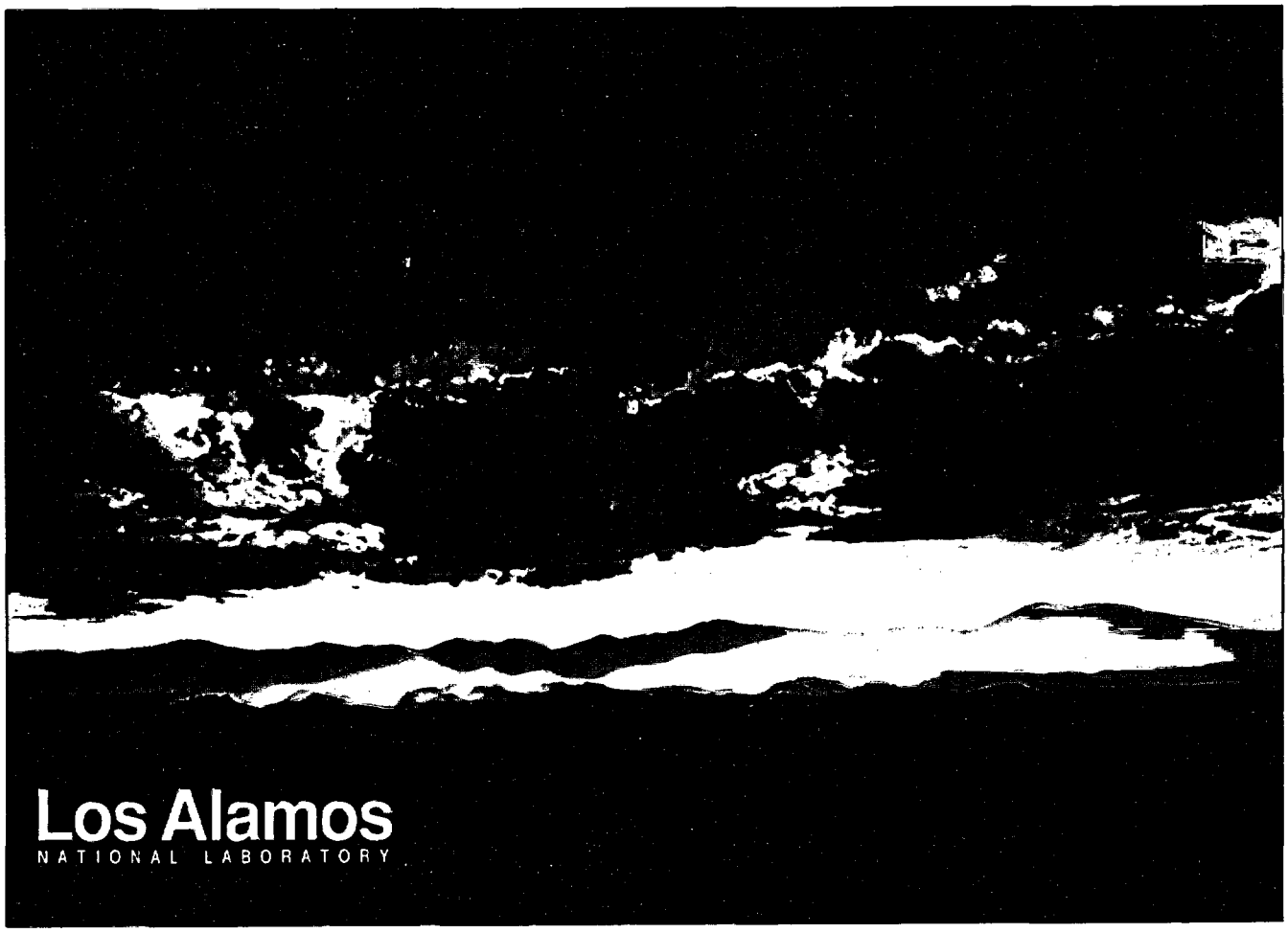
Yucca Mountain Site Characterization Project

Monthly Activity Report

February 1992



Attachment to TWS-EES-13-04-92-089

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This document has not received formal technical or policy review by Los Alamos National Laboratory or by the Yucca Mountain Site Characterization Project. Data presented in this report represent work progress and are not intended for release from the US Department of Energy.

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LOS ALAMOS NATIONAL LABORATORY

YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT

Monthly Activity Report
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WBS 1.2.1 Systems

Objective

The objective of this task is to integrate systems with the Geologic Repository Program, to describe the Yucca Mountain Site Characterization Project Mined Geologic Disposal System, and to evaluate the performance of the natural, engineered barrier, and total systems for meeting regulatory standards.

Technical Data (WBS 1.2.1.3.5)

Activities and Accomplishments

Staff attended Reference Information Base (RIB) and Parameter Normalization Working Group meetings on 3 February in Las Vegas, NV.

Staff met with principal investigators to discuss data that will be submitted to the Automatic Technical Data Tracking System (ATDT).

Data on colloidal agglomeration and chelation for WBS 1.2.3.4.1.2.2 was entered into the ATDT.

Staff presented information on technical data management to the Los Alamos Quality Assurance Liaisons.

Planned Activities

Submit data from 1.2.3.4.1.4 and 1.2.3.2.5 to the ATDT.

Update the Parameter Normalization List.

Caisson Experiment (WBS 1.2.1.4.6)

Activities and Accomplishments

Efforts were directed at completing preparation for the caisson experiment. In conjunction with Sandia National Laboratory (SNL), the porous materials for backfill and sorbing layer were identified. A silica sand will be the bulk background porous material, and an iron oxide (limonite) will be used to form a sorbing layer.

Staff obtained the time-domain reflectrometry (TDR) soil/water measuring system.

Continued on next page

Planned Activities

Travel to SNL to discuss the lower-boundary condition with SNL staff.

Prepare caisson for filling with sand.

Continue standard operating procedure to prepare for caisson experiment .

Continue writing paper for special issue of *Radioactive Waste Management.*

Publications

E. P. Springer and M. D. Siegel
An Integrated Intermediate-Scale Caisson Experiment to Validate Models of Fluid Flow and Contaminant Transport in the Unsaturated Zone
Journal article, *Radioactive Waste Management and the Nuclear Fuel Cycle, Special issue on the Yucca Mountain Project*
In preparation.

Performance Assessment Calculational Support (WBS 1.2.1.4.7)

Activities and Accomplishments

No activity to report.

WBS 1.2.3.1 Site Management and Integration

Site Management (WBS 1.2.3.1.1)

Objective

The objective of this task is to manage and integrate site characterization activities.

Activities and Accomplishments

A charter for the Radionuclide Solubility Working Group was written. For further information, see Appendix.

Publications

J. A. Canepa
Strategy for Testing the Applicability and Validity of Radionuclide Transport Models for Yucca Mountain, Nevada
Conference Paper, *Migration '91, Jerez de la Frontera, Spain, 14-18 October 1991*
In revision.

A. M. Simmons and J. A. Canepa
Recent Developments in the Integrated Approach Toward Characteristics of Radionuclide Transport, Yucca Mountain, Nevada
Conference Paper, Waste Management '92 Symposium
In preparation.

Surface-Based Test Management and Integration (WBS 1.2.3.1.1.)

Objective

The goal of this investigation is to provide coordination for Los Alamos surface-based test planning package development.

Activities and Accomplishments

The test planning package for UZ-16 in support of the Water Movement Tracer Tests (Study Plan 8.3.1.2.2.2 under the Site Characterization Plan Geohydrology Program) was approved for implementation. Wrote requirements letter requesting space for the Field Operations Center.

Planned Activities

Complete the job package and drilling start for the UZ-16.

WBS 1.2.3.2.1.1.1 Mineralogy, Petrology, and Rock Chemistry of Transport Pathways

Objective

The purpose of this activity is to define the important mineralogic and geochemical variables along fracture and rock-matrix transport pathways at Yucca Mountain, in support of performance assessment and to evaluate the impact of repository construction on natural waste-transport barriers.

Activities and Accomplishments

Participated in internal audit 3-21 February.

Fracture mineralogy efforts focused on writing a draft of journal article on fracture-lining manganese minerals at Yucca Mountain (Milestone 3123).

D. Broxton guided a field trip to Busted Butte at the Nevada Test Site on 28 February at which he presented information about a database of mineralogic, chemical, and petrographic information that might be used for locating adits at Busted Butte and other surface sites around Yucca Mountain.

To obtain additional information about mineralogy of rocks and fractures at depths greater than 200 feet below the water table, participants in the surface-based testing plan have been asked to deepen target depths for several future SD, UZ, and WT holes.

Cuttings from drill hole USW H-5 were analyzed by quantitative x-ray diffraction (XRD) methods. The results of these studies will extend our knowledge of mineral distributions beneath the northwestern part of the exploration block at Yucca Mountain.

Planned Activities

During the next few months we will (1) continue analysis of Mn-oxide fracture fillings in the Crater Flat and Paintbrush tuffs to determine their distribution and factors controlling that distribution; (2) complete paper on Mn-oxides for publication in a refereed journal; (3) continue analysis of calcites to understand transport and precipitation mechanisms; and (4) determine quantitative mineralogy from XRD data for Milestone 3137.

A new microdiffractometer (purchased for another program) is expected to arrive next month and will be used to analyze many fracture-coating minerals that occur in small patches rather than continuous coatings. As soon as the journal article (3123) on Mn-oxides is completed, work will resume on fracture coatings in the Topopah Spring Member.

Problem Areas

None

Milestones

3120
29 May 1992
Calcite in the Upper Paintbrush Tuff
35% complete.

3123
2 March 1992
Mn Fracture Minerals at Yucca Mountain
Undergoing extensive revision.

Continued on next page

3130
17 August 1992
Fracture Mineralogy of the Paintbrush Tuff

3137
30 September 1992
Mineralogy of Calico Hills for Adit Development
75% complete

Publications

D. Bish and S. Chipera
Detection of Trace Clays and Clay Minerals Amounts of Erionite Using X-ray Powder Diffraction: Erionite in Tuffs of Yucca Mountain, Nevada, and Central Turkey
Journal article, *Clay and Clay Minerals*
Published.

D. E. Broxton
Chemical Changes Associated with Zeolitization on the Tuffaceous Beds of Calico Hills at Yucca Mountain, Nevada
Conference paper, *Proceedings of the 7th Water-Rock Interactions Symposium*, July 1992
In YMPO review.

B. Carlos, D. Bish, and S. Chipera
Fracture-Lining Manganese Oxide Minerals in a Silicic Tuff
Journal article, *Chemical Geology*
Undergoing extensive revision.

G. D. Guthrie, D. L. Bish, and B. T. Mossman
Quantitative Analysis of Zeolite-Bearing Dusts Using the Rietveld Method
Journal article, Submitted to *Science*

D. Vaniman, D. Bish, D. Broxton, B. Carlos, S. Chipera, and S. Levy
Mineralogy as a Factor in Radioactive Waste Transport Through Pyroclastic Rocks at Yucca Mountain, Nevada
Journal article, *J. Geophs. Res.*
Draft complete; may be revised for a different journal.

WBS 1.2.3.2.1.1.2 Mineralogic and Geochemical Alteration

Objective

The objective of this task is to characterize past and present natural alteration processes that have affected the potential geologic repository and to predict future effects of natural and repository-induced alteration.

Activities and Accomplishments

G. WoldeGabriel completed mineral separations, weighing, and sample packaging in preparation for K/Ar analysis at Case Western Reserve University in March and sent samples to Case Western Reserve for preparatory degassing.

We received a new supply of Topopah Spring lower-vitrophyre core from the USGS, which will be characterized and used for steam-atmosphere experiments. Long-term zeolite heating experiments continued.

D. Vaniman processed root samples from Trench 14 in a low-temperature asher to obtain mineral residues. Mineralogy and chemistry of the residues will be determined in order to constrain the role of roots in generating calcite-silica deposits.

S. Levy is examined surface deposit samples for possible hydrothermal origin. They include concretions, fault deposits, breccias, fracture fillings, and altered tuffs.

Several quality assurance procedures were revised.

Planned Activities

S. Levy and B. Rundberg will examine outcrop sites of the Topopah Spring candidate host rock for possible sources of fractured blocks to be used in laboratory studies. S. Levy will work with USGS to map the deepened portion of Trench 14 and will revisit sample collection sites to study surface alteration.

G. WoldeGabriel will travel to Case Western Reserve University to conduct K/Ar analyses of secondary mineral separates from altered rocks in the Yucca Mountain area and other nearby locations.

Problem Areas

None

Milestone Progress

3138
30 October 1992
Chemical Transport in Zeolitic Alteration

3141
31 March 1992
Laminated Zone in Trench 14

3142
3 April 1992
K/Ar Dating of Clays and Zeolites
Research continuing; new draft in preparation.

3143
15 January 1992
Experimental Dehydration of Volcanic Glasses
Interim draft complete.

Continued on next page

Publications

G. WoldeGabriel, *et. al*
Preliminary Assessment of Clinoptilolite K/ARr Results from Yucca Mountain, Nevada: a Potential High-Level Radioactive Waste Repository Site
Conference paper, *Proceedings of the 7th Water-Rock Interactions Symposium*, July 1992
In YMPO review.

S. Levy and C. Naeser
Bedrock Breccias Along Fault Zones near Yucca Mountain, Nevada
Chapter in USGS Bulletin on Yucca Mountain studies
In USGS editorial review.

S. Levy
Natural Gels in the Yucca Mountain Area, Nevada, USA
Conference paper, European Materials Research Society Symposium
Approved by YMPO.

D. Vaniman, D. Bish, and S. Chipera
Dehydration and Rehydration of a Tuff Vitrophyre
Journal article, *J. Geophys. Res.*
Interim draft complete.

D. Vaniman, *et. al*
Precipitation of Calcite, Dolomite, Sepiolite, and Silica from Evaporated Carbonate and Tuffaceous Waters of Southern Nevada
Conference paper, *Proceedings of the 7th Water-Rock Interactions Symposium*, July 1992
In YMPO review.

WBS 1.2.3.2.1.2 Stability of Minerals and Gases

Objective

The objective of this activity is to produce a model for past and future mineral alteration in Yucca Mountain. The model is intended to explain the natural mineral evolution resulting from the transformation of metastable mineral assemblages to more stable assemblages and the effects of a repository emplacement.

Activities and Accomplishments

This activity has been deferred.

WBS 1.2.3.2.5 Postclosure Tectonics

Objective

The objective of these volcanism studies is to determine the hazards of future volcanic activities with respect to siting a high-level radioactive waste repository at Yucca Mountain.

Activities and Accomplishments

We evaluated the K-Ar and 40Ar/39Ar database for the Lathrop Wells volcanic center and found that both data sets are positively skewed, with mean larger than median. Both data sets also contain outliers that are greater than 1.5 times the interquantile range. Removing the outliers reduces, but does not eliminate, the positive skewness; including the outliers greatly modifies the weighted mean and associated error. Regression plots of the 40Ar/39Ar data have influential cases that control the slope and y-intercept of the regression plots; they should be examined for errors or suitability to the data set.

A poster session was prepared for the Waste92 meeting in Tucson next month. We have developed tables showing the recurrence rate of volcanic vents and the probability of repository disruption, using a range of alternative models for both attributes. Mean values of the two-part probability of Pr(E2 given E1)Pr(E1) where E1 is the recurrence rate and E2 is the disruption probability are less than 10^{-6} per year. A formal conservative value of the two-part probability has not been established. However, if the probability of E3 (Pr(E3) is less than 1, volcanism cannot be judged as a significant licensing issue based on the criteria established in 40 CFR 191, Appendix B.

Aerial photographs and digitized data for volcanic centers were ordered through EG&G.

A talk on volcanism was presented to a Nevada legislative group.

Volcanism staff participated in the DOE/HQ and M&O tours of Yucca Mountain.

We revised a detailed technical procedure, DP-605, "Preparation of powders from rock, cinder and ash samples."

We obtained and processed digitized data on the locations of basaltic volcanic vents in the San Francisco volcanic field using data from Tanaka *et. al.* (1986). We found that the field has a vent density of about 1.1 vents per square kilometer.

Work in Progress. We completed the first draft of Study Plan 8.3.1.8.1.2, and it is being processed for internal technical review.

We began an issue resolution report on the risk of volcanism; we are writing an introduction, that describes the history of volcanism in the Yucca Mountain.

We began a statistical analysis of trace-element geochemical data for the Lathrop Wells volcanic center. We are evaluating the data for use to discriminate field units established from mapping and trenching activity.

We began to revise Test Plan Package 91-32 to include construction of test pits in the Cima volcanic field.

Continued on next page

We have started compiling the geologic literature and examining the geologic setting of Quaternary basaltic volcanic vents in the southern Great Basin. These investigations are concerned with dike emplacement mechanisms, dike orientations relative to surface faults and vent locations relative to topographic features (valleys, range fronts, range interiors). Topographic and geologic maps needed for this work have been identified and ordered.

Planned Activities

We will begin trenching at the Cima Volcanic Field (permission has already been obtained from the Bureau of Land Management) and Lathrop Wells Volcanic Field next month. Trenching at the Lathrop Wells center and the Cima volcanic field will also begin next month.

We are evaluating field-study sites to test development chronology methods. Possible sites are the SP Crater in the San Francisco Volcanic Field and the Tabernacle Flow in Utah.

Problem Areas

None

Milestones

3174
8 January 1992
Effects of Magmatic Disruption on the Repository (Study Plan 8.3.1.8.1.2, R0)
First draft is complete.

3071
September 1992, expected completion April 1992
Status of Geochronology Studies at the Lathrop Wells Volcanic Center

3129
10 July 1992, expected completion April 1992
Geochemistry of Lathrop Wells Eruptive Sequences

3034
30 September 1992
Report on Magma System Dynamics

3035
30 September 1992, expected completion April 1992
Effects of Strombolian Eruption

3109
30 September 1992
Report of Subsurface Effects

Continued on next page

3111
30 September 1992
Preliminary Geologic Mapping of Volcanic Centers

3164
30 September 1992
Progress Report on Thermoluminescence

Publications

B. M. Crowe *et al.*
Lathrop Wells Volcanic Center: Status of Field and Geological Studies
Conference paper, American Nuclear Society International High-Level Radioactive Waste Management Conference, Las Vegas, NV, April 1992
In YMPO review.

B. M. Crowe *et al.*
Recurrence Models of Volcanic Events: Applications to Volcanic Risk Assessment
Conference paper, American Nuclear Society International High-Level Radioactive Waste Management Conference, Las Vegas, NV, April 1992
In YMPO review.

F. V. Perry and B. M. Crowe
Geochemical Evidence for Waning Magnetism and Polycyclic Volcanism at Crater Flat, Nevada
Conference paper, American Nuclear Society International High-Level Radioactive Waste Management Conference, Las Vegas, NV, April 1992
In YMPO review.

G. A. Valentine, B. M. Crowe, and F. V. Perry
Physical Processes and Effects of Magnetism in the Yucca Mountain Region
Conference paper, American Nuclear Society International High-Level Radioactive Waste Management Conference, Las Vegas, NV, April 1992
Approved by YMPO.

S. G. Wells, *et al.*
Multiple Eruptive Events at Small Volume Basaltic Centers: Evidence From the Cima and Crater Flat Volcanic Fields
Journal article
In preparation.

WBS 1.2.3.3.1.2.2 Water Movement Tracer Tests

Objective

The objective of the water movement tracer tests is to obtain measurements of chlorine isotope distributions to help quantify the percolation of precipitation in the unsaturated zone.

Activities and Accomplishments

J. Fabryka-Martin collected 66 surface-soil samples from locations within the conceptual Perimeter Drift Boundary (PDB). The samples, collected along a transect spaced about 400 m apart, are to be analyzed for chloride/bromide (Cl/Br) ratios as part of an effort to assess the spatial variability of the meteoric Cl/Br ratio. This ratio is important as an indicator of the extent to which meteoric chloride has mixed with rock chloride in the rock samples collected during drilling. to complete this set, approximately 24 more surface-soil samples will be collected from within the PDB on future field trips. Ninety ream-bit cutting samples collected from the first 2 of 12 neutron-access boreholes were received by the subcontractor and logged in. The collection of cuttings was completed for the third and fourth holes of this set and was begun on the fifth hole.

J. Fabryka-Martin presented guidelines for the collection of samples for the Water Movement Test task during drilling of UZ-16 and described other types of sampling activities planned for this study to Drilling Support Division staff at its YMP field office.

J. Fabryka-Martin made a presentation, "Proposed Sampling Program for the Water Movement Test: Who, What, When, Where, Why," to the Hydrology Integration Task Force. Its purpose was to make other YMP participants aware of the study's sampling program and to identify possible places for coordinating field sampling efforts. As a result of discussion following the talk, she arranged to collect soil profiles from pits to be excavated under the auspices of a USGS study in Midway Valley next month. Analytical work by Hydro Geo Chem focussed on defining precision and bias in the determination of chloride and bromide and revising the draft detailed technical procedure for ion chromatographic analysis accordingly.

Review comments on a detailed technical procedure (DP) for determining bulk density were addressed, and the DP is in the approval process.

Planned Activities

Complete additional DPs; process cuttings samples from neutron-access boreholes; process USGS water samples; collect soil samples from Yucca Mountain area.

Milestone Progress

3191
Procedure for Chlorine-36 Analysis of Unsaturated Zone Samples
30 September 1992

WBS 1.2.3.3.1.2.5 Diffusion Tests in the ESF

Objective	The objective of this task is to determine *in situ* the extent to which the nonsorbing tracers diffuse into the water-filled pores of the Topopah Spring welded unit.
Activities and Accomplishments	No significant activity in this study.
Milestone Progress	No level II milestones are planned this fiscal year.

WBS 1.2.3.3.1.3.1 Site Saturated Zone Ground-Water Flow System (Reactive Tracer Testing)

Objective

Experiments will be conducted at the C-Well complex (holes UE25 C#1, UE25 C#2, and UE25 C#3) and other wells in the vicinity of Yucca Mountain using reactive tracers to characterize retardation and transport properties at a larger scale than currently used in laboratory experiments.

Activities and Accomplishments

Software Qualification. Review comments of two software baselines are being processed: the software design document for the FRACNET application and the implementation baseline for the SORBEQ application.

LiBr Sorption Studies. Error statistics have been compiled for the analyses of all dissolved species being measured by ion chromatography. This requirement is specified by the detailed technical procedure (DP) for ion chromatograph analysis.

Planned Activities

Continue the effort to bring the computer codes FRACNET, FEHMN, GZSOLVE, and SORBEQ and other software into compliance with the SQAP. This consists of compiling existing documentation on these codes and writing any new material required by the SQAP.

Begin batch sorption experiments using lithium bromide.

Continue to develop techniques to measure the concentration of polystyrene microspheres in solution.

Problem Areas

None

Publications

W. L. Polzer, W. L., M. G. Rao, H. R. Fuentes, and R. J. Beckman
Thermodynamically Derived Relationships Between the Modified Langmuir Isotherm and Experimental Parameters
Journal article, *Environmental Science and Technology*
Undergoing revision.

B. A. Robinson
FRACNET-Fracture Network Model for Water Flow and Solute Transport
LA-series report
In preparation.

B. A. Robinson
SORBEQ-A One-Dimensional Model for Simulating Column Transport Experiments
LA-series report
In preparation.

Continued on next page

Milestone Progress

3188
16 January 1992
Documentation for SORBEQ

3194
1 April 1992
Batch Sorption Experiments with Lithium

T112
22 June 1992
Final Documentation for FEHMN

3196
27 July 1992
FRACNET Documentation

WBS 1.2.3.4.1.1 Groundwater Chemistry Model

Objective

The goal of this investigation is to provide conceptual and mathematical models of the groundwater chemistry at Yucca Mountain. These models will explain the present groundwater composition in relation to interactions of minerals and groundwater and will be used to predict groundwater compositions as a result of anticipated and unanticipated environments.

Activities and Accomplishments

A paper, "Water-rock interactions and the pH stability of groundwaters from Yucca Mountain, Nevada," is still in YMPO review. The paper describes compositional analyses of water samples from the tuff aquifer at Yucca Mountain and carbonate water from UE 25p#1, which were used in a modeling study of pH stability.

Modeling evaporation of different Yucca Mountain waters and waters from the surrounding area continued. A paper, "Precipitation of calcite, dolomite, sepiolite, and silica from evaporated carbonate and tuffaceous waters of southern Nevada," by D. Vaniman, M. Ebinger, D. Bish, and S. Chipera is still in YMPO review.

M. Ebinger attended a Geochemical Modeling short course sponsored by the USGS.

QA Activities. No additional progress to report on the IMOU between LLNL and Los Alamos. IMOU is in review in Las Vegas.

Planned Activities

Track Study Plan 8.3.1.3.1.1 during YMPO review.

USGS collaboration will continue. Dissolved gas compositions (e.g., fugacities of CO_2g and O_2g) from existing and new water-table wells will be used to determine Eh conditions independently of Pt electrode measurements. The gas composition data will also be used in further pH buffering capacity modeling and for refined models of the overall ground-water chemistry.

Continue support of QA efforts. Continue tracking IMOU mentioned above.

Problem Areas

None

Milestones

3006
31 March 1992
Eh and pH Buffering Capacity

3415
30 September 1992
Letter Report: Most Active Groundwater Chemistry

Continued on next page

Publications

M. Ebinger
Water-Rock Interactions and the pH Stability of Groundwaters from Yucca Mountain, Nevada
Conference paper, *Proceedings of the 7th* Water-Rock Interactions Symposium, July 1992
In YMPO Review.

D. Vaniman, D. Bish, M. Ebinger, S. Chipera
Precipitation of Calcite, Dolomite, Sepiolite, and Silica from Evaporated Carbonate and Tuffaceous Waters of Southern Nevada
Conference paper, *Proceedings of the 7th Water-Rock Interactions Symposium,* July 1992
In YMPO Review.

WBS 1.2.3.4.1.2.1 and 1.2.3.4.1.2.3 Batch Sorption Studies and Sorption Models

Objective

The objective of this task is to provide sorption coefficients for elements of interest to predict radionuclide movements from the repository to the accessible environment.

Activities and Accomplishments

The experiments to evaluate the effects of crushing on the sorption coefficients obtained by batch techniques have been completed. We are awaiting mineralogic analyses to properly interpret the data. Surface-area determinations have been completed on approximately 3/4 of the samples.

Testing of the atomic-force microscope continued. This instrument will ultimately be used to image substrates before and after sorption reactions that involve the important radionuclides. It will also be used to characterize the detailed textures of Yucca Mountain tuffs at the nanometer scale.

We began to conduct experiments in conjunction with the Stanford contract. This work will focus on the dependence of solution composition (i.e., ground waters) on sorption coefficients for uranium and neptunium on several pure mineral phases.

Planned Activities

Continue study of radionuclide sorption on pure mineral phases. Complete Study Plan revisions.

Milestone Progress

3009
20 February 1992
Variation of Water-Rock Ratio Sorption Coefficients on Zeolitic Tuff

3212
30 September 1992
Progress Report on Single Mineral Experiments

Publications

A. Meijer
A Strategy for the Derivation and Use of Sorption Coefficients in Performance Assessment Calculations for the Yucca Mountain Site
Conference proceedings, *Proceedings of a Workshop on Sorption*, Los Alamos, New Mexico, 11-12 September 1990.
In preparation.

WBS 1.2.3.4.1.2.2 Biological Sorption and Transport

Objective

The purpose of this research is to determine whether microbial activity can influence the movement of plutonium in tuff. Because fluids are used extensively in the exploration of locations for a nuclear repository, those micro-organisms capable of utilizing drilling fluids as growth substrates are of special interest.

Activities and Accomplishments

A paper, "Preliminary Evidence of Siderophore/Plutonium Complexation," submitted to *Applied and Environmental Microbiology* in May 1991, was revised and resubmitted.

Work was begun on Milestones 3080, "Chelation," and 3092, "Colloidal Agglomeration."

A preproposal "Biodegradation: Vadose Zone Column Studies" was prepared and sent to DOE Headquarters. A study of microbial activity, as affected by vadose-zone conditions in soil columns was presented. Results would be applied to YMP studies.

Planned Activities

Continue plutonium K_d experiments.

Continue colloidal agglomeration experiments.

Problem Areas

None

Milestone Progress

3080
30 September 1992
Report on Chelation
In preparation.

3092
30 September 1992
Report on Colloidal Agglomeration
In preparation.

3176
30 September 1992
Procedure for Determination of Formation Constants
In progress.

3177
30 September 1992
Procedure for Determination of Effects on Colloidal Agglomeration
In preparation.

Publications

L. R. Hersman, D. E. Hobart, and T. W. Newton
Preliminary Evidence of Siderophore/Plutonium Complexation
Journal article, *Journal of Applied and Environmental Microbiology*
Resubmitted.

WBS 1.2.3.4.1.3 Radionuclide Retardation by Precipitation Processes

Objective

The objective of the solubility determination task is to determine the solubilities and speciation of important waste elements under conditions characteristic of the repository and along flow paths from the repository into the accessible environment.

Activities and Accomplishments

The Study Plan is being revised in response to DOE comments; the revision should be complete by 15 August.

Speciation Studies. We prepared new Pu(IV) colloid and Pu(VI) stock solutions and continued efforts to produce a stable Np(V) stock solution (10^{-3} M in Np at pH=8.5) in J-13 water for the Sorption Task, 1.2.3.4.1.2.1/3. High-purity americium-243 was ordered from ORNL for nuclear magnetic resonance (NMR) studies, and synthesis on actinide model complexes continued.

We used new Pu(IV) stock solution to produce single crystals of the several Pu(IV)-EDTA complexes that have been shown to exist in the system. Our initial attempts failed because of competition for colloid formation; however, we subsequently discovered that an excess of EDTA was competitive with colloid formation and observed a color change from red/brown to yellow with increasing pH, consistent with our observations from UV-VIS-NIR experiments. We also observed that heating of Pu(IV) in the presence of EDTA results in reduction to Pu(III) under certain conditions. Our attempts to grow single crystals of Pu(IV)-EDTA complexes look promising. We plan to characterize these species by single crystal x-ray diffraction.

We continued to determine the speciation and stability quotients of actinyl carbonate complexes via solution NMR as this technique provides a species-sensitive probe for unequivocally unravelling molecular structure and solution dynamics in these complicated actinide carbonate systems. The dynamic behavior of ligand exchange between free and coordinated carbonate on actinyl carbonate complexes of Pu(VI) was examined by 13-C NMR line-broadening techniques. Scoping experiments were performed for Am(VI) under the same conditions, and these constitute the first direct observation of the Am(VI) carbonate species by NMR techniques. Eyring analysis provided average activation parameters of 38 kJ/M for the enthalpy of activation and -60 J/K for the entropy of activation for the plutonyl triscarbonate system at 295K. Our activation parameters agree with Stout, Sullivan, and Choppin for the uranyl and neptunyl triscarbonate systems, but disagree with Brucher, Glaser, and Toth for uranium. The origin of the discrepancy between activation parameters for uranium are not clear. With the exception of the data of Brucher *et al.*, the enthalpies of activation for each system are relatively small and positive, while the entropies are large and negative. The negative entropy values suggest a highly ordered transition state, and similar parameters have been reported for the acid-catalyzed aquation of bidentate carbonate complexes. The rate-determining step in the aquation reaction mechanism involves protonation of the carbonate ligand, which opens a chelate ring formed by one of the bidentate carbonates attached to the central metal ion. This is followed by rapid dissociation of the monodentate bicarbonate species. Stout, Choppin, and Sullivan proposed an analogous mechanism, which is also supported by our new data. In this mechanism, the addition of carbonate or bicarbonate (acid-catalyzed pathway) forms an intermediate stage in which four carbonates are bound, two in a monodentate manner, and such a transition state is expected to be highly ordered. Protonation of this complex is followed by a rapid dissociation of bicarbonate and the reforming of a metal-oxygen bond by one of the monodenate carbonate ligands.

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Additional NMR ligand-exchange studies of actinyl(VI) carbonate complexes are required before the intimate mechanism of carbonate exchange can be more accurately described. We have examined the variable temperature 13-C NMR of the plutonyl carbonate system at six different carbonate concentrations, but the line broadening was such that only two of these samples were suitable for actual pulsed NMR T2 measurement. It has been suggested that the effect of field inhomogeneity on such broad lines will be negligible and a standard approximation should be applicable providing that the NMR lines are lorentzian. Therefore, we anticipate that we will be able to extract T2 values from lorentzian line fits on the two samples for which we have experimentally determined T2. If, as anticipated, there is little difference in the T2 data, then rate constants as a function of carbonate concentration can be extracted from the six experimental spectra already collected. We also plan to examine the rate constants as a function of pH in order to probe the proposed acid-catalyzed mechanism. With these two studies completed, we can make more informed judgements concerning the intimate mechanism of carbonate self-exchange for the $^{242}PuO_2(^{13}CO_3)_3^{4-}$complex.

Experimental work on the PAS system continues to focus on the Pu(IV) carbonate systems. Specifically, we continue to map-out speciation boundaries as a function of both pH and total carbonate (i.e. combined bicarbonate and carbonate anion) concentrations. To explore the different peak intensities found as bicarbonate concentration is varied, we have recently used 250 nM Pu(IV) samples to complement the 1.0 μM samples used last month. The Pu solubility in J-13 water is >250 nM, so the new samples should not lose intensity because of Pu precipitation. The peaks have been found to be in the same ratios as in the 1.0 μM samples, implying an intrinsically weaker intensity at lower bicarbonate concentrations or a slower relaxation time resulting in lower PAS intensity. This latter possibility may suggest possible plutonium clustering. Because our signal to noise is still excellent at 250-nM Pu concentration, we are presently trying to extend our work to 25-nM Pu concentration. Weak interference from water/bicarbonate becomes important compared to the weak Pu signal at 25 nM, but initial results are encouraging. However, several days accumulation seems to be required to achieve a believable signal (signal to noise ratio of at least 2). Nonetheless, this would be a significant advance and would allow studies to be done to neutral pH's at environmentally relevant concentrations.

Solubility Studies. The neptunium (Np) solubility experiments have reached steady-state. We are unsure why the last two assays in the pH~ 7 experiment show a change in concentration, but we are looking into possible causes. Until an answer is found, this experiment will continue and more assays will be taken. UV/visible absorption-spectrophotometry studies of the Np experiments have been performed to determine the solution species, and the results are being worked up now. We will begin the undersaturation experiments soon, starting with Np at pH 6, then with pH 8.5 because these two oversaturation experiments have already reached steady-state for some time. The three plutonium solubility experiments have also reached steady-state, and we plan to perform oxidation-state separations to determine the Pu species present. After this, undersaturation experiments with the Pu solids will begin.

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The Am/Nd solubility experiments require much more work. The low Am solubility in UE25p#1 at 60°C leads to assays with very low count rates. Np and Pu samples usually have enough activity so that results can be obtained with relatively short counting times. The irregular approach to equilibrium plots for the Am experiments are probably caused by the relative concentration inaccuracy because of insufficient counting times and the lack of consideration of the low-level counter background. To avoid extra long counting times for the gamma-pulse height analysis of each sample, we tried to use alpha liquid-scintillation counting because of its high efficiency. We found, however, that this method will not work for the following reason: Am/Nd has a very low solubility in UE25p#1, while ^{237}Np the daughter of ^{241}Am, has a rather high solubility relative to Am/Nd. Even though the daughter impurity is very small in the initial stock solution, we have enriched the Am/Nd/UE25p#1 solution with ^{237}Np to a significant degree with regard to gross alpha activity. Liquid-scintillation counting does not have the resolution to distinguish between these alphas, and is, therefore, unsuitable for this situation. We must now perform low-level gamma-pulse height analysis of all Am/Nd samples, which necessitates the use of very long counting times as well as periodic background counts.

The problems we experienced with our personal computer multichannel analyzers have been corrected, and low-level gamma-pulse height analysis of Am/Nd assays has begun, including the assays from the second filtration experiment.

Regarding the Lawrence Berkeley Laboratory (LBL) QA effort, we completed a draft detailed technical procedure (DP), "Operating and Calibrating the Mettler H6T Analytical Balance," WS-LBL-DP-14, R0. Work continued on the draft DP, "Concentration Determination of Soluble Radionuclides from Data Provided by the Low Energy Gamma Counting System," TWS-LBL-DP-01, R0.

Meetings Attended or Planned. D. Clark presented a seminar on Am and Pu carbonate speciation probed by 13-C NMR at Lawrence Berkeley Laboratory (LBL) on 30 January. D. Hobart and P. Palmer met with H. Nitsche at LBL on 13 February along with I. Triay and A. Mitchell of WBS 1.2.3.4.1.4 to discus the solubility of Np(V) and problems in preparing stock solutions at Los Alamos for sorption experiments. Experimental differences in CO_2 pressures were identified as a possible problem (altitude difference between LBL at Sea Level and Los Alamos at 7,000 ft) and are now being investigated. D. Hobart met with G. Seaborg, Associate Director of LBL, and N. Edelstein to discuss actinide research and D. Hoffman, Director of the GTS-Institute for Transactinium Science (ITS), and C. Gatrousis, Deputy Director LLNL, to discuss potential Los Alamos collaborations with the ITS.

Problems

Problems with the gamma counters were solved by re-installing the old system until hardware problems can be corrected. The Am/Nd assays have had long counting times because of low solubility of these elements in UE25p#1 water. In the future, we plan to use liquid scintillation counting for the assays, which will reduce assay time for Am/Nd to ten minutes.

Planned Work

Efforts in all above mentioned areas will continue.

Milestone Progress

3031
30 September 1992
Speciation Measurements

Continued on next page

3329
30 September 1992
Report on Neptunium, Plutonium, and Americium Solubility Experiments from Oversaturation

3330
15 January 1993, (anticipated early completion)
Evaluation of Alternative Distribution Schemes in PAS

Publications

J. M. Combes, C. J. Chisholm-Brause, G. E. Brown, Jr., G. A. Parks, S. D. Conradson, P. G. Eller, I. R. Triay,
D. E. Hobart, and A. Meijer,
EXAFS Spectroscopic Study of Neptunium(V) Sorption at the a-FeOOH/Water Interface
Journal article, *Environmental Science and Technology*.
In press.

L. E. Hersman, P. D. Palmer, and D. E. Hobart, *Preliminary Evidence of a Siderophore/Plutonium Complex*
Journal article, *Journal of Applied and Environmental Microbiology*
Undergoing revision.

H. Nitsche, R. C. Gatti, E. M. Standifer, S. C. Lee, A. Miller, T. Prussin,
R. S. Deinhammer, H. Maurer, K. Becraft, S. Leung, and S. A. Carpenter
Measured Solubilities and Speciations of Neptunium, Plutonium, and Americium in a Typical Groundwater (J-13) from the Yucca Mountain Region
LA-series report
In preparation.

C. D. Tait, D. E. Morris, J. M. Berg and W. H. Woodruff
Evaluation of Alternative Detection Schemes in Photoacoustic Spectroscopy
In preparation.

C. D. Tait, D. E. Morris, S. A. Ekberg, P. D. Palmer, and J. M. Berg
Plutonium Carbonate Speciation Changes with pH
Abstract, American Chemical Society National Meeting, San Francisco, California, April 1992
In YMPO review.

Clark, *et.al*
Carbonate Complexation of Pu(IV)
LA-series report
In preparation.

Report
Molecular Models for Actinide Speciation
Submitted 5/30/91.
Internal technical review completed.

H. Nitsche
The Importance of Transuranium Solids in Solubility Studies for Nuclear Waste Repositories
Conference paper, European Materials Society Meeting
In YMPO Review.

WBS 1.2.3.4.1.4 Radionuclide Retardation by Dispersive, Diffusive, and Advective Processes

Objective

The objectives of this task are to determine the rate of radionuclide movement along the potential flow paths to the accessible environment and to examine the effect of diffusion, adsorption, dispersion, anion exclusion, sorption kinetics, and colloid movements in the flow geometries and hydrologic conditions expected to exist along the flow path to the accessible environment in the scenarios used for performance assessment.

Activities and Accomplishments

Staff continued the study of the transport behavior of radionuclides as a function of mineralogy. The most likely reasons for the discrepancies between batch sorption coefficients and sorption coefficients obtained via column experiments (reported in May 1991) are pseudocolloid formation, precipitation, slow speciation kinetics, or slow mass-transfer kinetics. Staff completed stability experiments with neptunium (Np) solutions of the type used for the column transport experiments.

Staff designed and completed a Np stability experiment in collaboration with P. Palmer and D. Hobart of WBS 1.2.3.4.1.3, (speciation studies). P. Palmer prepared a Np stock solution with a molarity of 1×10^{-2}, checked it spectrometrically, and found the Np to be Np(V). R. Lopez prepared two Np solutions with a molarity of 1×10^{-5} (from Palmer's Np stock solution). One solution was prepared in J-13 water and the second in a 1×10^{-3} M sodium bicarbonate solution (made with distilled water). After the 1×10^{-5} M Np solutions (in J-13 and 1×10^{-3} M sodium bicarbonate) were prepared, aliquots of these solutions were filtered. All solutions had a pH of approximately 8.0. No addition of NaOH was necessary for pH adjustment, and the filtered and unfiltered Np solutions were monitored by liquid-scintillation counting for 25 days. The unfiltered solutions were stable for 25 days, with a deviation from the average Np activity measured of +/- 2%. The filtered solutions appeared to increase in Np concentration (up to 4%); the reason for this is the in-growth of protactinium that appears in the liquid scintillation counting region, monitored for Np. P. Palmer monitored the unfiltered and filtered 1×10^{-5} M Np solutions spectrometrically; he reports spectra consisting of a neptunyl peak and a peak for the carbonato-Np complex (which agrees with the speciation data reported by H. Nitsche).

Consequently, it appears that the Np precipitation reported in the last two monthly reports was caused by the addition of NaOH when the pH was adjusted (during the preparation of Np solutions in J-13). The NaOH apparently converts some of the bicarbonate in the J-13 water to carbonate (causing precipitation of Np). The speciation and dynamic transport tasks have agreed on the optimal method for stable Np solutions preparation.

P. Palmer and D. Hobart of the speciation task and I. Triay and A. Mitchell of this task met with H. Nitsche to discuss several aspects of YMP Np work. Previous assumptions had been that conditions for Nitsche's solubility work at pH of 8.5 are similar to conditions encountered at Los Alamos (under atmospheric conditions). This is probably a reasonable assumption; however, the partial pressure of CO_2 at Los Alamos is 2.48×10^{-4} atmospheres and, the partial pressure of CO_2 used by H. Nitsche for his pH 8.5 solubility work is 5.73×10^{-4} atmospheres and this difference will affect the distribution of Np species in solution. However, our hypothesis is that this difference won't affect the Np sorption behavior

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to a significant extent. The spectra that H. Nitsche has collected for Np in J-13 at a pH of 8.5 agrees well with Palmer's spectra for Np in J-13 under atmospheric conditions at Los Alamos. Palmer, Mitchell, and Triay also discussed this potential problem with C. Bruton and B. Viani (at LLNL), and their assumption appears to be consistent with previous calculations performed by C. Bruton on Np speciation and solubility in J-13.

Upon return to Los Alamos, solubility task staff (Hobart and Palmer), dynamic transport task staff (Triay, Lopez, and Mitchell) and an expert in actinide chemistry (T. Newton) discussed the direction that this combined Np work should follow. The decision was made for speciation personnel (with the assistance of T. Newton) to begin developing signal-averaging UV/VIS spectrometric techniques to determine Np speciation in solutions down to the micromolar level. This effort will require development work that will be extremely useful to the radionuclide transport work at Los Alamos.

I. Triay, A. Mitchell and P. Rogers (of WBS 1.2.3.4.1.2.1/3) will coordinate sorption and transport experiments that integrate the knowledge of solution speciation (determined by the solubility task) and the interaction of Np with solid phases. The interaction among the LBL (Nitsche), LLNL (Viani and Bruton), and Los Alamos staff was very productive. This type of integrated approach will allow us to describe the interaction of Np with Yucca Mountain tuffs (which is needed for performance-assessment calculations).

Staff began Np transport work using crushed-tuff columns made from G4-1530 and G4-275 and concentrated on obtaining sharp breakthroughs for tritium elutions in order to determine the physical parameters of the columns.

Staff of the dynamic-transport column experiments and diffusion tasks met with P. Adams of Sandia National Laboratory to develop a format for input of all our dynamic transport and diffusion data to the SEPDB.

A detailed technical procedure (DP) to study radionuclide diffusive behavior using tuff wafers was implemented. The DP for the study of radionuclide diffusion behavior using diffusion cells was reviewed and sent to the QAL.

M. Ott and R. Lopez attended the YMP orientation.

I. Triay attended the Geochemistry Integration meeting at Las Vegas, NV.

Planned Activities

Continue work described above.

Milestone Progress

3040
30 September 1992
Kinetics of Sorption on Columns of Pure Minerals

3044
31 August 1992
Letter Report on Assessment of Available Techniques for Unsaturated Column Transport Experiments
In preparation.

Continued on next page

3027
31 March 1992
Report on Sorption by Batch and Column Techniques

Publications

I. R. Triay
Radionuclide Migration in Tuff under Diffusive Conditions
Conference Paper, *Proceedings of the Migration '91, Jerez de la Frontera, Spain, 14–18 October 1991*
In preparation.

I. R. Triay, A. J. Mitchell, and M. A. Ott
Radionuclide Migration Studies for Validating Sorption Data—Past, Present, and Future
Conference paper, *Proceedings of the Radionuclide Adsorption Workshop*, Los Alamos, NM, 11–12 September 1990
In preparation.

WBS 1.2.3.4.1.5.1 Retardation Sensitivity Analysis

Objective

The objectives of this task are to construct a geochemical/geophysical model of Yucca Mountain and to use this model to examine the physical and chemical controls on radionuclide transport along flow paths to the accessible environment.

Activities and Accomplishments

A paper, "Three-Dimensional Simulations of Radionuclide Transport at Yucca Mountain," by K. Birdsell, K. Eggert, and B. Travis was prepared for publication in a special issue of *Radioactive Waste and the Nuclear Fuel Cycle.*

QA and Programmatic. Certification of TRACRN continued. Code modifications to incorporate memory management, as specified in SVA-6, were completed with the exception of the restart capability. The design phase of TRACRN has been submitted to the SCM for an in-process review. Several verification examples for TRACRN have been completed, and the user's manual was almost completed.

Planned Activities

Staff attended the Los ALamos project orientation class.

Milestone Progress

3052
30 March 1992
Baseline Documentation for TRACRN

Publications

K. Birdsell, K. Eggert, and B. Travis
Three-Dimisional Simulations of Radionuclide Transport at Yucca Mountain
Journal article, Special issue of *Radioactive Waste Management and The Nuclear Fuel Cycle*
In preparation.

WBS 1.2.3.4.1.5.2 Demonstration of Applicability of Laboratory Data

Objective

The purpose of this study is to design and conduct experiments to evaluate the applicability of laboratory data and to test models used in the Radionuclide Transport Program to determine far field radionuclide transport. Both intermediate- and field-scale experiments and natural analogs will be assessed for their potential to provide the required data.

Activities and Accomplishments

A meeting was held with Lawrence Berkeley Laboratory (LBL) investigators 19 February to discuss current experimental design for testing radionuclide transport at Yucca Mountain. In the meeting held in January, ideas were proposed to use boreholes for both geophysical and hydrological measurements before alcove construction, and the February meeting expanded further on this idea. The length scale between fast paths for the proposed testing region at Yucca Mountain is currently unknown but it is expected to be long. Detecting fast paths is difficult, and one of the few tools that can be used particularly at a repository scale is geophysics. To test this potential, geophysics will be an integrated component of the radionuclide transport test proposed in this study.

The revised design will initially explore an area with two boreholes from the main drift to identify zones where fast flow may occur. If a zone is identified, then initial entry will be made, and two boreholes perpendicular to the first ones will be drilled. A suite of geophysical, hydrological, and transport tests will be conducted in these boreholes. The current assumption is that fast paths (most likely fractures or another discontinuity) can be identified. Flow and transport response times on these paths are expected to be short (days or weeks), and the lower alcove will provide a location for observing breakthrough. Following the effort to characterize and predict response of the zone through boreholes, the upper alcove will be mined, and the two alcove experiment will be implemented. Data obtained from the borehole phase of characterization can be used for model parameters to predict response of test block between alcoves thus providing data from another scale for model evaluation.

A key to this proposed design is the geophysical methods that will be used to detect test locations, and a prerequisite for implementation of this experiment will be to determine the required data for the geophysical methods. The feasibility will also be evaluated during the early phases of test implementation.

E. Springer was selected as the Los Alamos representative to the Integrated Test Evaluation (ITE); he attended the first meeting on 14 February. On 26 February he attended a second meeting to discuss consolidation of test categories for further evaluation.

A Hydrology Integration Task Force (HITF) meeting was held at Los Alamos on 6 February. Testing in the high-gradient area north of Yucca Mountain using an existing borehole, G-2, was the major focus of the meeting; however, a decision on this was postponed until better cost estimates for preparing G-2 are available. A workshop in conjunction with the Geochemistry Working Group was discussed; a date will be set following the Geochemistry Core Team meeting in February.

The SCPB change to break this study into four activities was submitted to the Project Control Branch following AP-06.1.

Continued on next page

Planned Activities

Continue to develop study plan.

Travel to Lawrence Berkeley Laboratory to discuss field test design, schedule and resources for this effort. This will have to entered into PACS.

Attend ITE meetings.

Problem Area

None

Milestone Progress

No FY91 milestones.

Publications

E. P. Springer
The Use of Anthropogenic Analogues in Site Characterization of Low-Level Radioactive Waste Sites
Conference Paper, *Proceedings of the 13th Annual DOE Low-Level Waste Management Conference, Atlanta, Georgia, 19–21 November 1991*
In preparation.

C. Woloshun
A Summary and Discussion of Hydrologic Data from the Calico Hills Nonwelded Hydrogeologic Unit at Yucca Mountain, Nevada
LA-series report
Received YMPO approval on 29 October 1991.
Accession numbers for references are being obtained.

WBS 1.2.5 Regulatory and Institutional

Objective

The purpose of this task is to coordinate the regulatory and institutional Project requirements within the Los Alamos programmatic structure. The focus of this coordination effort is on the integration of the technical work within the regulatory and institutional framework.

Study Plans

Water Movement Test, R1 (8.3.1.2.2.2). R0 has been approved by DOE and the NRC. R1 has been approved by DOE but not the NRC. A revision incorporating NRC and State of Nevada comments was submitted to the YMPO on 17 October 1991. We have not received a response.

Diffusion Test in the Exploratory Studies Facility, R0 (8.3.1.2.2.5). A revision incorporating DOE/HQ and Project Office comments was submitted to Dr. Dobson on 11 June 1991.

Testing of the C-Hole Sites With Reactive Tracers, R1 (8.3.1.2.3.1.7). Was issued by DOE/HQ as a controlled document, and sent to the NRC on 10 April 1990. On 13 January 1992 we were requested by DOE to revise NRC comments. We are in the process of doing this.

Mineralogy, Petrology, and Chemistry of Transport Pathways, R3 (8.3.1.3.2.1). Accepted by the NRC on 20 August 1990. On 24 October 1991 we were asked to revise study plan. On 27 January 1992 we submitted revised comments to T. Bjerstedt.

History of Mineralogy and Geochemical Alteration at Yucca Mountain, R0 (8.3.1.3.2.2). Project Office approved the study plan on 18 December 1991 and submitted it to the NRC on 31 January 1992.

Kinetics and Thermodynamics of Mineral Evolution and Conceptual Model of Mineral Evolution, R0 (8.3.1.3.3.2; 8.3.1.3.3.3). Comment resolution meeting for DOE/HQ and Project Office comments was held on 14–15 March 1990; revision activity has been deferred.

Sorption Studies and Sorption Modeling, R0 (8.3.1.3.4.1; 8.3.1.3.4.3). Comment resolution meeting for DOE/HQ and Project Office comments was held in February 1990; revision is in progress.

Biological Sorption and Transport, R1 (8.3.1.3.4.2). Revision, incorporating DOE/HQ and Project Office comments, were submitted on 20 May 1991. Additional revised text were submitted on 28 August 1991. The comment resolution verification was complete on 7 December 1991 and is in the process of being approved by the Project Office.

Dissolved Species Concentration Limits, and Colloid Formation and Stability, R0 (8.3.1.3.5.1; 8.3.1.3.5.2). Submitted to Project Office on 17 August 1990. Comments were returned to Los Alamos for a revision; that revision is in progress.

Dynamic Transport Column Experiments, R0 (8.3.1.3.6.1). Comment resolution meeting for DOE/HQ and Project Office comments was held on 28–30 August 1990; revision is in progress and is expected to be complete by March 1990.

Diffusion, R0 (8.3.1.3.6.2). Comment resolution meeting for DOE/HQ and Project Office comments was held on 28–30 August 1990; revision is in progress and is expected to be complete by March 1990.

Probability of Magmatic Disruption of the Repository, R0 (8.3.1.8.1.1). This study plan was approved by the Project Office on 19 September 1990 and by the NRC 5 October 1991.

Physical Processes of Magmatism and the Effects on the Repository, R0 (8.3.1.8.1.2). In preparation, expected target date is 30 May 1992.

Characterization of Volcanic Features, R0 (8.3.1.8.5.1). Accepted by NRC on 4 September 1990.

Retardation Sensitivity Analysis, R0 (8.3.1.3.7.1). A revision incorporating DOE/HQ and Project Office comments was submitted on 18 June 1991. On 17 October additional comments were received from SAIC, P. Cloke. We submitted revised comments to P. Cloke on March 6, 1992.

Ground Water Chemistry Modeling, R0 (8.3.1.3.1.1). Submitted to Project Office on 15 March 1991.

WBS 1.2.6 Exploratory Studies Facility

Objective

These Exploratory Studies Facility (ESF) tasks address the issues and information needs associated with the ES based characterization of Yucca Mountain to determine the suitability of permanently isolating high-level nuclear waste from biosphere in a geologic repository.

Activities and Accomplishments

Initiated work on developing Tracers, Fluids and Materials (TFM) management program consistent with plan issued by Project (YM 91-23) prepared by Los Alamos. Developed methodology to manage TFM. Held meeting at Las Vegas to brief participants on use of TFM at YMP. Continued to participate in Test Integration (TIG) meetings and Sample Management Facility meetings. Prepare briefings for weekly ESF management meeting on Fridays. Started activities to develop ESF-based sample requirements for laboratory tests and developing test information for tests to be performed in north-portal area.

Meetings. Met with participants regarding TFM. Participated in ESF replanning meetings and RSED-guided TIG meetings. Attended surface-based drilling and testing meetings, and Field Operations Center weekly meetings.

Planned Activities

Continue to support meetings on management of water used during site characterization.

Initiate work to identify administrative procedures to be changed to manage TFM during the site characterization.

Implement strategy to gather TFM information from participants.

Develop design related information for tests to be performed in the launch chamber.

Continue to support integration meetings such as ESF design, TIG, SMF surface-based testing and its interface with ESF testing.

Continue to replan Los Alamos effort.

Develop interfaces for testing and the ESF design.

Revise and update the PSAR, if required.

Prepare Title II Test Planning Packages.

Develop new networks for ESF testing.

Problem Areas

None

Milestones

None

WBS 1.2.6.8.4 Integrated Data System

Objective

The integrated data system (IDS) supports the Exploratory Studies Facility (ESF) test program by providing a central facility to automatically measure and control aspects of the ESF tests. The primary purposes of the IDS are to assist the principal investigators (PI's) in acquiring high-quality test data in a uniform, controlled fashion and to transfer those data to the PI's organizations for data management and analysis.

Activities and Accomplishments

This activity has been deferred.

WBS 1.2.9.1.2.4 Technical Software Management

Objective

The purpose of this activity is to manage the development, implementation, and use of all software employed on activities that will support a license application; to manage the configurations of all software and computational data; and to provide tools and procedures that support these activities.Technical software management continued to perform the quality assurance, configuration management, and engineering tasks that are required by the Los Alamos Software Quality Assurance Plan for the Yucca Mountain Project.

Activities and Accomplishments

Software configuration management (SCM) staff reviewed software, both formal, CCB-initiated reviews, and informal internal reviews of various baseline components of applications currently under development.

The DOCGEN application (October 1991 Monthly Report) continues in prototype development.

The design of the command-line parser, which will enable developers to easily define legal command lines for their applications and obtain information from the Unix command line, is almost complete. This is the first application that incorporates a full, object-oriented analysis and design.

Processed two baseline submissions, storing the submitted material in the certification environment, generating the attendant SCM documentation, performing the physical and functional configuration audits on each and generating software review packets to support CCB review of each. SCM sanctioned eight software applications and updated the Computer Program Library for each. Two CCB meetings were held at which six reviews were approved and two SCM Variance Authorizations were issued.

Planned Activities

Configuration Management:

- Continue management of submitted baselines and change requests.

Software Engineering:

- Continue work on the object-oriented design of the command line parser.
- Continue support of the schedule update effort for the Project Control Section.
- Continue support of the SCM effort.
- Continue technical support of the software review process.

WBS 1.2.9.1.4 Records Management

Objective

The objective of this task is to manage records and documents related to the licensing of a geologic repository for the disposal of high-level radioactive waste by developing, implementing, and maintaining a comprehensive, automated, and integrated information management system.

Activities and Accomplishments

The Records Processing Center rejected 9 records and accepted 238 records in February.

The records procedure was revised, and QP-17.4, R0, and 17.5, R0, were issued on 28 February 1992.

WBS 1.2.9.3 Quality Assurance

Objective

The Quality Assurance (QA) Program supports Los Alamos Yucca Mountain Site Characterization Project participants and ensures that their efforts provide data and evidence admissible for the repository-licensing process.

Activities and Accomplishments

Software. Two software Configuration Control Board (CCB) meetings were held (131 software change requests were submitted and 58 applications were approved). The process to approve commercial-grade software requests was streamlined.

Grading. Los Alamos has 33 approved grading packages and 1 package is in YMPO review. S. Bolivar attended a grading workshop in Las Vegas.

Document Control. Detailed technical procedure DP-609 "Balance Calibration", and quality administrative procedures QP-1.2, "Stop Work Control"; QP-1.3, "Conflict Resolution"; QP- 8.2, "Identification and Control of Samples"; QP-17.4, "Prepare Records"; and QP-17.5, "Process Records"; were issued.

Training. The new indoctrination class was attended by 25 YMP staff. R. Shay completed the Project Office lead auditor course.

Program Development. Twenty QPs are in various stages of revision. Efforts to stream line the QP process continued. The top ten QPs were prioritized, and a QP tracking mechanism was introduced. The Los Alamos quality assurance organization is conducting an internal assessment of 1991 activities.

Deficiencies. Actions for CARs YMP-92-002 and 003 were completed. SDR-597 was closed by the Project Office.

Audits. The audit (AR 92-01) of EES-1 was completed.

Planned Activities

Grading package and QP revisions will continue. Uncompleted survey reports and the criterion 18 audit report will be completed. The 1991 annual quality assurance progress report will be sent out for technical and editorial reviews. An indoctrination class will be offered in March. There will be an audit of EES-13/Las Vegas and associated subcontractor activities (AR 92-02,3,4,5) next month. The DOE will conduct a limited-scope audit of Los Alamos activities in March.

Problem Areas

The current software quality assurance plan is being examined, and modifications will be determined by budget constraints.

Publications

S. L. Bolivar
The Los Alamos National Laboratory Yucca Mountain Site Characterization Project Quality Program,
A Progress Report for January 1, 1990 - December 31, 1991.
In internal review.

APPENDIX

ATTACHMENTS AND LEVEL III MILESTONE REPORTS

RADIONUCLIDE SOLUBILITY WORKING GROUP

1. Role of Working Group

a. Integrate the radionuclide solubility and speciation activities supporting the waste package and near-field activities of LLNL and the far-field activities of Los Alamos.

This integration will allow Project programmatic changes such as new design concepts to be easily incorporated in site and performance activities. The meeting of the working group will allow more effective communication of technical progress in the YMP as well as sharing knowledge of progress in radionuclide research outside the YMP.

b. Function as a decision making body to determine the best radionuclide thermodynamic solubility and speciation data to be submitted to the Project geochemical data base, GEMBOCHS.

This will provide a better link between the data collection activities and data management activities for this complicated issue.

2. Process of Working Group for Evaluation of Data

GEMBOCHS is more than a data repository (the data base is interfaced with geochemical modeling codes), and therefore, it must continually be tested as new data is made available. Much of the thermodynamic data comes from the literature. For example, in a phosphate system some nuclide phosphate species have been measured. These literature data are included in the data base. New data on Pu from Nitsche was included in a user's version of the data base. Modeling done by Silva indicated a phosphate species should form. No phosphate species were observed by Nitsche. In Silva's considered opinion, the modeling results are unreasonable and he suggests that the phosphate data in GEMBOCHS may be suspect. He believes experiments should be carried out to corroborate or reject the literature data. This kind of modeling and evaluation is an example of the kind of data base testing required.

Only users with thermodynamic knowledge of chemical systems can know when the model is producing reasonable or unreasonable results; therefore, the testing and evaluation is conducted as part of the solubility/ speciation tasks. The working group would function as a liaison between the scientific data gathering and the data base management function for GEMBOCHS by providing evaluation and acceptance of the data and a recommendation for inclusion into the data base.

The solubility/ speciation task evaluates the present data base and decides whether testing is needed. Test problems are defined and sensitivity studies are identified. The modeler carries out the work and provides the results through written report and presentation. The results are brought to the working

group and evaluated. The working group decides if the data should be added to the GEMBOCHS and, if necessary, whether other data currently in the GEMBOCHS should be revised or deleted from the data base as a result of the modeling.

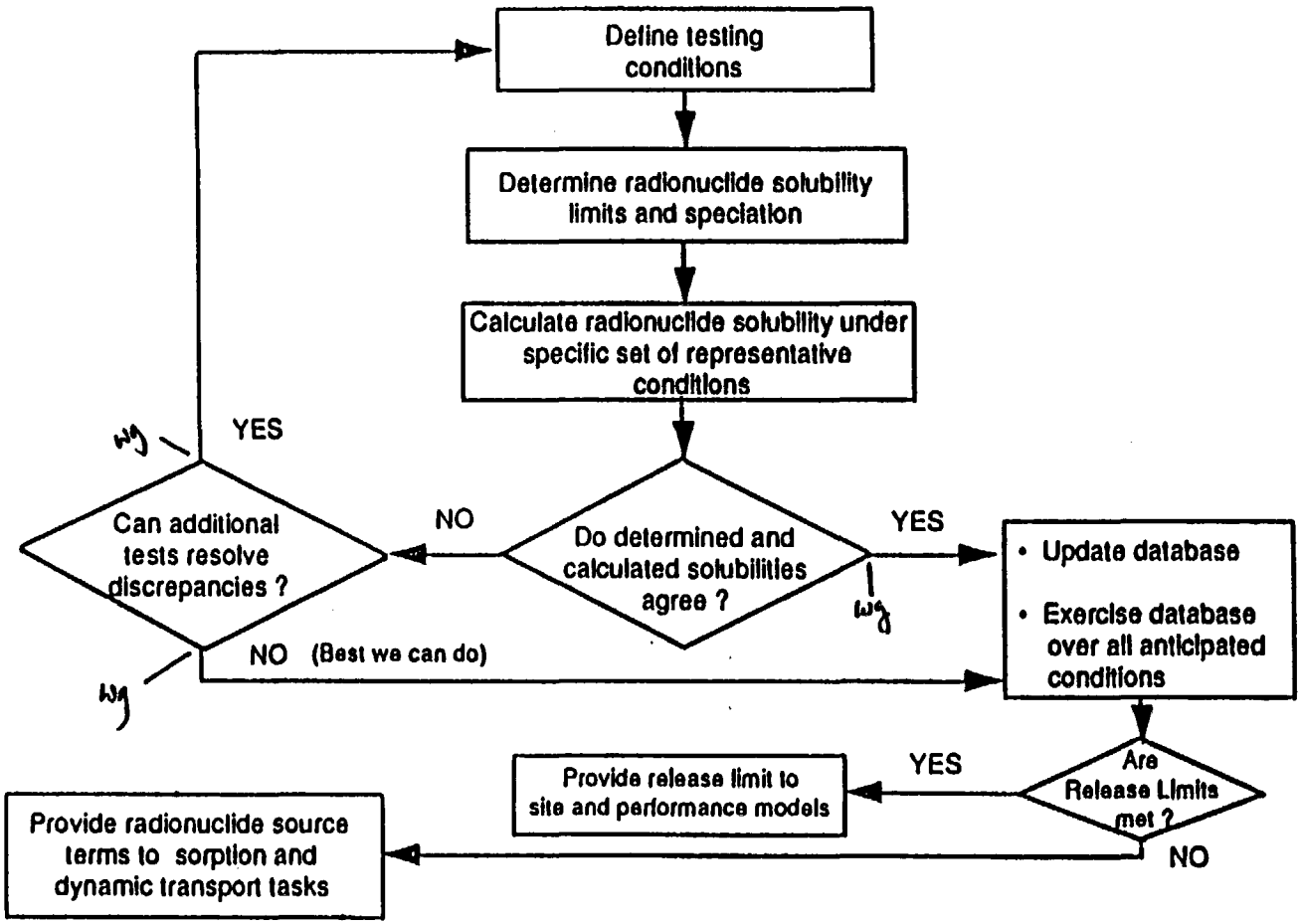
Data gaps may be identified as a result of the modeling. The solubility/speciation task decides whether sensitivity studies are needed to determine if laboratory work should be initiated. If lab work is necessary, the conduct of the work is evaluated against the current work scope and prioritized. This change is communicated to the working group so that necessary interfaces, contraints, or problems are identified.

The process described is shown in the attached Figure. The interface with the working group is shown. At certain points, interface with the working group would allow the data gathering tasks to tap expertise outside the existing work performing participant if necessary, and provide a vehicle for communication where clear overlap between the near- and far-field exist.

It is acknowledged that members of the working group may be called upon to provide formal review of data base submissions following prescribed data management procedures. The working group is not envisioned to function as the review body for the GEMBOCHS data base. The working group is not to be institutionalized i.e. management plans and procedures. The working group should be seen as a virtual team of the formal Geochemistry Core Team and only be a tool for integration, not the result of integration.

wg = interface with working group required

Strategy for Dissolved Species Concentration Limit Studies



RADIONUCLIDE SOLUBILITY WORKING GROUP-FUNDING SUPPORT

1. Los Alamos support requested of WBS 1.2.1.3.5

The working group is planning on meeting twice this Fiscal Year. The meetings would be scheduled for 2 days. Los Alamos participation would consist of 6 staff present for the meetings.

Staff hours supporting the meetings= 202

Staff preparation hours = 32

Staff post-meeting summary hours = 48

Additional hours-unanticipated effort = 50

Total = 300

(Cost- FTE + overhead) = $53K

Dave Morris will be the working group lead. His duties include:

a) preparation of meeting agenda

b) Conduct of meeting

c) Preparation of summary

d) identification of any milestones

e) direction of effort of working group participants

2. LLNL support

LLNL will be involved in the working group. Funding support for LLNL will be from other WBS elements or funds associated with International Programs.

P. T. Prestholt, NRC, Las Vegas, NV

Los Alamos Los Alamos National Laboratory
Los Alamos,New Mexico 87545