stress state, the effective stress principle as implemented in ABAQUS needs to be further investigated to determine if it is appropriate to use in partially saturated materials over all ranges of saturation. This concern is due to the strong fluid suction versus saturation relation apparently measured for the buffer in the laboratory and provided as input for the analysis. This strong relation resulted in the ABAQUS analysis predicting very high magnitudes of mechanical stress within the buffer. Experimental measurements, as well as results from other codes, showed much lower stress magnitudes.

1.3 INTEGRATED WASTE PACKAGE EXPERIMENTS

The Nuclear Regulatory Commission (NRC) in 10 CFR 60.113 requires that waste packages for high-level nuclear waste provide substantially complete containment of radionuclides for a minimum period of 300 to 1,000 yr. As stated in the License Application Review Plan (LARP) Section 5.4, the key technical uncertainties (KTUs) associated with the assessment of Engineered Barrier System (EBS) compliance with performance objectives include the prediction of environmental effects on the performance of waste packages and the EBS, and the extrapolation of short-term laboratory and prototype test results to predict long-term performance of EBS components. The goal of the Integrated Waste Package Experiments (IWPE) program is to provide a critical evaluation of the information available for assessment of compliance with regulatory requirements pertaining to the EBS by a suitable combination of literature surveys and critical experiments. To achieve its objectives, the IWPE program is divided into six tasks: Task 1–Corrosion, Task 2–Stress Corrosion Cracking, Task 3–Materials Stability, Task 4–Microbiologically Influenced Corrosion, Task 5–Other Degradation Modes, and Task 6–Report Preparation and Peer Review. The results of ongoing activities in Tasks 1, 2, and 3 are reported here.

Two of the key parameters in long-term life prediction of container materials under localized corrosion environments are the initiation and repassivation potentials. In performance assessment calculations, a single critical potential, which is the experimentally determined repassivation potential, is proposed for predicting the occurrence of localized corrosion of waste package containers. The assumption of a single critical potential is supported by the results reported in Chapter 3. Long-term localized corrosion tests (up to 14 months) show that the use of repassivation potential for deep pits or crevices is more conservative than the use of localized corrosion initiation potentials. The initiation potentials for pitting and crevice corrosion were found to decrease with time and approach the repassivation potential after long-term exposures. In addition, specimens held at potentials more negative than the repassivation potential have not yet shown any indication of localized corrosion. Further tests along this line are recommended to gain greater confidence in the use of this parameter for performance assessment.

The applicability of critical potentials for localized corrosion for predicting stress corrosion cracking (SCC) is being studied using slow strain rate and constant deflection tests on type 316L stainless steel (SS) and alloy 825. The results generated thus far are consistent with the assumption that the repassivation potential for localized corrosion constitutes a lower bound for the critical potential for SCC. However, the occurrence of SCC is apparently dependent on test technique. In contrast to slow strain rate tests in which SCC of type 316L SS was only observed at high chloride concentrations, SCC was observed using U-bend specimens in constant deflection tests conducted in either concentrated chloride solutions or in more dilute solutions with and without the addition of thiosulfate. Cracking was confined to the region above the solution/vapor interface for U-bend specimens in both a normal orientation, with the apex of the bend immersed in solution, and an inverted orientation, with the apex of the bend just above the solution/vapor interface. On creviced specimens, formed by using a double U-bend specimen, cracks were always located near the apex of the bend, independent of the specimen orientation. No differences in SCC susceptibility were observed with the two heats of type 316L SS currently being tested in the IWPE program. In the case of alloy 825, no apparent discrepancies were observed by comparing the results of the slow strain rate tests with those of constant deflection tests under environmental conditions similar to those used for testing type 316L SS. For alloy 825, SCC was observed only in a highly concentrated chloride solution (approximately 14 molal) in both slow strain rate and U-bend tests. However, since alloy 825 is far more resistant to SCC than type 316L SS, additional studies are needed to reach a conclusion. The need to further study the effect of crevice conditions and concentration processes at the vapor/solution interface on the initiation of cracks is emphasized to explore the full range of environmental and electrochemical conditions that can cause cracking of these alloys in chloride-containing solutions at temperatures close to the boiling point.

The thermal stability of alloy 825 was investigated and compared to the well-characterized type 304 SS. Sensitized alloy 825 has a high corrosion rate in standard boiling nitric acid tests but not in ferric sulfate/sulfuric acid tests. These results indicate that there is significant precipitation of high chromium-containing phases at the grain boundaries but comparatively little chromium depletion in the adjacent grains. Scanning transmission electron microscopy investigations of the sensitized material confirmed the results obtained in these standard corrosion tests. Chromium-rich $M_{23}C_6$ precipitates were found along the grain boundaries of the sensitized material, but unlike type 304 SS, no significant chromium-depleted regions near the grain boundaries could be detected. The precipitates were determined to contain as much as 71 wt percent chromium, in general agreement with literature values for $M_{23}C_6$ precipitates in Fe-Cr-Ni based materials. Cyclic potentiodynamic polarization tests conducted in 100 ppm chloride indicate that the repassivation potential, which has previously been shown to be sensitive to chromium depletion, decreased as the degree of sensitization increased. Further characterization of the precipitates and near-grain boundary regions of thermally treated alloy 825 is necessary for a comprehensive evaluation of the mechanism and effects of sensitization.

1.4 GEOCHEMICAL ANALOG OF CONTAMINANT TRANSPORT IN UNSATURATED ROCK

The technical objective of the Geochemical Natural Analog Research Project is to develop an understanding of the utility and limitations of natural analog studies in support of a license application for a high-level waste (HLW) repository and to provide fundamental data on the long-term behavior of a HLW repository. Natural systems that have evolved for periods of time comparable to that required for HLW disposal (i.e., 103 to 104 yr and greater) (U.S. Environmental Protection Agency, 1989) provide unique opportunities to obtain observational knowledge of the behavior of HLW repository subsystems. Such information is important in support of long-term predictive models of repository performance (Nuclear Regulatory Commission, 1987).

Qualitative and quantitative comparisons are made between field data for contaminant transport at Delta 3 in the Akrotiri, Santorini natural analog site, and a corresponding numerical flow and transport model. The archaeologic site has many features that are analogous to the proposed repository at Yucca Mountain (YM): silicic volcanic rocks, chemically oxidizing environment; partially saturated hydrology, semiarid climate, well constrained source of contaminant material, and a time scale of burial (approximately 3,620 yr) comparable to the regulatory period. Field samples have been collected and analyzed to detect and document the contaminant plume that emanated from bronze Minoan artifacts buried in silicic volcanic materials. Other meteorologic, hydrologic, geologic, and geochemical data have been collected to characterize the site to support numerical unsaturated flow and transport modeling. The flow and transport model was developed using data collected at the site, laboratory data on site materials, and literature data. Although site characterization data from Akrotiri are subject to considerable practical limitations, both the data and the limitations reflect fundamental facets of the development of performance assessments for the YM repository. Similarly, modeling presented in this report was conducted without knowledge of the character and extent of the contaminant plume at Akrotiri.

Cu is a primary component of the bronze artifacts and occurs in large concentrations in visible corrosion products located only immediately adjacent to artifacts. Cu occurs at slightly elevated concentrations associated with Mn in packed earth material. Zn shows a systematic pattern of decreasing concentration with depth in Hole IV. Both Zn and Cu show elevated concentrations in the deepest sample from Hole IV, suggesting a heterogeneous path to this point. Pb associated with the carbonate fraction reveals considerable heterogeneity. Relatively high values for Pb commonly occur in the top 15 cm, but never occur below 20 cm. Pb is also significantly enriched in Hole VII, which is adjacent to a major fracture.

The vertical, one-dimensional (1D) model system extends from the pre-excavation ground surface to the groundwater table at a depth of 24 m. At the top is a flux boundary with yearly sinusoidal infiltration reflecting the Mediterranean climate at the site. Four vertically disposed zones in the model correspond to the overlying Minoan tuff, the zone of Minoan deposits enclosing artifacts, a zone of packed earth floor material immediately beneath the zone of artifacts, and a zone of underlying Cape Riva tuff. No fractures or other heterogeneities are incorporated explicitly in the model. Porosity, hydraulic conductivity, moisture retention curve parameters, and distribution coefficients were assigned to the unsaturated matrix materials in the simulations. These data were determined in part from property values measured in the field and in the laboratory on samples from the Akrotiri site. Cu transport from the artifacts was modeled. The Cu source was fixed in the model by specifying a constant solubility-limited concentration in the zone containing artifacts.

Steady-state conditions are achieved rapidly in the model and correspond for most of the profile to initial conditions. The low permeability, highly sorptive packed earth layer has a dominant effect on modeled flow and transport. Sinusoidal infiltration has a small effect on steady-state hydraulic oscillations, which is detectable only above the packed earth. Aqueous Cu concentrations computed in the model show that concentrations beneath the source zone equal the constant value of the source over the time scale of millennia. Constant distribution coefficients in the model therefore produce no gradient in sorbed Cu over the same distances, except where the distribution coefficient changes for different materials.

Although some results from the field are qualitatively consistent with model results, important discrepancies result from poor representation of heterogeneity in the model and poorly constrained model parameters. System components that appear to have had major impacts on distribution of contaminants (i.e., Mn minerals in packed earth and the fracture adjacent to Hole VII) were neglected in the model. Identification of such components in relevant systems is confirmed as a major contribution that analog studies can make in support of repository modeling. Major assumptions, were required in the base model concerning both water chemistry and its control on the source term, retardation, and infiltration. Future data collection and interpretation will be used to refine these assumptions and tests will be performed to examine the sensitivity of model results to such parameters. This process may resolve discrepancies between field data and model results such as the apparent remaining transient nature of the Zn and Cu plumes in the field and the over prediction of sorption on packed earth in the model.

1.5 SORPTION MODELING FOR HIGH-LEVEL WASTE PERFORMANCE ASSESSMENT

To develop an understanding of radionuclide sorption processes and the important physical and chemical parameters that affect sorption behavior in the Yucca Mountain (YM) environment, experiments are being conducted to investigate the sorption behavior of U and other actinides on geologic media. During the second half of 1994, experiments were completed to determine the effects of pH, solid-mass to solution-volume (M/V) ratio, and U concentration on the sorption of uranium(6+) on quartz, which is a widespread and major rock-forming mineral at YM. The experiments were conducted using initial solution concentrations of 5, 50, or 500 ppb U, solution pH from 2 to 9, and M/V equal to 2, 20, or 50 g/L. The results show that uranium sorption on quartz is strongly dependent on pH. At an M/V ratio equal to 20 g/L and initial U concentration equal to 50 ppb, uranium sorption increases sharply at pH values above 4 ("adsorption edge"), reaches a maximum at pH approximately 6.8, and decreases sharply at pH greater than about 7.5 ("desorption edge"). Sorption data at M/V equal to 50 g/L indicate that, at a higher M/V ratio, the "sorption envelope" broadens, that is, the adsorption edge shifts to lower pH whereas the desorption edge shifts to higher pH, and the sorption maximum increases to higher values. Similar effects on the sorption envelope are observed when the initial uranium concentration is lowered (e.g., from 50 to 5 ppb). The experiments were conducted in a manner such that the amount of uranium sorbed on the quartz and the experimental containers could be independently quantified.

Modeling of uranium(6+) sorption on quartz was performed using a surface complexation modeling approach. A simplified diffuse-layer model (DLM) was used to reproduce the experimentally observed sorption behavior of uranium and to predict its sorption behavior under differing experimental conditions. Results of the modeling indicate that the sorption data could be fitted well by a simple DLM, but that at least two complexation reactions were required to appropriately model all data. Even in its simplified form, the DLM is capable of accounting for the effects of changing physicochemical conditions such as M/V or pH.

Results of the laboratory experiments and modeling activities provide the Center for Nuclear Waste Regulatory Analyses (CNWRA) with an understanding of the important parameters that control the sorption behavior of an actinide element. Because of the strong dependence on pH and sorbent-surface-area/solution-volume ratio, modeling of sorption processes will likely require that changes in groundwater chemistry and in rock/fluid ratio be properly accounted for in performance assessment calculations if retardation by sorption processes is included. However, the success of the surface-complexation model (SCM) in describing and predicting uranium sorption on quartz and other minerals suggests that SCMs offer a scientifically defensible approach that may be useful for performance assessment calculations.

The similarity in the pH-dependence of uranium sorption on quartz observed in experiments reported in this report and those reported previously for minerals such as a-alumina, montmorillonite, and clinoptilolite is important. It may help identify simplified approaches to modeling sorption and thus help in the development of Compliance Determination Methods (CDMs) relevant to the Key Technical Uncertainties (KTUs) identified in License Application Review Plan (LARP) Section 5.1 and in developing conceptual models related to the Performance Assessment Research Project and the Iterative Performance Assessment Phase 3. The information derived from the laboratory experiments may also help interpret data on uranium distribution and migration at the Peña Blanca field site of the Geochemical Analog of Contaminant Transport in Unsaturated Rock Research Project.

1.6 PERFORMANCE ASSESSMENT RESEARCH

In this research project, three general and interrelated technical objectives are being pursued. The first of these objectives is to provide modeling technology that will directly benefit the Nuclear Regulatory Commission (NRC) Iterative Performance Assessment (IPA) activity and be used in Compliance Determination Methods (CDMs). The second, and equally important, objective is to address Performance Assessment (PA) topics (e.g., conceptual models, mathematical models, model parameters, future system states, and model validation), which are designated as Key Technical Uncertainties (KTUs) in the License Application Review Plan (LARP). The third objective is to provide the technical basis for formulating guidance to the U.S. Department of Energy (DOE) in the specific areas of PA modeling approaches, particularly in the areas of disruptive scenarios and model validation. Studies conducted under the PA Research Project are divided among tne following three major tasks: Task 1–Conceptual Model Development, Task 2–Computational Model Development, and Task 3–Model Evaluation. In this reporting period, research emphasis was on topics associated with Tasks 1 and 3. As part of Task 1, a detailed study was conducted of multiphase flow and reactive transport models for the near-field zone. Under Task 3, a computer modeling study was performed to examine the relation between model predictive reliability and sampling schemes used to obtain data in heterogeneous media. Work was also performed on: (i) benchmark testing of DOE and NRC/Center for Nuclear Waste Regulatory Analyses (CNWRA) thermohydrologic codes, (ii) evaluating the Parallel Virtual Machine (PVM) computing technology, (iii) completing documentation on the new infiltration model for use in IPA Phase 3, and (iv) completing documentation of the analysis of hydraulic characteristics of tuff samples from the Peña Blanca site.

A study of near-field conceptual and mathematical models was given high priority to better position the NRC to review and critique the current DOE thermal loading strategy, which is referred to as the "extended-dry concept." The study involved a detailed technical review of the theoretical basis currently used in thermohydrologic models and codes. The review was conducted in a manner that identified the limitations and ranges of applicability of thermohydrologic models to unsaturated tuff. In addition, this review examined methods of estimating porosity and permeability changes that may occur in the thermohydrologic environment as a result of changes in pore fluid chemistry. This activity resulted in a CNWRA technical report (Lichtner, 1994) that is expected to be published as a NUREG/CR. In this semi-annual report, one aspect of that near-field study is highlighted, namely, an analysis of hydrochemical effects on porosity and permeability. A conservative hydrochemical model was formulated to estimate, as a function of temperature, the extent of mineral dissolution in the tuff. This model was then applied to bound adverse porosity and permeability changes in the tuff. For the case in which the K-feldspar completely dissolves, the model predicts that the matrix permeability could increase by one to two orders of magnitude, depending on pore-fluid temperature.

A hydrologic modeling study of predictive reliability and sampling design was also given high priority because of its potential benefits to addressing the related issues of conceptual model uncertainty and model validation. In the study, soil hydraulic data from the Las Cruces trench experiment were used to define properties of the hydrostratigraphy, assuming various sampling configurations. Predictions of water content obtained from a flow model were compared to in situ water content measurements for a long-term infiltration experiment. A single geometric representation of the layering was used in which the hydraulic properties were assigned to each zone using both purely random and stratified-random sampling configurations. For each sampling configuration, 10 infiltration simulations were performed to obtain estimates of the mean prediction error. Two measures are used to compare the predicted and observed moments of the infiltrated moisture plume. Both measures indicate a general improvement in the accuracy of the model predictions as the number of samples is increased, although the marginal increase in accuracy decreases rapidly as more samples are taken.

Based on the mean squared error measure, the purely random sampling configuration produced the most accurate predictions. This activity, which is highlighted in this semi-annual report, resulted in the paper by Wittmeyer et al. (1994), which has been submitted for journal publication.

1.7 VOLCANIC SYSTEMS OF THE BASIN AND RANGE

Investigations in the Volcanic Systems of the Basin and Range Research Project are directed primarily toward development of probability models of potential volcanic events in the Yucca Mountain Region (YMR), based as far as possible on geologic insight into tectonic processes and geological controls on small volume basaltic volcanism. The project is directed toward addressing several key technical uncertainties (KTUs) including: (i) prediction of future system states (disruptive scenarios), and (ii) development and use of conceptual tectonic models of igneous activity. During the last 6 months, work has included a critical review of the Volcanism Geographic Information System (GIS) database (delivered as a Major Milestone in January 1995), peer review of volcanism research projects (results delivered as an Intermediate Milestone in January 1995), and development of two new nonparametric models of the probability of volcanic disruption of the proposed repository (submitted as a contribution to the Journal of Geophysical Research).

Research at the Center for Nuclear Waste Regulatory Analyses (CNWRA) into the probability of volcanic disruption of the proposed repository has led to recognition of several scales of spatial and temporal patterns in cinder cone volcanism that must be incorporated into any viable probability model. The patterns include: (i) shifts in the location of volcanism, either by migration or more abrupt changes in the locus of volcanism; (ii) development of clusters; and (iii) development of regional alignments and local vent alignments. Research in this project has documented and quantified these aspects of vent distribution in a comprehensive fashion for the first time. Recognition of these aspects of basaltic volcano distribution provides the Nuclear Regulatory Commission (NRC) with a direct means of assessing the utility and applicability of any volcanism probability model. A model that cannot capture these aspects of basaltic volcano distribution may not be adequate in the formulation of disruptive scenarios unless conservative results can be assured.

Planned research is now essentially complete on the development and implementation of nonparametric, nonhomogeneous probability models, which includes spatio-temporal nearest-neighbor, kernel, and nearest-neighbor kernel models. This research represents the first application of nonparametric and nonhomogeneous probability models to volcanism in the YMR, and the first time these models have been developed for use in volcanic fields in general. Together, these models indicate that the probability of volcanic disruption of the repository is between 1×10^{-4} and 5×10^{-4} in 10,000 yr. These estimates encompass broad uncertainty in the ages and number of volcanic events in the YMR. However, currently these models take only extrusive volcanic events into account. Development of these models has provided insight into the spatial scale of probability variation in the YMR that was not otherwise available. Although probability estimates of volcanic disruption of the proposed repository based on nonparametric, nonhomogeneous models are broadly similar to those based on simpler techniques, such as homogeneous models, they also indicate that probability varies by more than two orders of magnitude within 20 km of the center of the repository block, due to the position of the repository at the edge of the Crater Flat Cluster. Thus, these models show that much of the uncertainty in prediction of the probability of disruptive scenarios lies in the constraints that can be placed on this spatial scale of variation.

Several broad and preliminary statements can be made regarding the utility of structural models in igneous disruptive scenario modeling, based on literature review and development of the Volcanism GIS. Correlation between regional rates of extension and volcanism is clear; yet, given available data, this correlation does not, in itself, provide insight in the likelihood of continuing volcanism in the YMR on the spatial and temporal scales of most concern. Rates of deformation are poorly known compared with geochronological data available for most volcanic fields. Episodes of volcanism may occur synchronously with episodes of extension, but this occurrence has not been demonstrated conclusively in any western Great Basin volcanic field. On a regional scale, volcanism in the western Great Basin is sometimes localized in pull-apart zones and similar structures. Broad, regional fault patterns in the YMR may be consistent with this relationship. However, the scale of this correlation, for example, in the Coso volcanic field, is coarse compared with the proximity ot the repository to Crater Flat. Fault and dike interaction is a viable means of focusing magmatism, particularly in areas like the YMR, where regional fault patterns and principal stress orientations are sympathetic. Therefore, the fault pattern should be considered in formulating probabilistic models on a detailed local scale, such as in Iterative Performance Assessment (IPA). Yet little data are available related to the extent to which this interaction controls the ascent and localization of basaltic magmas. One conclusion from these observations is that current probability models based on structural control are tentative at best. It is questionable whether these models have a predictive value on the temporal and spatial scales of interest for volcanic disruptive scenarios. Nonetheless, incorporation of structural and tectonic data does remain as one of the most likely avenues for introducing a mechanistic basis for probability models development and evaluation.

1.8 TECTONIC PROCESSES IN THE CENTRAL BASIN AND RANGE REGION

The primary objectives of the Tectonics Research Project are to compile and integrate tectonic data for the Central Basin and Range and Yucca Mountain (YM) regions, and to develop and assess models of tectonic processes. The purpose of the project is to evaluate the adequacy of existing data, methods, and models for determining compliance with regulatory requirements involving tectonics. Of particular concern is the adequacy of existing and anticipated data for quantitatively evaluating compliance with waste-isolation performance objectives and design criteria for a geologic repository operations area. Data and references compiled by Tectonics Research Project staff have been used to develop Compliance Determination Strategies (CDSs) on Structural Deformation [License Application Review Plan (LARP) Section 3.2.1.5], Evidence of Igneous Activity (LARP Section 3.2.1.9), and Structural Deformation and Groundwater (LARP Section 3.2.2.8). Digital terrain and boundary data, and visualization methods developed for tectonics research are also being used in the Regional Hydrogeologic Processes and Volcanism Research Projects.

Significant technical accomplishments by the Tectonics Research Project to date include: (i) development of digital terrain models of the YM and central Basin and Range regions; (ii) production of integrated maps of Quaternary faults, Quaternary basaltic volcanic fields, historic earthquake seismicity and in situ stress data using the Tectonics Geographic Information System (GIS); (iii) compilation of an initial database of geodetically measured regional strain and geologically determined slip rates for individual fault systems; (iv) evaluation of historic earthquakes with emphasis on the relationships between earthquakes and mapped faults, temporal and spatial clustering of earthquakes, and the 1992 Landers earthquake sequence in the southern Mojave desert; (v) sampling at Bare Mountain, Nevada, for fission track analyses; (vi) reconnaissance field work in the Black Mountains, California; (vii) participation in the NRC/CalTech YM/Death Valley Global Positioning System (GPS) Survey; and (viii) conducting collaborative research, with the Regional Hydrogeologic Processes Research Project, on the effects of in situ stress on transmissivity and regional groundwater flow in the Death Valley region.

Significant accomplishments since the last semi-annual report include: (i) development of an interactive computer program to analyze slip tendency and dilation tendency for mapped faults and fractures; (ii) performance of slip tendency analyses of existing fault sets (including YM faults) to evaluate relative risk of slip in contemporary stress state; (iii) dilation tendency for faults and fractures to investigate potential for magmatic intrusion of faults/fractures and to evaluate potential effects of in situ stress on transmissivity and regional groundwater flow; (iv) field research on fault and dike interaction along the Mesa Butte Fault in the San Francisco Volcanic Field, Arizona; (v) sampling at Bare Mountain, Nevada, for paleomagnetic, microstructural, and additional fission track analyses; (vi) participation in the 1994 campaign of the NRC/CalTech YM/Death Valley GPS Survey; and (vii) continued collaborative research, with the Regional Hydrogeologic Processes Research Project, on the effects of in situ stress on transmissivity and regional groundwater flow.

1.9 FIELD VOLCANISM

The Field Volcanism Research Project is designed to better characterize the effects of basaltic igneous activity on repository performance. This characterization will be possible through investigations of the (i) mechanics of basaltic eruptions, (ii) extent and characteristics of shallow hydrothermal systems and diffuse degassing associated with basaltic volcanoes, and (iii) nature of basaltic intrusive geometries in the shallow subsurface. Successful completion of the Field Volcanism Research Project, which began in April 1993, will require study of Plio-Quaternary basaltic volcanoes in the western Great Basin (WGB) and comparison with historically active basaltic volcanoes located elsewhere. Key technical uncertainties (KTUs) related to the Field Volcanism Research Project are (i) low resolution of exploration techniques to detect and evaluate igneous features, (ii) inability to sample igneous features, (iii) development and use of conceptual tectonic models as related to igneous activity, and (iv) prediction of future system states (disruptive scenarios).

Activities designed to address issues related to the probability and consequence of igneous activity in the Yucca Mountain Region (YMR) that have been initiated or completed during the last 6 months include:

- An independent expert-panel review of the Center for Nuclear Waste Regulatory Analyses (CNWRA) volcanism research projects
- Extensive field work at Tolbachik volcano, Kamchatka

- Initial comparisons of YMR and Tolbachik eruption products
- Continued modeling of temperature and soil-gas data from Parícutin volcano, Mexico
- Continued modeling of fault-dike interactions

The details of the expert-panel review are reported in an Intermediate Milestone, Expert-Panel Review of CNWRA Volcanism Research Programs (Hill, 1995), which was completed during this reporting period. In addition, some results of fault-dike modeling studies (Draper et al., 1994) and degassing studies at Cerro Negro, Nicaragua (Conway et al., 1994), were presented as posters at the Annual Meeting of the Geological Society of America. CNWRA contributions to melt-inclusion research at Cerro Negro, Nicaragua, were presented at the Fall Meeting of the America Geophysical Union (Roggensack et al., 1994). A paper on the significance of amphibole crystals in Quaternary YMR basalts, which was reported in Connor and Hill (1994), also was accepted for presentation at the 1995 International High Level Radioactive Waste Management Conference.

The main conclusions of the peer review were: (i) CNWRA volcanism research projects are scientifically defendable, relevant to addressing important geological problems in the YMR, and are being undertaken by well-qualified personnel; (ii) increase the scope of studies of basaltic volcanism in the YMR, including Miocene basaltic activity associated with waning stages of caldera magmatism; (iii) conduct independent physical volcanological studies of Quaternary YMR basaltic volcanoes and supplement these studies with data from other appropriate Basin and Range and modern analog volcanoes; (iv) continue to evaluate the relationships between YMR and modern analog volcanoes as data from planned studies becomes available; (v) prioritize project goals to focus on the most urgent tasks; and (vi) allocate more time for in-depth studies that result in peer-reviewed journal publications by decreasing the number of administrative reports.

The 1975 eruption of Tolbachik volcano, Russia, had a relatively large range in explosivity throughout the eruption. Earlier phases of the eruption sustained columns of ash to over 10 km high and dispersed that material hundreds of kilometers from the vent. In contrast, later stages of the eruption had intermittent ash columns only several kilometers in height and of limited dispersal. However, the cinder-fall deposits from all phases of this eruption have characteristics that are classically defined as low energy (i.e., strombolian). This contradiction indicates that commonly applied definitions of basaltic eruption energetics may be inaccurate, when determined from cinder-fall deposits. A limited sampling of the Lathrop Wells cinder-fall deposits shows that these deposits have granulometric and crystallographic characteristics that are similar to the 1975 Tolbachik deposits. Quaternary volcanoes in Crater Flat also have crystallographic characteristics of the Tolbachik deposits, but their cinder-fall deposits have not yet been sampled. The 1975 eruption of Tolbachik volcano thus appears very analogous to Quaternary eruptions in the YMR. Ongoing research will continue to investigate the possibility that YMR volcanoes may have had periods of highly explosive and dispersive eruption activity.

Degassing and thermal studies conducted at the Tolbachik volcano support initial work at the Parícutin volcano. These studies show that degassing occurs over a broad area at cooling cinder cones, for at least decades after cessation of the eruption. In addition, the detailed thermal studies at Tolbachik and Parícutin are being used to evaluate the Sandia National Laboratories (SNL) Total-System Performance Assessment (TSPA) models that simulate cooling of igneous features. Initial results of this analysis are that the numerical models used in the SNL TSPA analysis predict a rate of cooling that is much faster than observed at the Tolbachik volcano.

1.10 REGIONAL HYDROGEOLOGIC PROCESSES OF THE DEATH VALLEY REGION

Yucca Mountain (YM) has been proposed as a potential high-level nuclear waste (HLW) repository, in part because of the favorable geochemical and hydrologic environment provided by its 700-m-thick unsaturated zone. Siting the repository in the unsaturated zone may limit the potential for waste canister corrosion and dissolution of the waste form. Low water fluxes which are postulated to exist in the unsaturated zone, limit the likelihood that dissolved radionuclides will be rapidly transported to the accessible environment. One mechanism that may saturate the repository horizon and compromise favorable conditions at the YM site would be an increase in the elevation of the regional water table. Elevation of the water table may occur due to increased recharge to the regional hydrogeologic system from areas up to 100 km to the north and northeast of YM. Even if elevation of the regional water table does not saturate the repository block, the reduced thickness of the unsaturated zone may significantly diminish travel times in the vadose zone. The research project on Regional Hydrogeologic Processes of the Death Valley Region was initiated to improve understanding of the saturated groundwater flow regime at YM and to assess the influence of the regional flow system on the height of the water table beneath YM. The objectives of this research project are to analyze existing conceptual models and develop new conceptual models of the regional hydrogeologic flow regime in the Death Valley region that contains YM, and to construct numerical models of regional flow that may be used to assess the potential for the water table beneath YM to rise in response to wetter climatic conditions.

Predictions made with numerical models will be used by the U.S. Department of Energy (DOE) in its license application to demonstrate that the YM site meets the overall performance standards outlined in 10 CFR 60.112 and the geologic subsystem performance standard defined in 10 CFR 60.113(a)(2). In addition, the DOE may choose to use numerical models to demonstrate the absence or influence of potentially adverse conditions including: (i) the effects of future pumping on the regional flow system [10 CFR 60.122(c)(2)]; the potential for deleterious changes to the hydrologic system [10 CFR 60.122(c)(5)]; (ii) the potential for changes to the hydrologic conditions resulting from climate change [10 CFR 60.122(c)(6)]; (iii) the potential for water table rise [10 CFR 60.122(c)(22)]; and (iv) the presence and influence of favorable conditions, including the clear absence of fully saturated pathways connecting the repository to the water table [10 CFR 60.122(b)(8)(ii)]. Understanding of the regional hydrogeologic system developed from this project will be used to guide the review of the DOE license application and to assess the adequacy of the models used by the DOE to demonstrate compliance with the regulatory requirements and environmental standards.

During the past 6 mo, efforts focused on developing alternative conceptual models of flow in the Death Valley region and the constructing and calibrating of numerical models of flow and transport, respectively. An accurate steady-state water level map has been prepared, and a straightforward procedure for estimating the areal distribution of average annual precipitation and average annual recharge has been developed. Work on obtaining prior estimates of the mean values and variances of model parameters, such as hydraulic conductivity and areal recharge, that are required for statistically based model calibration procedures has also progressed. The work presented in this semi-annual report details the development of a new geostatistical procedure for estimating average annual precipitation and recharge in the Death Valley region.

Obtaining reasonably accurate initial estimates of the distribution and magnitude of natural recharge is essential for constructing and calibrating numerical models of the regional flow system. The areal distribution of recharge will be used to define the number and extent of the areal source terms in the numerical flow model. In addition, estimates of the magnitude of recharge are needed to provide the prior information used to stabilize the inverse problem, as well as to provide initial parameter estimates for the optimization algorithm used in the automatic calibration routine. The spatial variation of average annual precipitation within the Death Valley region is caused by mesoscale and synoptic effects. The predominant mesoscale effect is orographic precipitation resulting from the extreme relief of Basin and Range topography. Two separate synoptic scale effects cause the average annual precipitation in the western and northwestern portions of the Death Valley region to be less than that in the southern and southeastern portions, at any specified elevation. The predominant synoptic scale effect is the rain shadow produced in the lee of the Sierra Nevada during the winter months when low-pressure centers generated in the western Pacific Ocean and Gulf of Alaska are driven onshore by the Canadian High. A secondary synoptic effect is caused by the Southwest Monsoon, which produces summertime convective storms in the southern and southeastern portions of the Death Valley region.

Coefficients of a logarithmic equation describing the mesoscale orographic effect are estimated by regressing measured average annual precipitation against the elevation of the precipitation stations. Residuals obtained by subtracting the average annual precipitation predicted by this logarithmic equation from the measured average annual precipitation exhibit a spatial structure indicative of both the Sierra Nevada rain shadow and the Southwest Monsoon effects. Previous researchers have taken advantage of the strong correlation of precipitation with elevation and the relative abundance of elevation data to cokrige the spatial distribution of average annual rainfall. However, geostatistical analysis conducted in this report suggests that neither the precipitation field nor the elevation field is stationary, and thus calls into question the validity of using cokriging. A new co-estimation procedure for average annual precipitation is described in this semi-annual report. The new procedure makes use of the relative abundance of elevation from digital elevation maps (DEMs), and combines residual kriging in the presence of an external drift function with polynomial trend surface fitting. An especially appealing aspect of the procedure is its use of drift and trend models that explicitly represent the orographic precipitation effect and the combined leeward rain shadow and Southwest Monsoon effects. Moreover, because the trend in the residuals caused by the synoptic effects is removed by fitting a polynomial trend surface, the resulting random field is stationary, and straightforward kriging can be used. Initial estimates of recharge within the Death Valley region are obtained by using the empirical Maxey-Eakin formula, which specifies that recharge is a fixed percentage of average annual precipitation.

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