ONWI-9(3)

Technical Progress Report for the Quarter 1 April—30 June, 1980

Office of Nuclear Waste Isolation

Battelle Memorial Institute
505 King Avenue
Columbus, OH 43201

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OVERVIEW

BY

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General Manager

The ONWI Technical Program

This report describes the technical accomplishments during the period from April through July, 1980, on the commercial nuclear waste management programs under the direction of the Office of Nuclear Waste Isolation (ONWI). These programs are described in the Report ONWI-19 (Rev. 1), ONWI Technical Program Plan, December, 1979 [see Public Information Section for availability of this document and the previous Technical Progress Report, ONWI-9(2)].

The National Waste Terminal Storage program (NWTS) was established in 1976 and given the responsibility of developing a system for the permanent isolation of nuclear wastes. NWTS is part of the Office of Nuclear Waste Management in the U.S. Department of Energy. The establishment of NWTS signaled the acceleration of the national program.

ONWI has lead responsibilities in the NWTS structure for oversight and coordination of all programs, for development of the general technology, and for geologic exploration on non-DOE land. A project management group, ONWI directs and evaluates studies, research, and development performed by subcontractors on repository sites and designs.

The scope of ONWI activities includes providing the technology and facilities for the terminal isolation of these wastes by disposal in mined repositories deep underground in stable geologic formations. Steps leading to the accomplishment of that purpose include:

- Site exploration, characterization, and recommendation
- Design, licensing, construction, and operation of a commercial geologic repository (or repositories)
- Technology development to support these steps.

Throughout the process, ONWI has the responsibility to provide public information on all aspects of the program and to encourage public interaction.

It is recognized that safety of the public is the overriding program objective. The technical programs have been formulated to meet the challenge of the NRC licensing process, which is the institutional mechanism for assuring that public protection has been accomplished.

The site investigation portion of the program involves a comprehensive geologic, hydrologic, and environmental characterization of candidate repository sites throughout the United States. Included are studies in salt formations in Mississippi, Louisiana, Texas, and Utah. Investigations of other geologies are also being conducted and accelerated. The investigation process requires extensive field activity including deep-hole drilling, associated supporting geologic and hydrologic investigations, and environmental characterization. Comprehensive site qualification criteria are being developed to guide the site investigation and evaluation process.

The technology development program is designed to provide experimental data and validated analytical modeling of the various phenomena involved in repository design and performance assessment. We have attempted to define and anticipate technological issues that will be addressed in the licensing process and to initiate experimental and analytical programs for providing adequate information to justify a technical consensus that the performance of the barrier system utilized in geologic disposal can be modeled and predicted with confidence over long time frames associated with the safe disposal of nuclear waste. The experimental information and analytical techniques will eventually become incorporated in a validated, predictive model of long-term repository performance and used to define the risk potential of geologic repositories to man and his environment.

The repository design and licensing programs are structured to assure that all designs and supporting information are developed in a format consistent with the licensing process. To assure attaining this objective, documents are being prepared such as the licensing plan, formats for the environmental report and safety analysis reports required for the licensing process, and preliminary information reports, which will provide an opportunity for early interaction with the NRC and subsequent discussions about program strategy. In addition, the ONWI staff is closely monitoring the development of criteria and regulations developed by the EPA and the NRC to assure that these are properly integrated into the programs.

The programs required are enumerated in the Work Breakdown Structure (WBS) shown in Figure 1. Progress on various elements of this Work Breakdown Structure is reported in this Quarterly Report in accordance with the WBS elements.

Quarterly Highlights

Major accomplishments during this quarter are listed below.

Science and Technology

- Detailed analyses of the long-term (up to 15 years) creep data being obtained in the Salt Model Pillar Studies show that the exponent on time continues to increase (approaching one) for all samples. In general, these data suggest that the deformation rate is becoming constant even for the samples tested at room temperature.

- Work is continuing in the WRIT program on waste form leaching and radionuclide sorption. The Leach Test Methodology effort addresses both static and flow methods for measuring radionuclide release from candidate waste forms.

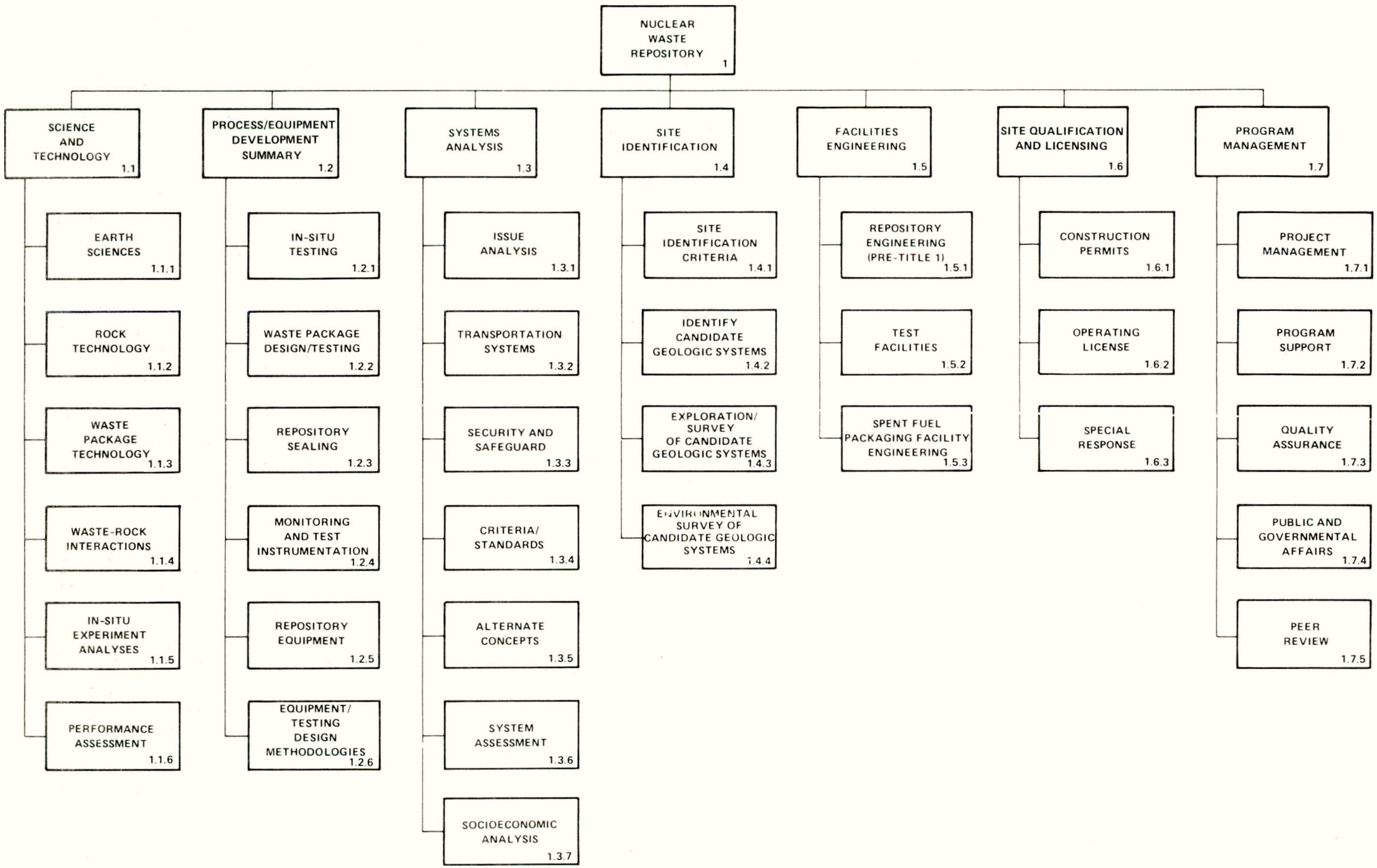


FIGURE 1. ONWI WORK BREAKDOWN STRUCTURE

• In the performance assessment area, AEGIS completed the documentation of the codes used in the initial site assessments. With documentation of the codes complete, they were transferred to the SCEPTER program as planned and on schedule.

• The development of the numerical code ROCMAS for the thermomechanical-hydrological model development was initiated. The flow-stress part of the program has been validated against a number of fracture flow problems for plane two-dimensional and axisymmetric systems.

• Thermomechanical simulations of the planned accelerated borehole closure experiments to be executed at Avery Island, Louisiana, were performed. After the field experiments are completed, these simulation results will be compared with the field results. The results of the comparisons will allow an assessment of the laboratory-determined constitutive relations and material properties and the modeling procedures.

Process/Equipment Development

• A repository waste package design studies program was initiated. The objective of the program is to develop initial designs.

• Work on the borehole cement and rock properties study continues. Potential borehole plugging and shaft-sealing materials, including cementitious formulas modified for field tests and new experimental types, are being investigated.

• Excavation of the flatjack slots was completed by Terra Tek on the Heated Block Flatjack test in granitic gneiss.

• Blast damage assessment technique evaluation and geologic mapping procedures were initiated at the Colorado School of Mines Experimental Mine.

Systems Analysis

• Researchers on the Social-Institutional Aspects of Nuclear Waste Management have developed, by means of topical papers, a set of tentative recommendations for impact assessment.

Site Characterization

• The final Gulf Coast Salt Dome Regional Summary and Area Recommendation report and the draft Permian Area Environmental Characterization report were transmitted to DOE.

• Field work in the Gulf Coast Salt Dome Region was conducted in Louisiana, Mississippi, and Texas. Water supply wells at five sites have been installed, and nine deep wells at four sites have been completed. Pump tests have been conducted at two deep well sites, and site restoration has been completed at two of the sites. Thirty additional shallow borings at Cypress Creek and ten shallow borings at Richton Dome are complete. A third high-resolution reflection seismic line was completed at Cypress Creek and three lines completed at Richton Dome.

- The report, *Results of Hydraulic Tests of Wells DOE-1, -2, and -3 Salt Valley, Utah*, was printed and distributed (USGS Open File Report 80-205), and analysis of data from the hole-to-surface resistivity, cross-hole seismic, and surface electromagnetic surveys at Salt Valley continued.

- Coring and open-hole hydrological testing of the Gibson Dome No. 1 borehole (GD-1) was completed to a depth of about 2,700 feet. Hole-to-surface resistivity measurements at GD-1 out to radial distances of approximately 6,300 feet from the hole were completed.

- The extent of salt dissolutionand contiguous ground collapse has been determined for the northern margin of the Palo Duro basin and adjacent margins of the Dalhart and Anadarko basins.

Major Public Information Events of the Quarter

Revisions were made in the multiimage slide/tape presentation to incorporate specific recommendations made in the President's Policy Statement on a Comprehensive Radioactive Waste Management Program. Several showings of the presentation were held. These included:

Millsaps College, Jackson, MS, Energy Symposium, April 1
American Nuclear Society, Dayton, OH, April 13
American Planning Association, San Francisco, CA, April 14
Michigan Educators' Energy Forum, East Lansing, MI, April 19
Ascension Lutheran Church, Columbus, OH, April 20
Joint Symposium on Hazardous Nuclear Waste Disposal, Raleigh, NC, April 25
Rotary Club, Cleveland, OH, May 1
Association of Engineering Geologists, San Francisco, CA, May 3
Community-Oriented Energy and Nuclear Waste Symposium at Louisiana Technical University, Ruston, LA, (meeting developed by ONWI for the Department of Energy), May 8
RE/SPEC, Inc., Rapid City, SD (May and June, several showings)
American Society of Mechanical Engineers, Canton Chapter, Canton, OH, May 14
Linden Lions Club, Columbus, OH, May 27
American Society of Mechanical Engineers Symposium on Nuclear Waste, Idaho Falls, ID, May 29
Basalt Waste Isolation Project (BWIP) Technical Society Meeting, May 29
Society of Women Engineers, New Jersey National Convention, June 27

The Film Management contract between ONWI and the Media Group was approved by the DOE. The Media Group has been employed to provide guidance and facilities for technical films and multislide presentations. One of the first tasks is a program-wide NWTS film for public dissemination.

ONWI's technical exhibit panels were designed, updated, reviewed, and approved by DOE. The panels were used in major exhibits at meetings of the American Institute of Chemical Engineers (June 8 to 11, Philadelphia), American Nuclear Society (June 9 to 11, Las Vegas), and American Society of Mechanical Engineers (May 11 to 14, Washington, D.C.).

Briefing packages were prepared for the appropriate DOE representatives in NWTS briefings for USGS Province 9 states. Material was also transmitted to DOE for briefings for Wisconsin, Minnesota, and Michigan officials on granitic investigation. A draft news release on national screening of geologic systems was submitted to DOE.

Six fact sheets were resubmitted for DOE review, incorporating DOE suggestions, and seven additional new fact sheets were submitted. The fact sheets are being developed for wide dissemination to the public of brief, factual information.

Public Information Program

ONWI publishes technical reports on nuclear waste isolation which result from scientific and technical investigations conducted by more than 100 subcontracting organizations. This Technical Progress Report issued quarterly is a summary of progress by these subcontracting organizations. The reports cover the subject areas of geology, hydrology, drilling, rock mechanics, and socioeconomics and licensing, among others.

Reports are distributed to the public, government agencies, universities, and libraries, and are available in limited numbers to interested individuals. Readers who would like to receive the *ONWI Library Reports List* or other publications are invited to write or call:

ONWI Library
505 King Avenue
Columbus, Ohio 43201
(614) 424-7697.

The ONWI Library is open to the public from 8 a.m. to 5 p.m., Monday through Friday. Interested users may arrange to visit the Library during these hours by contacting the Library at the above address.

TECHNICAL PROGRESS REPORTS

In this section the progress reports of the programs in the various waste management technologies are presented according to the organization of the Work Breakdown Structure (WBS). Each report carries a WBS number for the convenience of the reader. The content of the second level of the WBS follows:

WBS 1.1 Science and Technology. The reports describe methodologies and data relative to physical and chemical properties of radioactive waste forms, geologic media, and isolation materials for use in NWTS projects. Methods and criteria are developed for evaluation of seismic, thermal, hydrological, climatic, and other potentially disruptive events; and models and techniques for assessment of public risk and safety in support of licensing activities are developed.

WBS 1.2 Process/Equipment Development. These reports are of projects which deal with engineering feasibility or confirmation testing of equipment and processes to meet the requirements of the repository and related support functions. They include engineering test programs, execution of in situ tests; borehole plugging; waste canister, cask, and transporter technology; and generic engineering design criteria for use in the NWTS projects.

WBS 1.3 Systems Analysis. These reports deal with key issues related to waste isolation, including studies on transportation of waste, spent fuel disposal, and waste projections.

WBS 1.4 Site Identification. The reports in this section deal with geologic exploration, and the identification and development of potential sites for repositories. The emphasis of the work in these areas is to study regional geologies from which study locations will be identified, and finally recommend specific sites for the NWTS repositories.

WBS 1.5 Facilities Engineering. These reports deal with conceptual engineering for repositories, and support activities such as the Generic Environmental Impact Statements and the International Nuclear Fuel Cycle Evaluation (INFCE). Other studies concern design safety, licensing plans, and environmental assessments.

WBS 1.6 Site Qualification and Licensing. The work reported in this area is concerned with the development and procedures necessary for the identification, selection, and qualification of proposed sites for isolation of radioactive wastes. This includes preparation of a site selection plan; development of siting criteria; performance of environmental surveys; preparation of environmental characterization reports; preparation of a licensing plan, a safety analysis report, an environmental report, and an environmental impact statement; and conducting safety analyses and environmental impact assessments.

SUMMARY

1.1 SCIENCE AND TECHNOLOGY

The scope of Science and Technology investigations covers Earth Sciences, Rock Technology, Waste Package Technology, Waste-Rock Interactions, In Situ (Field) Experiment Analyses, and Performance Assessment. The objective of this task is to assure adequate technological bases for providing the generic foundation for the concept of geological isolation and for supporting specific repository projects. In addition to the progress reported herein for individual projects, the Earth Science Technical Plan and the Waste Package Program Plan were completed this quarter.

Detailed analyses of the long-term (up to 15 years) creep data being obtained in the Salt Model Pillar Studies show that the exponent on time continues to increase (approaching one) for all samples. In general, these data suggest that the deformation rate is becoming constant even for the samples tested at room temperature.

Work is continuing in the WRIT program on waste form leaching and radionuclide sorption. The Leach Test Methodology effort addresses both static and flow methods for measuring radionuclide release from candidate waste forms. The Sorption/Desorption Methodology effort involves factors influencing retardation of radionuclide migration and describes and compares static and dynamic methods of measurement. In another aspect of work in this technical area, substantial progress has been made in developing methods to attain the low partial pressures of oxygen required for conducting laboratory leaching and sorption tests under expected repository conditions.

Some of the irradiation experiments with brines in small Pyrex ampoules have been completed. The analyses of the brines for the quantities of gases produced by radiolysis indicate that the only significant effect of the dissolved chloride salts is to increase the rate of deposition of gamma energy.

In the performance assessment area, AEGIS completed the documentation of the codes used in initial site assessments. With this done, the codes were transferred to the SCEPTER program as planned and on schedule. The codes transferred include most of the AEGIS hydrologic, transport, and dose codes.

A statistical sensitivity analysis was done using a simple nuclear waste repository to demonstrate the sensitivity methodology for the heat transfer aspects. Factors found to be most important included thermal loading, package spacing and size, and rock thermal properties. The important feature of this work is the use of the technique for other aspects of repository performance.

Monitoring of the transport of thorium from the Morro do Ferro deposit has continued. A weir and continuous sampler have been installed on a small stream below the deposit and should be operational in a few months. Until that time grab samples will continue to be collected at four locations along the stream.

Work has continued on the laboratory study of clay membranes with efforts toward calibration and testing the two membrane testing machines. Also, five gas samples have been collected from the deep crystalline ground water.

Work on diagenesis of clay minerals indicates that chlorite minerals begin forming at relatively low temperatures and are present in rocks that have been exposed to burial temperatures on the order of 400 C.

Studies on thermodynamic properties of actinides have concentrated on improving computer facilities by implementing a more stable system and extending the memory.

Empirical measurements on fission product release from spent fuel show that the distributions of products released do not correlate with physical features within the fuel.

The development of the numerical code ROCMAS for the thermo-mechanical-hydrological model development was initiated. The flow-stress part of the program has been validated against a number of fracture flow problems for plane two-dimensional and axisymmetric systems.

Three papers were prepared based on studies with ROCMAS. The first, entitled *Numerical Modeling of Thermohydrological Flow in Fractured Rock Masses*, summarizes the efforts of the past few years that have culminated in the development of the coupled stress-fluid flow analysis code ROCMAS. The other two papers give more detailed discussions of the background and rationale of the program.

A system for hydraulic fracturing was built at LBL. The system includes two innovations —a downhole assembly for measuring packer pressure and injection pressure with simultaneous surface readout, and a wireline impression packer for obtaining fracture orientation.

Thermomechanical simulations of the planned accelerated borehole closure experiments to be executed at Avery Island, Louisiana, were performed. After the field experiments are completed, these simulation results will be compared with the field results. The results of the comparisons will allow an assessment of the laboratory-determined constitutive relations and material properties and the modeling procedures.

Textural and fabric data were obtained on specimens of WIPP site rock salt and on a suite of experimentally deformed warm-sintered, synthetic specimens. These data permit comparison of the sintered specimens with the undeformed and experimentally deformed naturally occurring ones from WIPP.

WBS 1.1.1

Project: Geothermometry Methods for Determining the Thermal History of Shales

Principal Investigator: Georgia Institute of Technology (C. E. Weaver)

ONWI Project Manager: J. O. Duguid

Objective

The objective is to establish geothermometry methods for determining the thermal history of shales. A secondary objective is to determine the geochemical, mineralogical, and structural changes that occur in shales when they are subjected to burial temperatures between the range of 100 to 400 C.

Progress Reported Previously

The program started 1 February 1977. A suite of Cambrian Conasauga shale samples subjected to varying burial temperatures was collected from Georgia, Tennessee, and Alabama. Detailed X-ray analyses of various size fractions showed there are at least 20 parameters that correlate well with the burial temperature gradient.

Chemical data also varied as a function of paleotemperature. Chlorites which were exposed to a high degree of burial diagenesis are more magnesium rich than chlorites having undergone only shallow burial (MgO varies from 8.7 to 16.6 percent). The distribution of iron and magnesium changes with increasing burial temperature (MgO/Fe_2O_3 varies from 0.34 to 0.92).

Acid dissolution was used to determine rate constants for the release of cations from chlorite and illite during acid treatment. Rate constants for the release of all of the structural cations in chlorite and potassium in illite change with increasing degree of diagenesis. Chlorite becomes more resistant to acid attack as the Mg/Fe ratio increases or as chlorite becomes better crystallized. With increasing degree of burial diagenesis, the amount of total potassium in illite increases (3.2 to 6.8 percent K_2O) as well as the percentage of fixed potassium (84 to 95 percent).

K-Ar apparent ages were determined for size fractions of 25 samples. Within each particular size range ($<$0.2, 0.2-2, and 2-44 μm) the apparent ages show a consistent pattern of decrease with increasing temperature. A decrease in the apparent age of each sample with decreasing particle size is also evident. Detailed study of K-Ar relationships in the silt size range of several samples, in conjunction with mineralogic and chemical data, indicates that the apparent age patterns reflect (1) an increase in the abundance of diagenetically formed illite, and (2) a decrease in the abundance of detrital illite/mica and K-feldspar as a result of dissolution reactions and in response to increasing burial depth and temperature toward the southeast. The 300 to 350 million year apparent age minimum approached in each size fraction may reflect the time at which temperatures were lowered to the extent that diagenesis stopped.

The ^{39}Ar-^{40}Ar incremental release spectra from selected sample fractions indicate that radiogenic argon is released from feldspars at higher temperatures (>500 C) than from clay minerals in the Conasauga shale. Spectra from a series of progressively metamorphosed samples demonstrate the decreasing influence of detrital feldspars in samples representing increased burial depths and temperature.

Isotopic temperatures based on the ^{18}O content of illite and quartz, and temperatures estimated on the basis of color alteration of phosphatic fragments (conodonts, brachiopods), indicate that the burial temperatures involved a range from about 150 to 300 C.

Si from layer silicates or quartz is mobilized in the early stages of diagenesis and precipitates as small disseminated grains or in thin sheets. The sheets consist of stacks of thin flakes of quartz honeycombed with 1 to 10-μm voids. This suggests the Si migrated in a fluid phase. At the more advanced stages of diagenesis the quartz crystallizes in the form of parallel laths. At this stage the detrital quartz is almost completely destroyed.

Vacuoles or bubbles are abundant in the layer silicate minerals (physils). Shales subjected to the lowest stage of diagenesis (~100 C) contain swarms of tiny round bubbles. With increasing burial temperature the bubbles become elongate (10 to 20-μm long), more oriented, and concentrated. As pressure solution and recrystallization progress, the newly formed phases are relatively free of inclusions. The vacuoles, Ti, and some Mn and Fe are concentrated as residues in thin sheets parallel to the cleavage and inside the vacuoles. They constitute zones of weakness along which the rocks cleave. The vacuoles can probably be used to construct a "degree of diagenesis" or temperature scale.

A study of Conasauga shales from the heater experiment indicated minor changes in addition to those reported by Sandia. The samples subjected to the highest temperature did not disperse, had minor changes in the X-ray peaks of chlorite, and lost some argon from the fine fraction.

A minor adjunct project was to confirm the presence of graphite as inclusions in Gulf Coast salt domes. Scanning Electron Microscopy (SEM) and electron diffraction studies of water insoluble anhydrite residue confirm the presence of graphite. In addition, quartz, dolomite, pyrite, illite, chlorite, and talc are present. The association of pyrite with the graphite suggests the graphite may have formed from organic material that had been subjected to a relatively high burial temperature (deep burial).

Activities During the Reporting Period

A considerable amount of time was spent examining the vacuoles in the shale with the SEM and electron microscope. Figure 1 is a typical field of view showing the distribution of elongate vacuoles in a shale that is in the advanced stages of diagenesis. The distribution gives a banded appearance to the shale. The vacuole bands have a relatively high Fe content and a slight pleochroism, suggesting chlorite or phengite are concentrated with the vacuoles. The intervacuole bands are nearly pure chlorite.

With increasing temperature and pressure, kinking develops and the vacuoles are rotated from horizontal to vertical. Fe and Ti are concentrated in these vertically aligned vacuoles. The Ti occurs as discrete, small ovoids.

FIGURE 1. DISTRIBUTION OF VACUOLES IN SHALE

Once the elongate vacuoles form, probably during flake rotation, they persist and move in response to directed stress. They are present in rocks exposed to burial temperatures on the order of 400 C and subjected to high pressure. They are structurally stable, suggesting they are sealed and contain fluid under high pressure.

In some areas rows of illite flakes have grown perpendicular to the main cleavage. These rows also have a high void area, with the voids aligned perpendicular to the vacuoles parallel to bedding.Visually, the void area of these rocks appears to be on the order of 20 percent. This is unusual and some way must be found to measure it. The vacuoles are so well sealed that even after heating the rock to 500 C the vacuoles appear unaffected.

Energy dispersive X-ray fluorescence (EDX) analysis confirms that the Mg and Al content of chlorite increases and Fe decreases with increasing burial temperature. A re-evaluation of the chemical data indicates that the Fe, Mg, and tetrahedral Al content of the chlorite increases with increasing temperature up to 300 C. At higher temperatures, Mg continues to increase but Fe and tetrahedral Al decrease. This may explain some of the conflicting statements in the literature. Contrary to what might be expected, the Fe and Mg content of illite increases with temperature and the Al content decreases. This suggests that phengite, an Fe-rich illite, formed.

The $^{18}O/^{16}O$ measurements were completed on the Conasauga heater experiment samples. The data have not been analyzed. A few large field samples were collected for physical measurements; an attempt will be made to obtain more. An X-ray technique is being developed to measure orientation.

K-Ar measurements of size fractions of a sample exposed to a burial temperature higher than that of any sample previously analyzed showed that all size fractions were reclocked. This tends to confirm the temperature trend. All of the mica has apparently been recrystallized.

Limestone samples have been taken from the Upper and Middle units of the Conasauga Shale. These samples are associated with the limestone outcrops and quarries near where the shale samples were collected. They are being analyzed by X-ray, petrographic, and radiometric dating techniques. X-ray analyses of thin sections show various degrees of dolomitization, with dolomitization increasing with burial temperature and along the edge of the Cartersville fault. Recrystallization also increases with temperature.

Preliminary K-Ar analyses show that apparent ages increase with increasing burial temperature. The ages calculated for the samples are over a magnitude of order greater than the age of the formation. This is due to an excess of ^{40}Ar in the samples. It is possible that the excess Ar was derived from the shales associated with the limestones. To test this possibility the insoluble residues (clays) will be 'dated'.

WBS 1.1.1

Project: Technology Development Studies for Geologic Disposal; Dating Ancient Ground Water by the Accumulating Radioactive Decay Products

Principal Investigator: Savannah River Laboratory (SRL) (I. W. Marine)

ONWI Project Manager: J. O. Duguid

Objective

Samples from several wells which are in proximity will be dated using helium accumulation methods. These samples should give similar age dates because of the close proximity of the wells. If there is substantial variation, the method will need to be reevaluated.

Activities During the Reporting Period

Five gas samples have been collected from three deep-water wells at the Savannah River Plant. These samples were submitted for analysis to determine the elements in the effervescent gas and in the residual gas in the water, and to determine the quantity and nature of dissolved solids in the water.

WBS 1.1.1

Project: Technology Development Studies for Geologic Disposal; Study of Membrane Phenomena in Geologic Material

Principal Investigator: Savannah River Laboratory (I. W. Marine)

ONWI Project Manager: J. O. Duguid

Objective

The objective is to determine the effects of natural osmotic membranes on natural hydraulic gradients in argillaceous formations.

Activities During the Reporting Period

Two completed membrane testing machines are now in use. There are two types of osmosis experiments with compacted clay slurries: (1) a "U-tube" type of experiment in which solution reservoirs on either side of the membrane are open to the atmosphere; and (2) a system that is closed to the atmosphere in which little net flux across the membrane is allowed. In the U-tube experiment, osmosis is gaged by measuring the net flux of solution from one side of the membrane to the other by means of calibrated capillary tubes. In the closed system experiment, osmosis is determined by the continual buildup of osmotically induced hydrostatic pressure as measured by a differential pressure transducer.

In the U-tube method, variations of laboratory temperatures (18 to 23 C) and atmospheric pressure make the fluctuating levels in the capillary tubes difficult to interpret. However, by monitoring a nonosmotic system (i.e., with water in both reservoirs) for weeks, the fluctuation of a truly osmotic system can be measured. Response in this system is very slow.

Response time in the closed system is more rapid. The low measured pressures are probably caused by the present inability to make certain that, during flushing of the fresh water reservoir with 0.1M NaCl solution, the membrane is in contact with all of the solution.

Diffusion measurements have been carried out after cessation of the experiments. Both reservoirs are flushed with water and the recovered volume is analyzed for NaCl content. Fluxes of salt and water across the membrane occurred, with the diffusion of salt across the membrane being about 20 percent of that calculated for free diffusion in an open body of water.

WBS 1.1.1

Project: Oklo Natural Fission Reactor Program

Principal Investigator: Los Alamos Scientific Laboratory (A. J. Gancarz and A. E. Norris)

ONWI Project Manager: D. P. Moak

Objective

The objective is to determine mechanisms of reactor product transport in geologic media that indicate natural fission reactors or rich uranium ore bodies.

Activities During the Reporting Period

No progress report was submitted for the period.

WBS 1.1.1

Project: Study of Thorium Transport from Morro do Ferro

Principal Investigator: New York University Medical Center (M. Eisenbud)

ONWI Project Manager: J. O. Duguid

Objective

The objective of this project is to study the natural transport of thorium and other elements from Morro do Ferro. The thorium deposit on the Morro do Ferro, a hill on the Pocos de Caldas plateau in Minas Gerais, Brazil, offers what may be a unique opportunity to improve understanding of the behavior of plutonium over geologic time. Thorium is an actinide with chemical properties similar to plutonium in the +4 state. The Morro do Ferro deposit is estimated to contain 12,000 MT of thorium, and the deposit is believed to be about 80 million years old.

Activities During the Reporting Period

Geology of the Morro do Ferro

Existing cores are being located and assembled in one place for study. It is believed that 19 hard rock cores are available to various depths up to about 200 meters, as well as 70 bags of material obtained by means of Empire drills to a depth of about 15 meters. Additional cores will be drilled as required to achieve the objectives. The extent to which thorium, uranium and rare earths can be used as analogs for studies of the environmental behavior of other cations will be investigated theoretically and experimentally. Emphasis will be on the thorium-plutonium analogy.

A preliminary examination has been completed and it shows that the behavior of plutonium is sufficiently similar to thorium to justify intensive study of the mobility of thorium at Morro do Ferro.

Mechanism of Hydraulic Removal of Thorium
and Other Elements of Interest

A meterological station is being installed on the Morro do Ferro to provide a continuous record of rainfall and other appropriate variables. It consists of a weather station (MRI Model 1082), rain collector (MRI Model 383), and rain gage recorder.

A weir is being constructed downstream from the hill. Continuous flow measurements will be recorded by appropriately calibrated instruments in a hut to be constructed atop the weir. A Manning composite sampler has been delivered and should be in operation soon. Calibration will be completed as soon as flow conditions permit.

The water passing through the weir will be sampled continuously at a rate proportional to the flow. Depending on flow conditions, continuous sampling may be deferred until the start of the rainy season in mid-October. Grab samples at four sites on the stream have been obtained at intervals during the past year and isotopic analyses for the three thorium isotopes (228/230/232) are under way.

Grab samples of water from the stream on the north side of the hill and from the first two gullies downstream from the weir will be sampled to ascertain if significant concentrations of thorium or other elements are leaving the hill by those routes. These samples will be obtained as soon as flow conditions permit.

The thorium content of surface waters from other representative streams in the Pocos de Caldas plateau and from other parts of Brazil and the U.S. will be measured.

There is little information about the natural thorium content of surface waters. A recent review by Langmuir and Herman (1980) summarizes the relatively few data reported in the literature. Samples of Hudson River water have been analyzed and are two orders of magnitude lower than stream samples from Morro do Ferro. Additional samples will be collected both in Brazil and the U.S. during the coming year.

Ten wells are to be drilled near the end of the dry season on the Morro do Ferro to a depth of about 3 meters below the water table.

Sedimentary Deposits of Material from the Morro do Ferro

The purpose of this work is to determine the extent to which the plume of debris from the Morro can be mapped, and to make an estimate of the quantities of deposited material.

The location of the plume is determined initially by gamma-ray scanning in the field using a single-channel analyzer tuned to the 2.62 MeV radiation from the Tl-208 daughter of Th-232. The ratio Th-232/Th-228 is measured in representative samples to determine if disequilibrium exists.

The radiation fields on and in the immediate vicinity of the Morro do Ferro were mapped in July and August of 1979. Additional measurements will be made this summer. In particular, the stream bed will be surveyed as far downstream as practical, and measurements by gamma-ray scanning will be completed in the flood plains. A limited number of sediment samples have been examined.

Six cores to the greatest possible depth will be obtained from the two swamps downstream from the hill. Core profiles are described by Th, U, and rare earth analyses. Rates of accumulation are determined by dating methods.

The first cores will be taken during the months of July and August. There is an Empire drill in Pocos de Caldas and this will be used to obtain the first cores. Drawings were obtained for a core sampling system that should be superior to the Empire drill, and two such devices have been fabricated.

Mathematical Modeling

A mathematical model will be developed to describe the transport of elements of interest from the Morro do Ferro. All of the information obtained in the overall project will be integrated into this mathematical model that will describe the environmental behavior of the elements.

REFERENCE

Langmuir, and J. S. Herman. 1980. "The Mobility of Th in Natural Waters at Low Temperatures." Accepted for publication in *Geochimica et Cosmochimica Acta,* July.

WBS 1.1.1

Project: Radionuclide Mobilization by Organic Complexing Agents

Principal Investigator: Battelle's Columbus Laboratories (BCL)
(J. L. Means, D. W. Hastings)

ONWI Project Manager: J. Kircher

Objective

The objective of this program is to fully evaluate the possibility that organic complexing agents from a variety of sources, including the ground water, the repository rock, or the waste itself, may form strong complexes with certain radionuclides and significantly increase transport rates from the repository.

Activities During the Reporting Period

No progress report was submitted for the period.

WBS 1.1.1

Project: Directional Antenna

Principal Investigator: Lawrence Livermore Laboratory (H. M. Buettner)

ONWI Project Manager: J. E. Monsees

Objective

The overall objective is to construct a directional antenna system, usable within a single borehole, for locating anomalies near the borehole. The goals are to:

- Show experimentally that miniature, directional antennas can be produced by enclosing the antenna elements in a sheath made of a ferrite or ferroelectric material

- Provide an assessment of the most appropriate sheath materials.

Progress Reported Previously

A computer code which predicts the shortening effect of a ferrite or ferroelectric sheath on a wire antenna has been written and verified.

Commercially available materials for the sheath have been surveyed, with an emphasis on ferrites. Additionally, the possibility of using new, unique, composite materials has been investigated.

A computer code has been written which predicts the far-field radiation pattern for a center-driven, dipole antenna surrounded by a cylindrical sheath of a ferrite or ferroelectric.

Several attempts to measure the radiation pattern of a ferrite-sheath, dipole antenna were made. The methods used were: (a) continuous wave (CW) measurements in air using a large ground plane, (b) CW measurements in air in a uniform electric field, and (c) CW measurements in a local lake.

Methods (a) and (b) were abandoned early in the program, owing to numerous difficulties. Method (c) was believed workable and was therefore pursued.

Activities During the Reporting Period

A major unsolved problem is whether the computer code for predicting the radiation pattern of a center-driven, dipole antenna surrounded by a ferrite or ferroelectric sheath correctly predicts the radiation pattern. A good deal of effort has been expended in trying to measure the radiation pattern using method (c) above (with numerous modifications) to either verify or refute the computer code. Method (c) was finally abandoned because of numerous, continuing difficulties.

New methods of determining the radiation pattern are now being pursued. One involves using the ferrite-sheath (30-mm-diameter) antenna as a monopole, driven against a ground plane in lake water. The apparatus has been designed and is now being built. The other methods involve the use of a cylinder of water and ferrites as antenna sheaths in air.

Some new materials have been purchased (not yet arrived) for use as the "sheath" in future antennas. The materials are a ferrite (relative permeability and dielectric constants 15 and 10, respectively), and ferroelectric (relative dielectric constant of 1350). The materials are in the form of 3-inch-diameter, 1-inch-thick discs which can be stacked to form antennas of various sizes.

WBS 1.1.1

Project: Hydrology of Nearly Impermeable Rock

Principal Investigator: Lawrence Berkeley Laboratory (W. Thur)

ONWI Project Manager: J. O. Duguid

Objective

The FY 80 objective for one task under this project is to develop a workable theory of analysis for the constant head well injection testing technique, and to verify this theory through field tests on simple fractures in crystalline rock. The technique uses the transient flow rates resulting from a suddenly applied constant head as a means of studying near- and far-field flow conduits.

The FY 80 objective under the second task is the modeling study of theoretical permeabilities of fractured rock systems. Anisotropic media and varying fracture geometries will be modeled to explore the relationships between detailed fracture geometries and the resultant average system permeabilities.

In later years, data from the first task well testing techniques are to be interfaced with the second task modeling studies to develop a system for the stochastic determination of the flow characteristics of anisotropic heterogeneous media.

Progress Reported Previously

This is the first quarterly report for this project.

Activities During the Reporting Period

During 1980, the goal has been to develop well test solutions for transient flow rate under constant head injection conditions for single fractures. Such a test is more rapid and simpler to run than the more common constant flow rate techniques. The single fracture analytical techniques are being developed for closed boundaries (finite fractures) and partially open boundaries (fractures which intersect other fractures).

During the quarter, the main activities have been to develop a mine computer data acquisition system for well testing. The system has now been assembled and software development is under way. A 100-foot-deep test well in granite is available. This test well was logged with a borehole television to determine fracture locations. This hole will be used to test the constant head single fracture technique planned for the future.

Under the second task, the survey of existing literature was completed, as was the numerical study of infinite, regular fractures. A fracture mesh generating program was developed, and a simple finite-element line model was chosen for flow analysis.

WBS 1.1.2

Project: Technology Development Studies for Geologic Disposal; Effects of Earthquakes on Subsurface Facilities

Principal Investigator: Savannah River Laboratory (SRL) (I. W. Marine)

ONWI Project Manager: M. R. Wigley

Objective

The project objective is to evaluate the potential for seismic disruption of underground facilities. The program is divided into the following tasks:

- Review the existing knowledge to document the damage or nondamage to mines, tunnels, wells, and other underground facilities due to earthquakes, and to evaluate the significance of these data. The report documenting this damage and nondamage was published by the Savannah River Laboratory as USDOE Report DP-1513, *Earthquake Damage to Underground Facilities*.

- Perform a detailed mathematical analysis of displacements in the vicinity of faults.

- Through the use of numerical techniques, perform a generic study to determine the effect of an earthquake on underground facilities, with emphasis on how and to what extent seismic waves might affect or create fractures which could permit increased water circulation in the rock surrounding a repository.

Activities During the Reporting Period

Additional work on the Numerical Simulation of Earthquake Effects on Tunnels for Generic Nuclear Waste Repositories, aimed at enhancing the results of the model, was completed. This work included: (1) alteration of the code to permit the simulation of longer duration earthquakes, (2) alteration of the code to treat joints as existing cracks, (3) additional runs for a simulated low-magnitude, high-frequency, high-acceleration, close-in earthquake, (4) re-examination of the material properties of shale used in the model, and (5) additional runs using different horizontal-to-vertical stress ratios. Tables 1 through 3 show the complete results for salt, granite, and shale, respectively.

Conclusions from the SRL studies thus far are described below. Subsurface damage to underground facilities from far-field earthquakes is virtually nonexistent, as shown by both the model studies and by observations. The longer wavelengths in the far-field are closer to the natural periods for surface structures and thus cause damage. These wavelengths are, however, much longer than subsurface tunnel dimensions, and thus cause little subsurface damage.

TABLE 1. RESULTS FOR SALT COMPARED WITH DEFINED CRITERIA

Property	Computer Model Study, Salt				
	Case 1	Case 2	Case 3	Case 4	Case 5
Joint Geometry	X	X	X	X	X
Pore Pressures	X	X	X	X	X
In Situ Stresses	σH = σV	σH = σV	σH = σV	σH = σV	σH = σV
Fault	X	X	X	X	*
Thermal Loading	*	*	*	X	*
Earthquake (g = acceleration gravity)	Oroville (0.41 g)	Parkfield (0.35 g)	EPRM (0.95 g)	Oroville (0.41 g)	Oroville (0.41 g)
Failure Criterion	0	0	Failed (Earthquake Phase)	0	0
Damage Criteria	Fracturing Void Strain	0	Fracturing Void Strain	0	0
Permeability Criterion	0	0	0	0	0

Legend: X = None; * = Yes; 0 = Does not exceed criterion.

Very-near-field earthquakes, even of small magnitude, can be damaging to subsurface facilities because they are rich in short wavelength motions that are attenuated at greater distances.

In situ stress is a critical parameter in determining the subsurface effects of earthquakes. This parameter is, of course, nonexistent in evaluating the causes for surface damage. Model studies in which the horizontal stress was twice the vertical stress showed stability problems, even during the heating phase before the earthquake occurred. The state of in situ stress needs to be considered in the site selection process even though this is a difficult parameter to measure.

Model studies indicate stability problems with shales having the properties presented in the Generic Environmental Impact Statement (GEIS) for geologic storage of radioactive waste. Massive mudstones might be more stable.

TABLE 2. RESULTS FOR GRANITE COMPARED WITH DEFINED CRITERIA

Property	Computer Model Study, Granite							
	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8
Joint Geometry	AI	AI	AI	AI	AI	AI	AI	AI
Pore Pressure	X	X	X	*	*	X	X	X
In Situ Stresses	$\sigma H = \sigma V$	$\sigma H = \sigma V$	$\sigma H = 2\sigma V$	$\sigma H = \sigma V$	$\sigma H = \sigma V$	$\sigma H = \sigma V$	$\sigma H^1 = 2\sigma V$ $\sigma H^2 = \sigma V$	$\sigma H = 3/2\sigma V$
Fault	X	X	X	X	X	X	X	X
Thermal Loading	*	*	*	*	*	*	*	*
Earthquake Intensity (g = gravity unit)	Oroville (0.41 g)	Oroville (0.41 g)	Oroville (0.41 g)	Oroville (0.41 g)	Oroville (0.41 g)	ERPM (0.95 g)	Oroville (0.41 g)	Oroville (0.41 g)
Failure Criterion	0	0	Failed (before earthquake phase)	0	0	Failed (earthquake phase)	Failed (before earthquake phase)	0
Damage Criteria	0	0	Slip	0	0	Failed (earthquake phase)	Slip	0
Permeability	0	0	Exceeded	0	0	Exceeded	Exceeded	0

Legend: X = None; * = Yes; 0 = Does not exceed criterion; AI = Orthogonal joints at 45° to horizontal.

TABLE 3. RESULTS FOR SHALE COMPARED WITH DEFINED CRITERIA

Property	Computer Simulated Model Studies Case 1	Case 2
Joint Geometry	*	*
Pore Pressures	X	*
In Situ Stresses	H = V	H = V
Fault (No Fault)	X	X
Thermal Loading	*	*
Earthquake Intensity (g = acceleration of gravity)	Oroville (0.41 g)	Oroville (0.41 g)
Anisotropy	*	*
Failure Criterion	Failed (earthquake phase)	Failed (heating phase)
Damage Criteria	Slip Void-Strain	Slip Void-Strain
Permeability	Exceeded	Exceeded

Legend: X = None; * = Yes; 0 = Does not exceed criterion. Orthogonal joints with spacing of 1 m by 0.2 m at angle of 3° to horizontal.

WBS 1.1.2

Project: ONWI Support Program; Thermal Property Measurements

Principal Investigators: Oak Ridge National Laboratory (J. G. Moore and M. T. Morgan)

ONWI Project Manager: G. E. Raines

Objective

The objective of this program is to obtain accurate thermal data to be used in thermal analysis of possible repository sites. Methods and procedures will be established for making thermal property measurements, and data will be obtained on selected specimens of cores from possible repository sites and standard natural materials.

Progress Reported Previously

The report entitled *The Thermal Conductivity of Rocks in the Bureau of Mines Standard Rock Suite* was published in January.

Studies were started on methods for determining the thermal conductivity of fragmented and/or friable materials. A cell was devised that uses water as the secondary phase for measurements at temperatures less than 100 C. Initial measurements were inconsistent. A refrigerated heat exchanger was obtained for installation on the thermal conductivity instrument for more accurate measurements at the lower temperatures.

A computer program for determining the radial power loss in a cut-bar thermal conductivity apparatus was adapted for use with the Hewlett Packard 2647A computer.

Activities During the Reporting Period

Additional decade boxes were installed in the scanner of the thermal conductivity analyzer to allow more thermocouples to be used and to allow each of the six primary thermocouples to be parallel through two relays, one connection in reverse polarity. This procedure would cancel any biased EMF introduced in the scanner.

The thermal conductivity of Pyrex 7740, measured as a calibration check using Pyroceram 9606 as a reference, was 5 percent higher than the NBS value at 100 C.

The use of nickel powder in silicone grease between contact surfaces in the cut-bar stack failed to improve interfacial conductivity between metal, Pyroceram, and Pyrex. This material might still be of use for more porous surfaces.

Computer calculations of bypass heat flow to be used in correcting thermal conductivity measurements were completed. Approximately 900 tables were produced.

Thermal conductivity measurements were made on the Pyroceram 9606 disk being used as a comparative standard to calibrate thermal conductivity measurements. The results at 50 to 180 C were within 1 percent of values used for the ORNL Pyroceram 9606 reference meters, and 18 to 25 percent higher than values obtained at a subcontractor.Sections of the Pyroceram disk taken from the waste trim were prepared for laser diffusivity measurements to provide absolute thermal conductivity values. Results from ORNL measurements on the comparative standard using Pyroceram meters reserved for calibration checks averaged

$$k\ 2.5692 + 424.13/T\ (W/m{\cdot}K)$$

where T is in degrees Kelvin. Results from the top and bottom meters were within 3 percent of the average.

Graphite cloth was used by the subcontractor to improve thermal contact at interface surfaces in their apparatus. Pieces of graphite cloth have been received at ORNL and will be used in final measurements on the comparative standard.

WBS 1.1.4

Project: ONWI Support Program; Effects of Water in Salt Repositories

Principal Investigators: Oak Ridge National Laboratory (A. J. Shor, C. Canonico, C. F. Baes, Jr.)

ONWI Project Manager: J. F. Kircher

Objective

The objective of this program is to predict from experimental and modeling studies those consequences of the presence or the ingress of water to a salt repository that might compromise the integrity of the repository.

Progress Reported Previously

Following initial studies of salt deposition onto beds of salt crystals from flowing brine in a negative temperature gradient, studies of the isothermal consolidation of salt beds under uniaxial stress in flowing brine were begun. The initial results on consolidation of 1.27-cm columns could be represented adequately by the expression

$$\phi = 0.827 - 0.0627 \log ([\exp (0.046\, \sigma^0) - 1]\, t/z^2) \;,$$

where the observed void fraction ϕ is below 0.4, the applied stress σ^0 is in the range 20 to 155 bar, the root-mean-square particle size z is in the range 0.012 to 0.035 cm, and the time t is in minutes. The permeability of these beds was found to decrease considerably faster with the void fraction than is predicted by the Blake-Kozeny equation. A simple model was evolved for salt consolidation (based on the effect of pressure on salt solubility) which accounted approximately for the dependence of consolidation rate on the stress and the particle size, but failed to account for the time dependence.

The consolidation results from the 1.27-cm-ID column apparatus gave evidence of a wall effect, i.e., the void fraction was found to increase with distance from the (top) end of the salt column where the stress was applied. Consequently, a larger (2.54-cm-ID) column was built and used for additional measurements. These indicated that while a wall effect was still present, it was considerably smaller.

A microscope stage assembly was constructed for the observation of salt consolidation and deformation of salt crystals in brine and under stress.

An apparatus was fabricated to measure the permeability of a grain boundary between stressed crystal surfaces, and measurements began on the decrease of permeability with time.

Activities During the Reporting Period

Salt Consolidation

During this period a series of salt consolidation runs has been completed, in the larger apparatus (2.54-cm ID), for which the crystal size, the applied stress, and the length of the column were systematically varied. It has been found that the data for each run can be represented usually within experimental error by a three-parameter equation of the form

$$\phi = a - b \ln (c + t) .$$

Each run was fitted with this equation by a least-squares computer program and the resulting parameter values are summarized in Table 1. The values of a, b, and c obviously depend on the particle size, the stress applied, and the amount of salt in the column (a wall effect). But they also covary quite strongly with each other, and a model is needed to rationalize this general form of equation before the dependencies of these parameters on the independent variables can be assigned reliably.

At the end of each run producing a salt column consolidated well enough to section and sample, the distribution of brine was determined. The profiles of void fraction versus distance up the column (plotted in Figure 1) are seen to be linear within experimental error, confirming previous measurements on the smaller columns. The magnitude of the wall effect (the slope of these plots) seems to be greater the larger the particle size but not very dependent on the applied stress. It is planned to include this wall effect in the final treatment of the consolidation data by formulating an equation for the void fraction as a function of time, particle size, and stress,

$$\phi = \phi (t,z,\sigma) ,$$

and an equation that relates the stress at a distance x down the column to the applied stress σ^{o},

$$\sigma = \sigma(x,\sigma^{o}) .$$

The observed overall void fraction can be obtained from the integration

$$\phi = \frac{\int_{o}^{L} \phi dx}{L} ,$$

where L is the length of the column.

Consolidation runs were made with mixtures of the smallest (0.0075 to 0.015 cm) and largest (0.025 to 0.042 cm) crystal sizes. The results are compared with previous runs with the separate crystal sizes in Figure 2. The mixtures produced lower initial void fractions and the 50–50 wt % mixture produced the most rapid consolidation. Even a 4 wt % addition of the small crystals (about an equal number) to the large ones produced an appreciable lowering of the void fraction after a given time.

TABLE 1. SMOOTHING FUNCTION FOR VOID FRACTION OF 2.54-CM-DIAMETER COLUMNS OF SALT CRYSTALS STRESSED IN BRINE

$$\phi^0 = a - b \ln (c + t)$$

Crystal Size[a], cm	Applied Stress, bars	Weight of Salt, g	a	b	c, min	Standard Error of Fit[b]
0.0119	20	38	0.4745	0.025741	3.7	0.001
0.0119	20	75	0.4965	0.034934	10.2	0.009
0.0119	20	75	0.5047	0.032051	11.0	0.003
0.0119	155	38	0.4039	0.043011	2.0	0.005
0.0119	155	75	0.4501	0.044408	5.4	0.009
0.0119	155	75	0.4386	0.044613	3.9	0.008
0.0119	155	150	0.5010	0.048093	10.2	0.002
0.0164	20	75	0.5126	0.031142	56.7	0.004
0.0164	50	38	0.4868	0.035266	12.4	0.002
0.0164	50	75	0.5039	0.035119	16.1	0.002
0.0164	100	75	0.5226	0.045306	21.6	0.002
0.0164	1551	75	0.4477	0.040219	2.3	0.018
0.0217	50	75	0.4924	0.034544	41.4	0.003
0.0217	100	75	0.4808	0.036193	22.5	0.002
0.0346	20	38	0.4740	0.021195	51.1	0.002
0.0346	155	38	0.4151	0.031918	18.5	0.002
0.0346	155	75	0.5037	0.040568	44.2	0.005

(a) Root-mean-square particle size. The size ranges were 0.0075 to 0.0150 cm, 0.0150 to 0.0177 cm, 0.0177 to 0.0250 cm, and 0.0250 to 0.0420 cm.

(b) Standard deviation of the calculated from the observed void fraction.

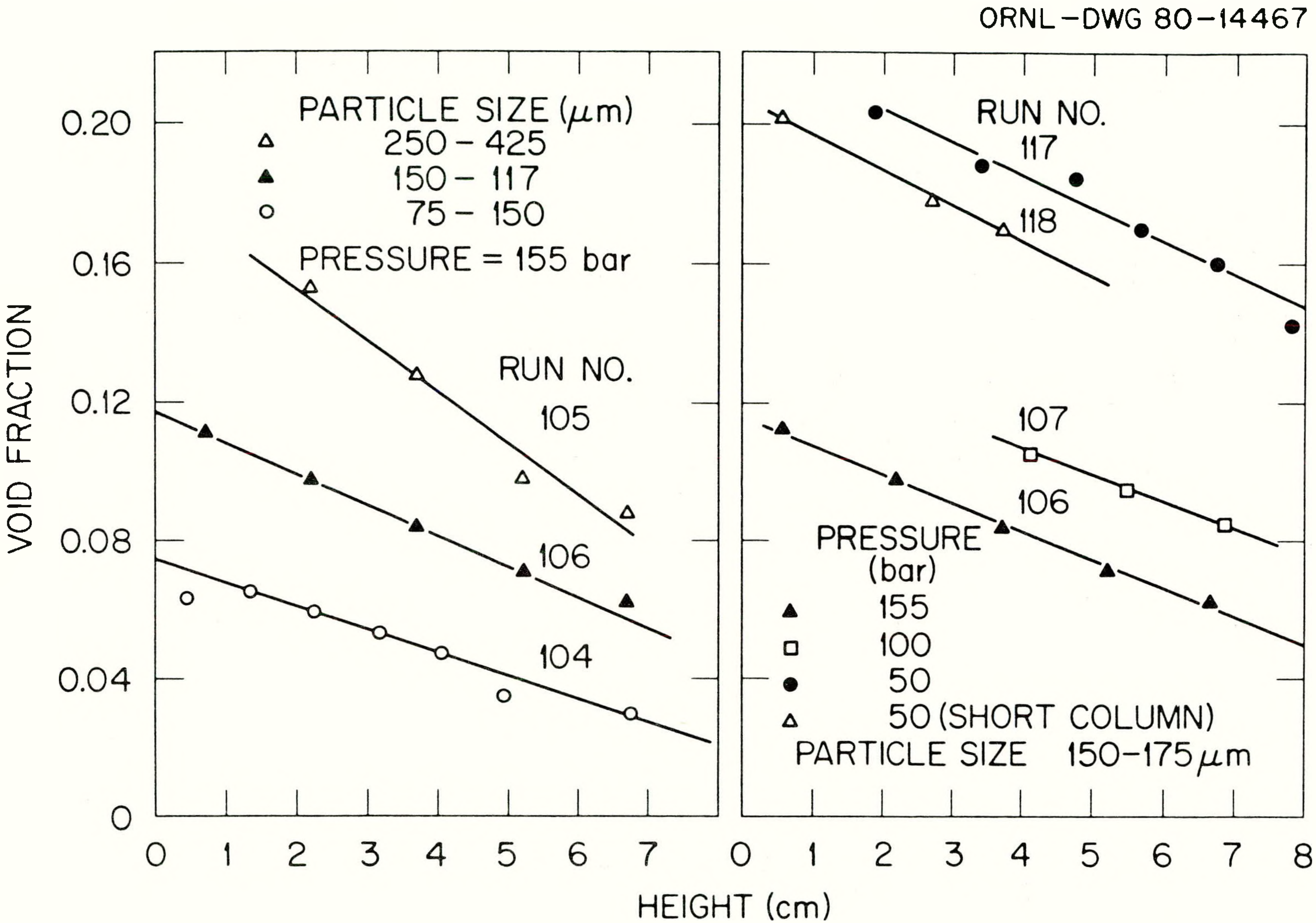


FIGURE 1. VOID FRACTION OF SALT COLUMNS VERSUS HEIGHT FOR VARIOUS PARTICLE SIZE RANGES AND APPLIED STRESSES

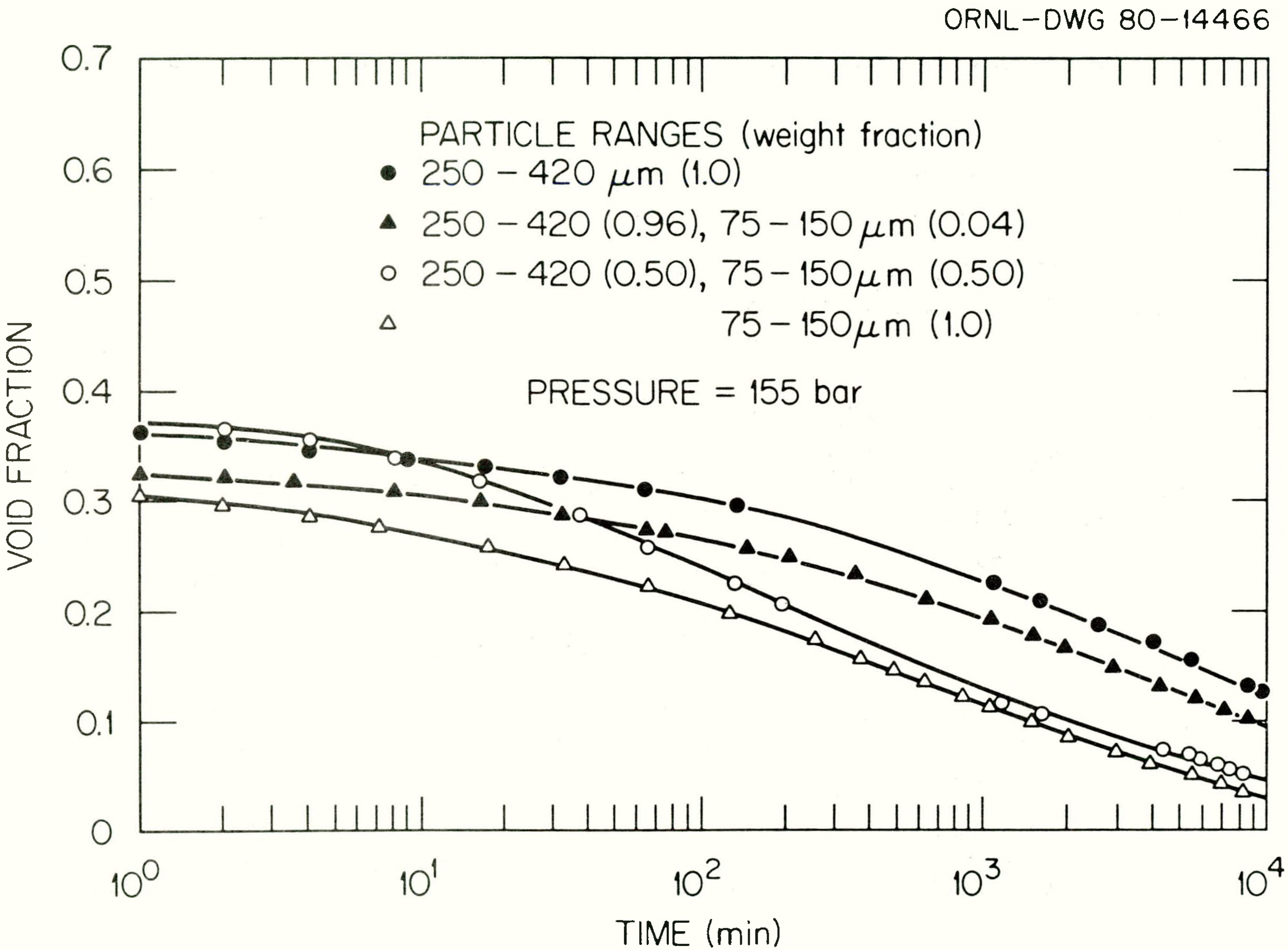


FIGURE 2. CONSOLIDATION OF COLUMNS OF SALT (2.5 CM IN DIAMETER) IN BRINES FOR VARIOUS COMBINATIONS OF PARTICLE-SIZE RANGES

A consolidation run was also made using a 5 molal $MgCl_2$ brine in which NaCl is much less soluble, and this considerably decreased the amount of consolidation.

Deformation of Salt Crystals in Brine

In studies with the microscope stage assembly, increasing uniaxial stress was applied stepwise over a period of hours to a salt crystal in brine. After each increase in the stress, the rate of deformation was initially rapid and then decreased almost to zero in a period of hours. The total strain showed a linear variation with stress in the range 94 to 329 bars (Figure 3). The amount and the rate of strain also seemed to depend on the rate at which the stress was applied. In Runs 112 and 113, the stress was applied more rapidly than in Run 111 and the resulting limiting smaller strains were reached much more rapidly. Also plotted in Figure 3 is the average behavior observed for aggregates of dry salt reported by Serata and Gloyna (1959).

Permeability of Grain Boundaries to Brine

The permeability of a single NaCl grain boundary was measured. Several tests were first performed to perfect techniques for sealing the salt crystals to the Monel surfaces. Epoxy cement proved to be satisfactory when exposed to saturated brine at pressure differences up to 10 bars.

Trials were conducted on single-crystal NaCl of optical quality. Crystal axes were colinear with the ram axis and closely fitted the ½-inch confining space. At first the opposed crystal faces were formed by cleavage; but better results were obtained later by dressing the surfaces using V block gages as guides to get a better fit between the surfaces. No temperature control was used at first and results were erratic. Thermostating of the entire unit at 20.0 C has led to improved results. Monel construction for all surfaces exposed to brine was found to be necessary and satisfactory.

Each succeeding refinement in procedure has led to a reduction in the measured permeation. Flow rates were measured while applying a steady axial pressure to the crystal faces of 75 to 125 bars and independently varying the pressure on the saturated brine from 2/3 to 7½ bars. It was demonstrated that measured permeation was nearly independent of brine pressure (i.e., flow was proportional to fluid pressure). On a longer time scale of days, permeation shows a steady decrease with time at constant conditions. This decrease is the expected result and demonstrates the "sealing" effect due to deformation and/or pressure solution. A more precise understanding and description of this phenomenon at a single well-defined crystal boundary is the purpose of this study.

Decreases in measured permeation with time, however, were not continuous as expected, but showed some discontinuities. These are currently attributed to the discontinuous wall seizure on the surface of the moving (upper) crystal. Modifications have been made in the apparatus to incorporate a Monel sleeve around the upper crystal to confine lateral forces on the NaCl due to creep caused by the axial pressure. This allows all of the axial pressure to be accurately applied to the crystal interface continuously.

Radial fluid flow between two circular plates is described by the transport relation of Bird, Stewart, and Lightfoot (1962).

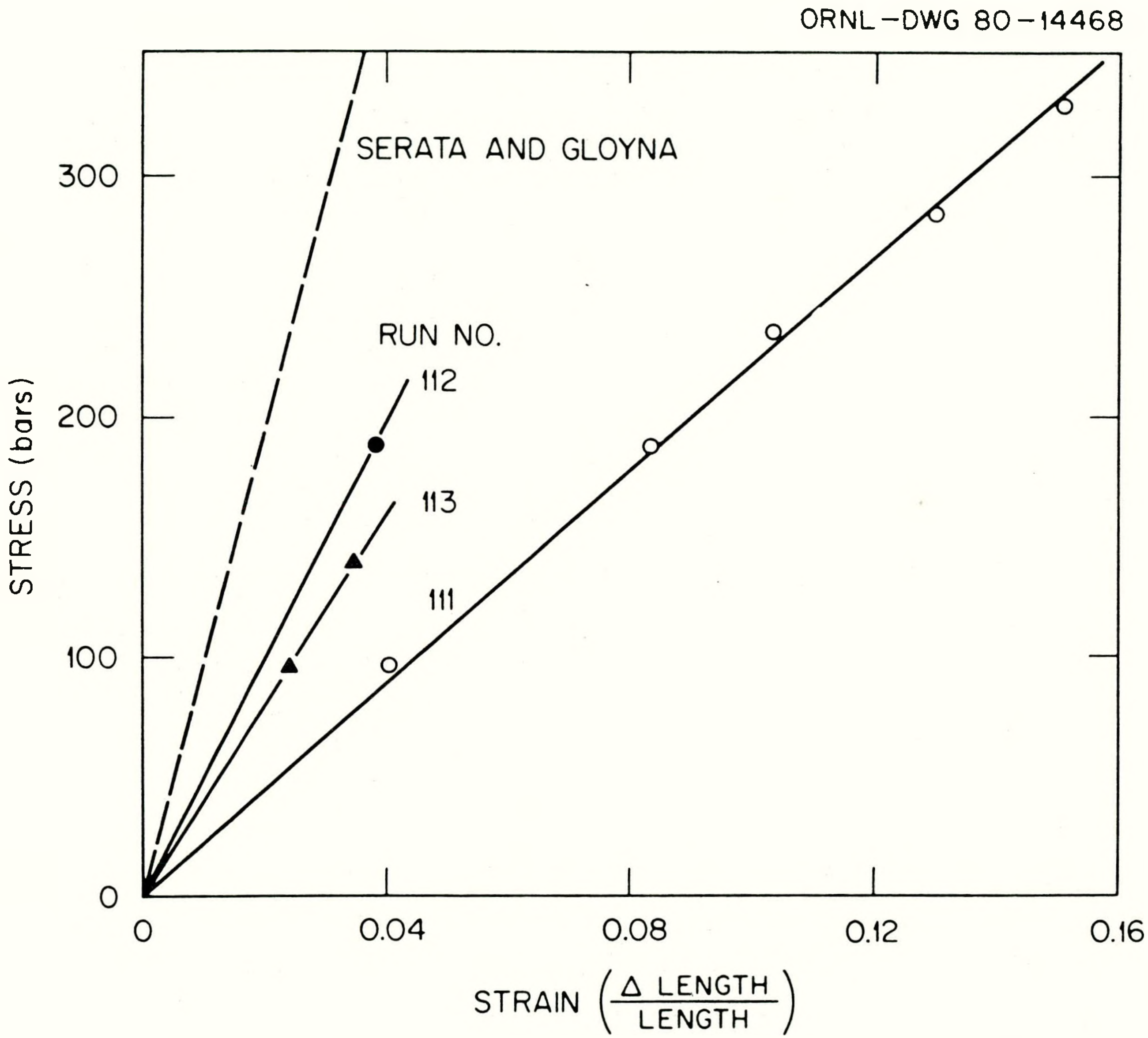


FIGURE 3. STRESS-STRAIN CURVE FOR A SALT CRYSTAL IN BRINE

$$Q = 4/3 \; \frac{\pi z^3}{\eta} \; \frac{(P - P_o)}{\ln \frac{r}{r_o}} \quad = \text{volume flow/sec,}$$

where z and η are the surface separations and viscosity of the fluid, while P and P_o represent the fluid pressure across the opening. The inner and outer radii of the salt surfaces are r_o and r. It is therefore possible to estimate the crystal separations from the experimentally observed viscous flow under controlled conditions.

Flow rates are observed to decline steadily with time at 20 C and an axial loading pressure on the surfaces of 75 and 124 bars. At these conditions the permeation is approaching the experimental limit of detection at a driving pressure of 7 bars in 24 hours of integrated flow (~0.00015 ml).

This study is continuing, with automated data collection now being adapted to the equipment. Pressure effects on the interface and the effects of temperature on the rates of change of permeability of salt-crystal boundaries are now being examined.

REFERENCES

Bird, R. B., W. E. Stewart, and E. N. Lightfoot. 1962. *Transport Phenomena,* John Wiley, New York, p. 114.

Serata, S., and E. F. Gloyna. 1959. "Reactor Fuel and Waste Disposal Project", A.E.C. Contract AT (11-1)-490.

WBS 1.1.2

Project: Bench-Scale Salt Creep Tests, Phase III

Principal Investigator: South Dakota School of Mines and Technology (W. H. Grams)

ONWI Project Manager: M. M. Lemcoe

Objective

The objective of this program is to provide bench-scale, time-dependent deformation information on samples of dome-type rock salt. These data will be used by other research groups to check existing computer codes or models which were based upon laboratory-scale testing.

Progress Reported Previously

Laboratory-scale testing of photoelastic coating on rock salt has been done. Good correlation was found between strain gage and photoelastic testing. Bonding of the birefringent material over long periods of time does not seem to be a problem.

The biaxial load frame has been fabricated, assembled, and checked out. No problems were found when assembling the unit, although care must be taken because of the large size and weight of the individual components.

Activities During the Reporting Period

Final analysis of the photoelastic testing was complete. Continued efforts were made to remove the large blocks of salt from the mine.

WBS 1.1.2

Project: Transient Creep in Rock Salt

Principal Investigator: Texas A & M Research Foundation (M. Friedman)

ONWI Project Manager: M. M. Lemcoe

Objective

The objectives are to (a) develop a transient creep constitutive relation for rock salt based on operative deformation mechanisms, (b) measure, experimentally, additional flow variables required for evaluating transient creep theories, and (c) determine the deformation mechanisms during transient and steady-state creep.

Activities During the Reporting Period

Transient-Creep Laws

A nonlinear least-squares-fitting program has been written for the HP 9825 programmable desk computer. It is based on similar programs written earlier to fit steady-state-creep data and constant-strain-rate data (see Parrish and Gangi, 1977 and 1981).

The program assumes that the strain (creep) curves can be represented by functions of the form:

$$e(t) = e_o + \sum_{m=1}^{M} e_{Tm} (1 - e^{-r_m t}) + \dot{e}_{ss} t \qquad (1)$$

where

e_o = elastic strain

e_{Tm} = transient-creep strain associated with creep mechanism

r_m = its rate constant = $1/T_m$

T_m = the time constant for the transient-creep mechanism

$\dot{e}_{ss}$ = the steady-state-creep rate.

This equation can be derived if it is assumed that: (1) each mechanism is independent of every other one and each has its own constitutive equation, and (2) first-order kinetics hold for each mechanism; that is, the rate of change of the strain rates of each mechanism is proportional to the strain rate of that mechanism (Gangi, 1981). This latter assumption also means that the differential form of each constitutive equation is linear so that superposition can be used. This, in conjunction with the first assumption, leads to the condition that the total strain of the material is just the sum of all the strains due to each mechanism.

The steady-state strain rate may be an artifact of the experimental procedure and not a true property of the material. If a mechanism has a time constant (call it T_m) that is long relative to the duration of the experiment or test, it can appear to give "steady-state" behavior because

$$e_{Tm}\,(1-e^{-t/T_m}) \simeq e_{Tm}[(t/T_m) - 0.5(t/T_m)^2]$$

$$\simeq (e_{Tm}/T_m)t \quad \text{if} \quad (t/T_m) << 1 \qquad (2)$$

where the "steady-state strain rate" would then be

$$\dot{e}_{ss} = e_{Tm}/T_m = r_m e_{Tm}.$$

The nonlinear, least-squares-fitting program was used to fit creep data from WIPP site, experimentally deformed rock salt specimens obtained from Sandia Laboratories. Data were supplied for three deformed specimens (9-2624, 9-2677, and 9-2668) and portions of each specimen, along with an undeformed specimen (9-2671), for textural and fabric characterization. Experimental conditions are given in Tables 1 and 2. Results of the creep data curve fitting are given in Table 1 and plotted in Figures 1 through 4. The first column (M) of the table gives the number of (transient) mechanisms fitted to the data. The next column (S.S.) has a Y (for yes) if steady-state flow is assumed and an N (for no) if there is no steady-state flow in the fitting function. When more than one mechanism is fitted and no steady-state flow is assumed, the product $e_{T2}r_2$ is inserted in the $\dot{e}_{ss}$ column. This value is generally close to the previous $\dot{e}_{ss}$ value if the rate constant, r_2, is small compared with the reciprocal of the experiment's duration. Note, for the first two experiments, that this product is quite different from the fitted values of $\dot{e}_{ss}$ (by a factor of 10 in the first experiment and by factors 2 to 3 in the second one) and the r_2 values are large (between about 5 and 10 Khr^{-1}) compared with the $1/t_E$ values (about 1.6 and 3.3 Khr^{-1}, respectively) of the experiments. On the other hand, the $e_{T2}r_2$ value for the third experiment (35.3 mstr/Khr) differs by only about 20 percent relative to the fitted value of $\dot{e}_{ss}$ (30.7 mstr/Khr); in this case, the r_2 value (0.276 Khr^{-1}) is small compared with the $1/t_E$ value (1.6 Khr^{-1}). The same is true for the last experiment, where $e_{T2}r_2$ (1060 mstr/Khr) is about 25 percent larger than the fitted $\dot{e}_{ss}$ value (782 mstr/Khr) and the r_2 value (2.83 Khr^{-1}) is fairly small relative to the $1/t_E$ value (6.7 Khr^{-1}).

From the results of the first experiment, it can be seen that fitting two transient mechanisms instead of one transient mechanism and steady-state flow causes a big change in the e_{T1} and r_1 values (0.632 versus 0.380 and 21.9 versus 67.6, respectively) but little change in the e_o value (0.589 versus 0.536). When two mechanisms and steady-state flow are fit to the data, almost no change occurs in the e_o value (0.536 to 0.534) and only small changes occur in the e_{T1} and r_1 values (0.380 to 0.311 and 67.6 to 86, respectively). Large changes occur in the e_{T2} and r_2 values (0.602 to 0.499 and 4.98 to 8.56, respectively). This identical pattern can be seen to hold for the second experiment (C2).

The rms errors of the fit, E (in millistrain), is given in the last column for each case. In both of the first two experiments, significant changes in the rms error are obtained when two mechanisms are fit, rather than just one mechanism and steady-state flow. The improvement in the fit is also apparent from the curves plotted in Figures 1 and 2. The improvement in rms error is not great when the "two-mechanism plus steady-state-flow" fit is made. This is also seen from the plotted data and fitted curves.

TABLE 1. RESULTS OF CREEP DATA CURVE FITTING

M	S.S.?	e_o(mstr.)[a]	e_{T1}(mstr.)	r_1(Khr^{-1})	e_{T2}(mstr.)	r_2(Khr^{-1})	e_{ss}(mstr/Khr)	E(mstr.)
Experiment 9-2677 T = 22 C P = 20.63 MPa $\Delta\sigma$ = 7.79 MPa t_E = .65 Khr N = 17								
1	Y	0.589±.026?	0.632±.038	21.9±.3	—	—	.460±.0001	.033
2	N	0.536±.010?	0.380±.047	67.6±5.1	0.602±.026	4.98±.012	$(e_{T2}r_2=3.00)$	.012
2	Y	0.534±.020?	0.311±.101	86±17	0.499±.061	8.56±.16	0.247±.0003	.009
Experiment 9-2677; T = 22 C; P = 20.69 MPa; $\Delta\sigma$ = 23.10 MPa; t_E = 0.30 Khr; N = 22								
1	Y	4.18±.54?	9.27±.75	54.7±.2	—	—	60.4±.01	.98
2	N	3.07±3.25?	5.88±.50	380±18	28.0±3.5	4.79±.001	$(e_{T2}r_2=134)$	.46
2	Y	3.06±22.7?	5.37±.82	461±41	12.1±38.4	10.24±.04	35.4±.36	.45
Experiment 9-2624; T = 100 C; P = 3.45 MPa; $\Delta\sigma$ = 7.41 MPa; t_E = .65 Khr; N = 39								
1	Y	1.25±.22?	6.83±.39	10.10±.01	—	—	30.71±0.01	.20
2	N	1.27± ?	5.73±7.2	11.71±.03	128±73,000	0.276±.001	$(e_{T2}r_2=35.3)$	.20
Experiment 9-2688; T = 200 C; P = 20.69 MPa; $\Delta\sigma$ = 6.90 MPa; t_E = .15 Khr; N = 21								
1	Y	2.36±1.4?	25.9±3.4	48.83±.05	—	—	782.0±.3	1.28
2	N	0.68± ?	14.22±3.6	142.1±1.4	374±3,300	2.82±.001	$(e_{T2}r_2=1060)$	1.24

(a) 1 mstr. = 1 millistrain = .001 m/m

TABLE 2. OBSERVATIONAL DATA ON UNDEFORMED AND EXPERIMENTALLY DEFORMED WIPP ROCK SALT

Specimen	Deformation Conditions	Grain Size[a] X/s, mm (N)[b]	Grains Containing Intragranular Cubic Inclusions[a], % (N)	Polygonized Grains[c], % (N)	Free Dislocation Density[c], cm^{-2} (N)	Evidence of {110} Slip[c], (N)	Bubble Density, cm^{-2} (N)	Grain Boundary Bubble Size[a], $\bar{X}$/s, mm (N)	Tube Length $\bar{X}$/s, mm (N)
W9-2671	Experimentally Undeformed	3.9/2.5 (25)	85 (62)	10 (10)	10^6 (10)	None (10)	4×10^5 (14)	0.01/.01 (91)	0.17/.15 (40)
W9-2624	$\Delta\sigma$ = 1075 psi; T = 100 C P_c = 500 psi; t = 650 hr e = 2.8%	3.5/2.2 (25)	39[d] (95)	None (10)	10^7 (10)	Yes (10)	7×10^5 (19)	0.01/.01 (234)	0.12/.08 (78)
W9-2677	$\Delta\sigma$ = 1130 psi; T = 22 C; t = 670 hr $\Delta\sigma$ = 3350 psi; T = 22 C; t = 320 hr $\Delta\sigma$ = 4800 psi; T = 22 C; t = 130 hr P_c = 3000 psi e = 13%	4.4/1.7 (25)	56[d] (55)	10 (10)	10^7 (10)	Yes (10)	4×10^5 (20)	0.01/.006 (317)	0.14/.08 (98)
W9-2668	$\Delta\sigma$ = 1000 psi; T = 200 C P_c = 3000 psi; t = 165 hr e = 15.2%	4.3/2.1 (25)	60 (80)	80 (10)	10^6 (10)	Yes (10)	3×10^5 (23)	0.01/.01 (222)	0.06/.06 (126)

(a) Determined from thin section.
(b) N is sample size, $\bar{X}$ is the mean, and s is the standard deviation.
(c) Determined from etched cleavage faces.
(d) Intragranular cubic inclusions greatly reduced in size.

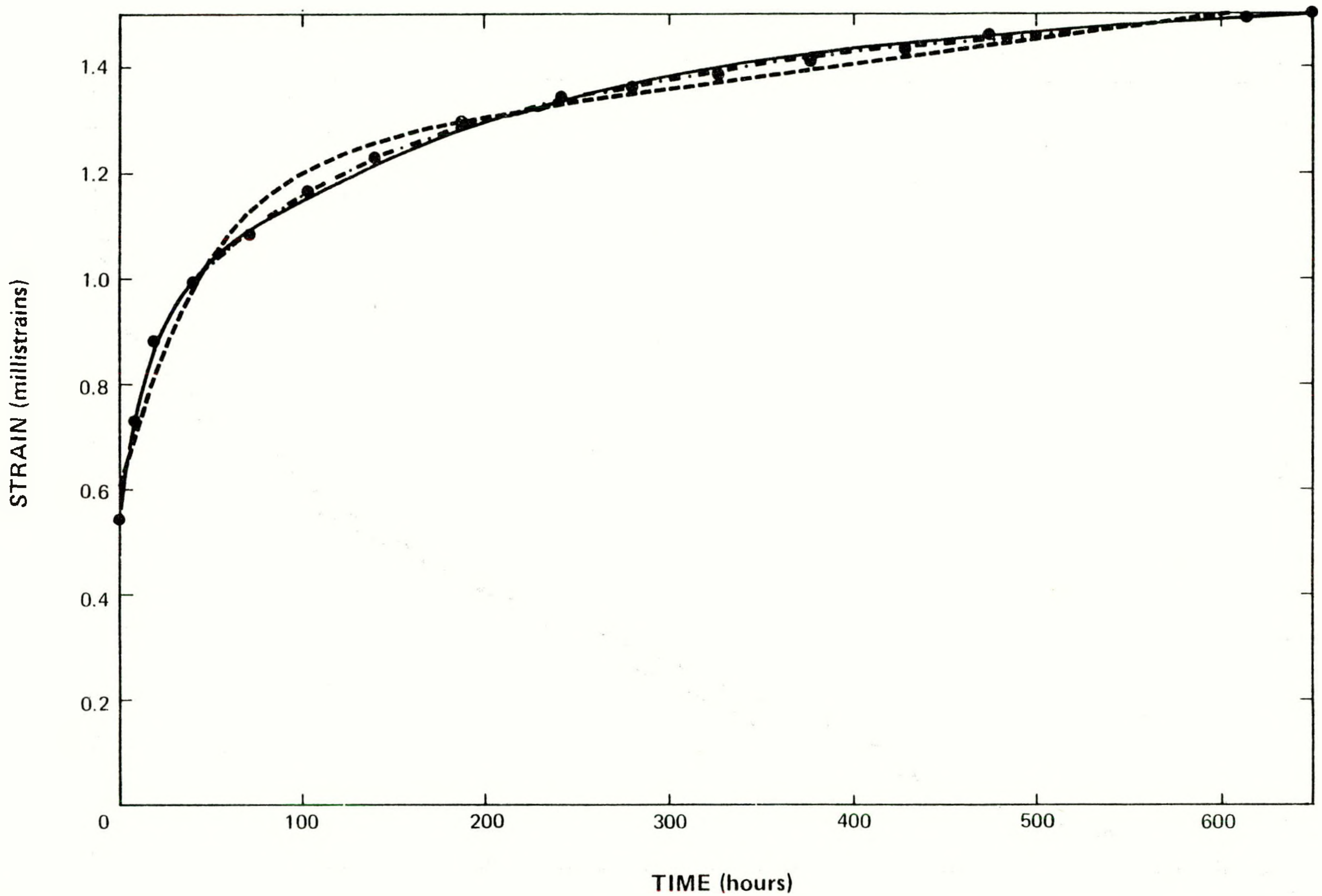


FIGURE 1. LEAST-SQUARES FIT TO DATA FOR EXPERIMENT 9-2677 RUN AT 22 C, 20.7-MPA CONFINING PRESSURE, FOR 670 HOURS AT A DIFFERENTIAL STRESS OF 7.8 MPA

Solid dots are the experimental data. Dashed curve is a fit to one transient mechanism plus steady-state flow; solid curve is a fit to two transient mechanisms; dot-dash curve is a fit to two transient mechanisms plus steady-state flow. See Table 1 for parameter values.

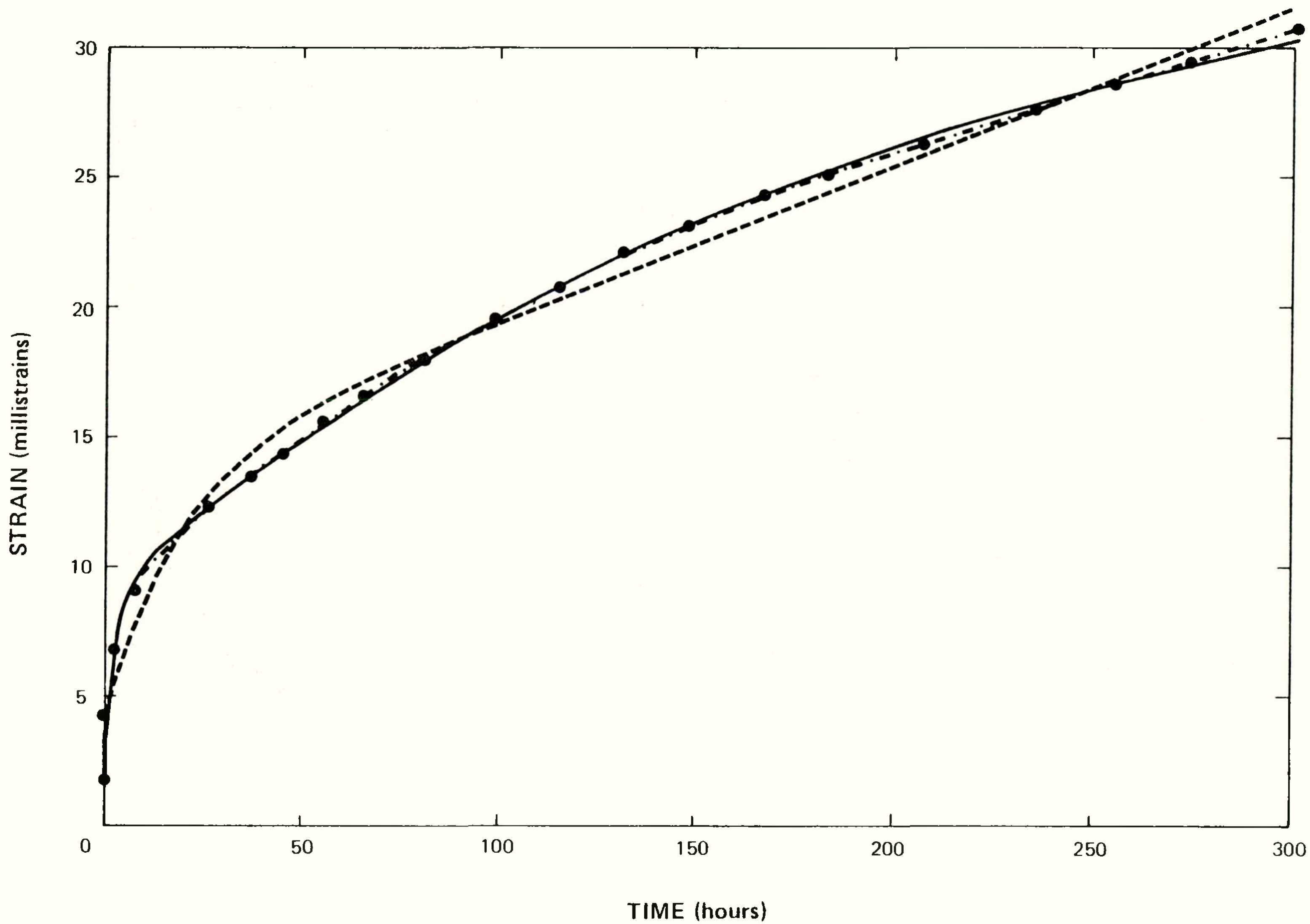


FIGURE 2. LEAST-SQUARES FIT TO DATA FOR EXPERIMENT 9-2677 RUN AT 22 C, 20.7-MPA CONFINING PRESSURE, FOR 320 HOURS AT A DIFFERENTIAL STRESS OF 23.1 MPA

Definition of dots and the three types of curves is same as in Figure 1. See Table 1 for parameter values.

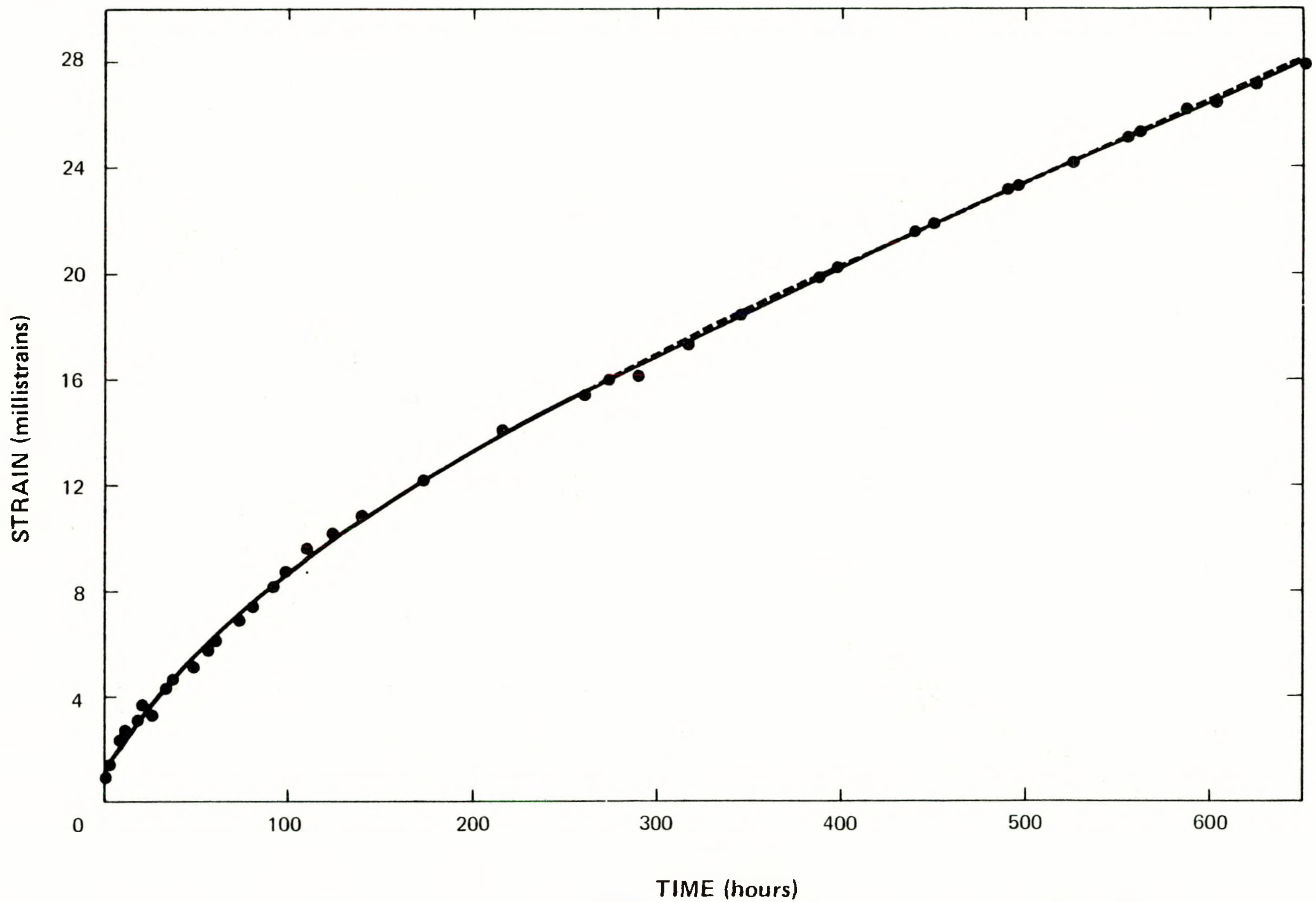


FIGURE 3. LEAST-SQUARES FIT TO DATA FOR EXPERIMENT 9-2624 RUN AT 100 C, 3.5-MPA CONFINING PRESSURE, FOR 650 HOURS AT A DIFFERENTIAL STRESS OF 7.4 MPA

Solid dots and solid and dashed curves have same definition as in Figure 1. See Table 1 for parameter values.

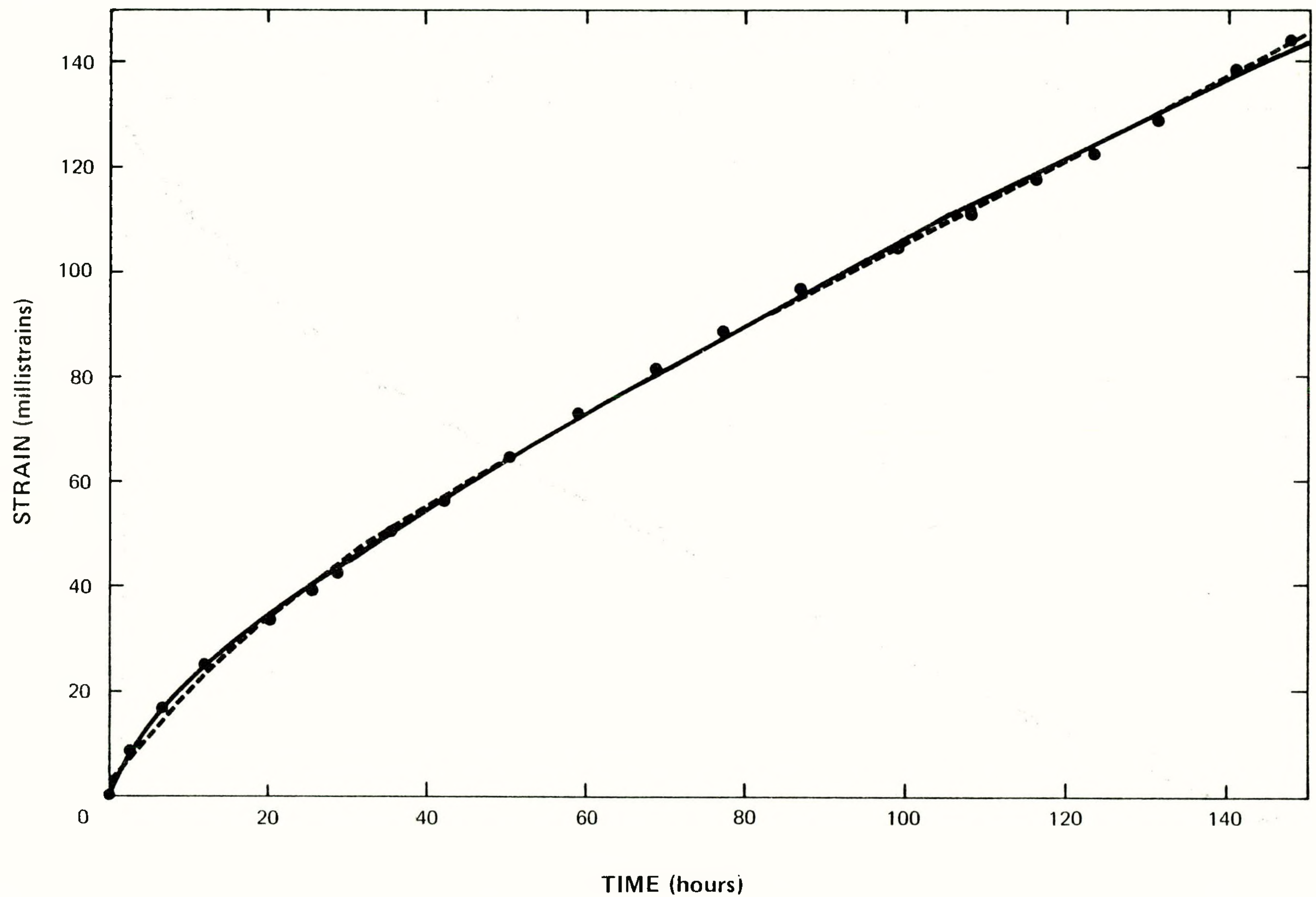


FIGURE 4. LEAST-SQUARES FIT TO DATA FOR EXPERIMENT 9-2688 RUN AT 200 C, 20.7-MPA CONFINING PRESSURE, FOR 165 HOURS AT A DIFFERENTIAL STRESS OF 6.9 MPA

Solid dots and solid and dashed curves have same definition as in Figure 1. See Table 1 for parameter values.

It is clear both from Table 1 and Figures 3 and 4 that no improvement is made by assuming two transient mechanisms instead of only one mechanism and steady-state flow for these experiments. There is little difference in the rms errors (E) and the variations of the e_{T2} parameters (in particular) become very large. This is a manifestation of the fact that the duration of the experiments is too short to conclusively extract the parameters of the second transient mechanism.

The rms deviations of the parameters have been determined using the method suggested by Bevington (1969). This method assumes that ". . . the variation of the squared error with respect to each parameter is independent of the values of the other parameters (at least near the minimum) . . ." and this is not a valid assumption for these fitting functions. Nevertheless, they give some idea of the expected variation in the parameters. In particular, it is difficult to obtain the rms deviation for e_o because we compute the parameter Σe_{Tm} ($e_{To} \equiv e_o$) and get a value (assuming the above independence holds) for e_o by subtracting the squares of the deviations of all the e_{Tm} from that of the sum to obtain an estimate of the squared deviation of e_o. Again this assumes no correlations and is obviously incorrect because in two instances (in the last two experiments) the rms deviation for the sum was smaller than that of just one of the terms, namely, that of e_{T2}.

The correlations of parameters may also explain the unusually low (unrealistically so) rms deviations for the rate parameter, r_2, in the experiments.

These "rms deviations" are reported even though they have obvious shortcomings, because they do provide some insight into how the variations vary with different fitting functions and because they probably are good approximations for e_o, $\dot{e}_{ss}$, e_{T1}, and r_1.

Clearly, the fits between the theoretical curves and the experimental data are excellent. The most interesting point of these fits is that steady state appears to be an approximation to another transient mechanism—one that has a long relaxation time ($T_M = 1/r_M$) relative to the duration of the experiment.

Synthetic Rock Salt Specimens

Synthetic cylinders of pure rock salt are being prepared routinely by filling a 20-cm-long by 3.8-cm-diameter polyolefin, thermo-shrink-tube with granular salt, inserting the tube into the pressure vessel, evacuating, raising the temperature to 100 C, and applying 150-MPa confining pressure for 15 minutes. The density of these "warm-pressed" specimens is 98 to 99 percent of the density of a single crystal of halite. The sintered aggregate is easily cored and polished into right-circular cylinders for deformation tests. Sixteen such billets from which two cylindrical specimens each are obtained were made during this reporting period. Texture and fabric data of this "starting material" are listed in Table 3, discussed later.

Experimental Deformation

Thirty-three successful experiments were made during this quarter with stress relaxation data obtained at the end of five of the tests. Of the 33 experiments, 20 were on specimens of synthetic pure rock salt and 13 were on specimens composed of specific homogeneous mixtures of halite and anhydrite. The former were run at temperatures of 100, 200, and 300 C,

TABLE 3. OBSERVATIONAL DATA ON UNDEFORMED AND EXPERIMENTALLY DEFORMED WARM-SINTERED, SYNTHETIC ROCK SALT SPECIMENS[a]

Specimen	Deformation Conditions P_c (MPa)	T (C)	ϵ (%)	Average Grain Size, $\overline{X}$/s, mm (N)[b]	Axial Ratio, $\overline{X}$/s (N)	Grains Containing Intragranular Cubic Inclusions, % (N)	Abundance of Intragranular Cubic Inclusions, % (N)	Polygonized Grains, % (N)	Average Polygonized Subgrain Size, $\overline{X}$/s, mm (N)	Dislocation Density, cm^{-2}, (N)	Bubble Density, cm^{-2}, (N)	Grain Boundary Average Bubble Size, $\overline{X}$/s, mm (N)	Tube Length $\overline{X}$/s, (N)
CV85	Undeformed			0.30/.011 (25)	1.55/.004 (25)	80 (100)	12 (100)	11[d] (100)	(d)	10^7 (10)	2×10^6 (25)	.003/.002 (220)	.027/.02 (100)
812	100	100	10	0.39/.015 (25)	1.44/.003 (25)	82 (100)	6 (100)	37[d] (100)	(d)	10^7 (10)	1×10^6 (25)	.004/.003 (200)	.037/.02 (100)
819	100	200	10	0.39/.013 (25)	1.53/.004 (25)	33[c] (100)	< 1 (100)	79 (100)	.017/.01 (25)	10^7 (10)	1×10^6 (25)	.005/.002 (232)	.029/.01 (100)
816	100	300	10	0.37/.016 (50)	1.61/.004 (50)	1[c] (100)	trace (100)	97 (100)	.023/.01 (25)	10^7 (10)	1×10^6 (25)	.005/.002 (241)	.031/.01 (100)

(a) All data determined from thin section study.
(b) N is sample size, X is the mean, and s is the standard deviation.
(c) Intragranular cubic inclusions are greatly reduced in size.
(d) Only incipient polygonization. Subgrains formed have incomplete (not closed) boundaries.

at confining pressures of 50, 100, and 200 MPa, and at a strain rate of 10^{-4} sec^{-1}. The latter were run at 200 C, confining pressures of 100 and 200 MPa, and also at 10^{-4} sec^{-1}. All specimens are cylindrical, 2.5 cm in diameter and 5 cm long. The stress-shortening curves in Figures 5-9 illustrate pertinent results, first for the pure halite specimens and then for the halite-anhydrite ones. Stress relaxation data have not been analyzed to date, although time was spent determining machine stiffness in preparation for that analysis.

With extreme care taken to manufacture identical starting material and to duplicate each step in the experimental procedure, satisfactory reproducibility of the experimental data (Figure 5) has been achieved. Occasionally, however, an anomalous result will occur (Figure 6, strongest specimen, solid curve, at 100 C). In general, the reproducibility is sufficient for all practical purposes.

The effects of temperature and confining pressure on the pure halite specimen are shown in Figures 6, 7, and 8. Ultimate strength is enhanced by confining pressure and decreased by increasing temperature, as expected. The confining-pressure, strengthening effect diminishes with increasing temperature and all but vanishes at 300 C (Figure 6).

Work is being done on homogeneous mixtures of halite and anhydrite. The purpose is to evaluate the influence of anhydrite composition on the strength and ductility of impure rock salt. This work should be completed by late August. Figure 9 shows the influence of composition on ultimate strength as determined at 100-MPa confining pressure, 200 C, and a strain rate of 10^{-4} sec^{-1}. Clearly, strength decreases with increasing halite content, but the addition of the first 25 percent of halite produces the most dramatic change. This trend can be explained by a shift in the dominant deformation mechanism from slip and polygonization in the halite to cataclastic flow in anhydrite with increasing anhydrite content. An increase in ductility with increasing halite content has also been observed at 10-MPa confining pressure.

Structural Characterization of Starting Materials and Experimentally Deformed Specimens

Textural and fabric data were obtained on specimens of WIPP site rock salt (Table 2) and on a suite of experimentally deformed warm-sintered, synthetic specimens (Table 3). These data permit comparison of the sintered specimens with the undeformed and experimentally deformed naturally occurring ones from WIPP.

WIPP Specimens. Examination of Table 2 and corresponding photomicrographs in Figures 10 through 14 indicates the following major points:

(a) The undeformed starting material contains abundant intragranular cubic inclusions (Figure 10a, b), a very few polygonized grains (Figure 11a), and no evidence of $\{110\}\langle 1\bar{1}0\rangle$ slip. It has recovered largely from any natural deformation.

(b) All deformed specimens show evidence of $\{110\}\langle 1\bar{1}0\rangle$ slip (Figure 12).

(c) Specimen 2668, deformed at 200 C, shows evidence of slip plus recovery (polygonization [Figure 11b] and somewhat reduced dislocation density). This would suggest that a two-mechanism constitutive equation should fit the creep data for this specimen better than a one-mechanism equation. Gangi's (1981) analysis (Table 1 and Figure 4) shows, however, that the one- and two-mechanism fits for this specimen are about the same.

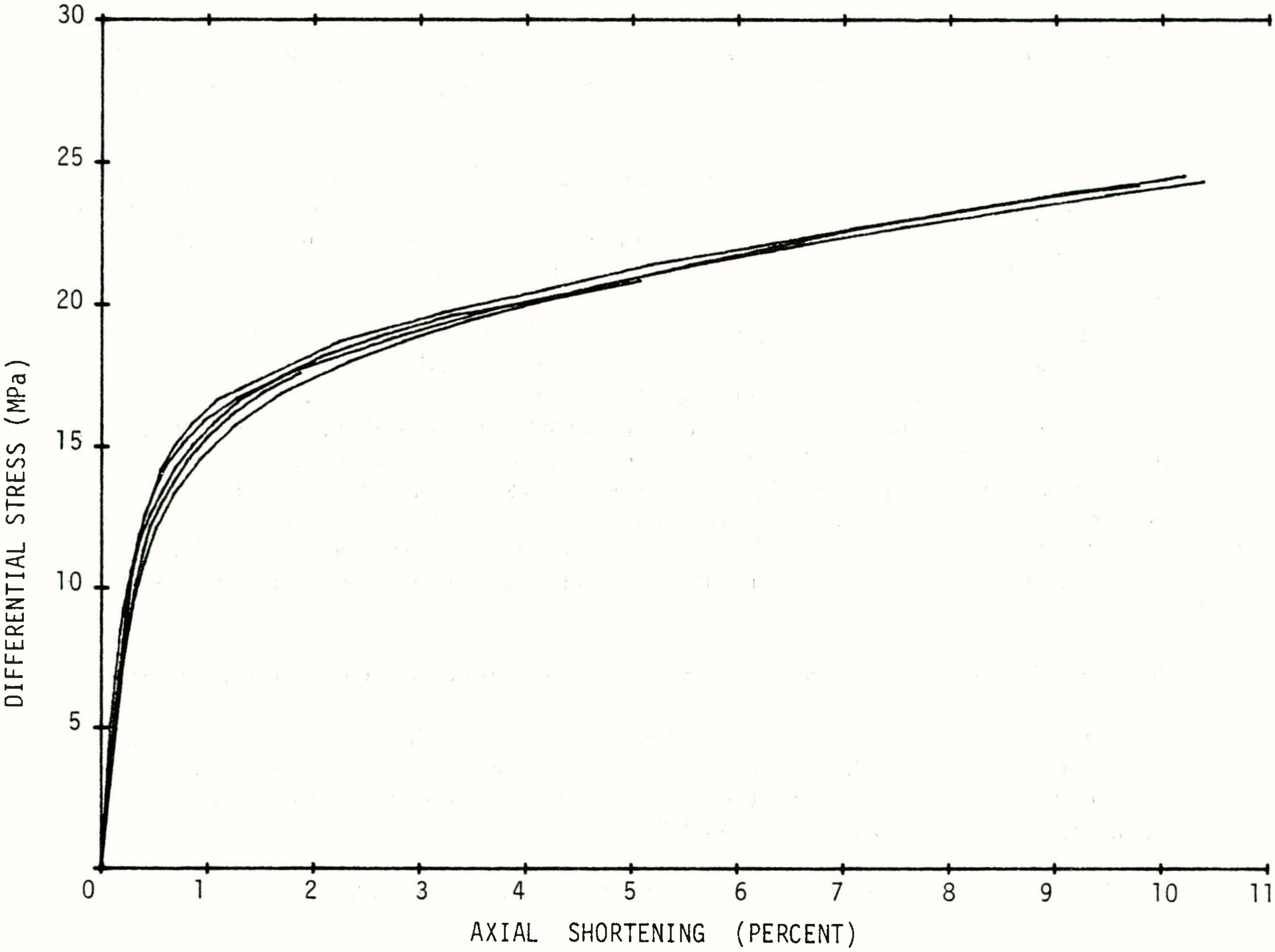


FIGURE 5. FIVE STRESS-SHORTENING CURVES SHOWING DEGREE OF REPRODUCIBILITY FOR SYNTHETIC SPECIMENS OF ROCK SALT DEFORMED AT 200-MPA CONFINING PRESSURE, 100 C, AND A STRAIN RATE OF $10^{-4}sec^{-1}$

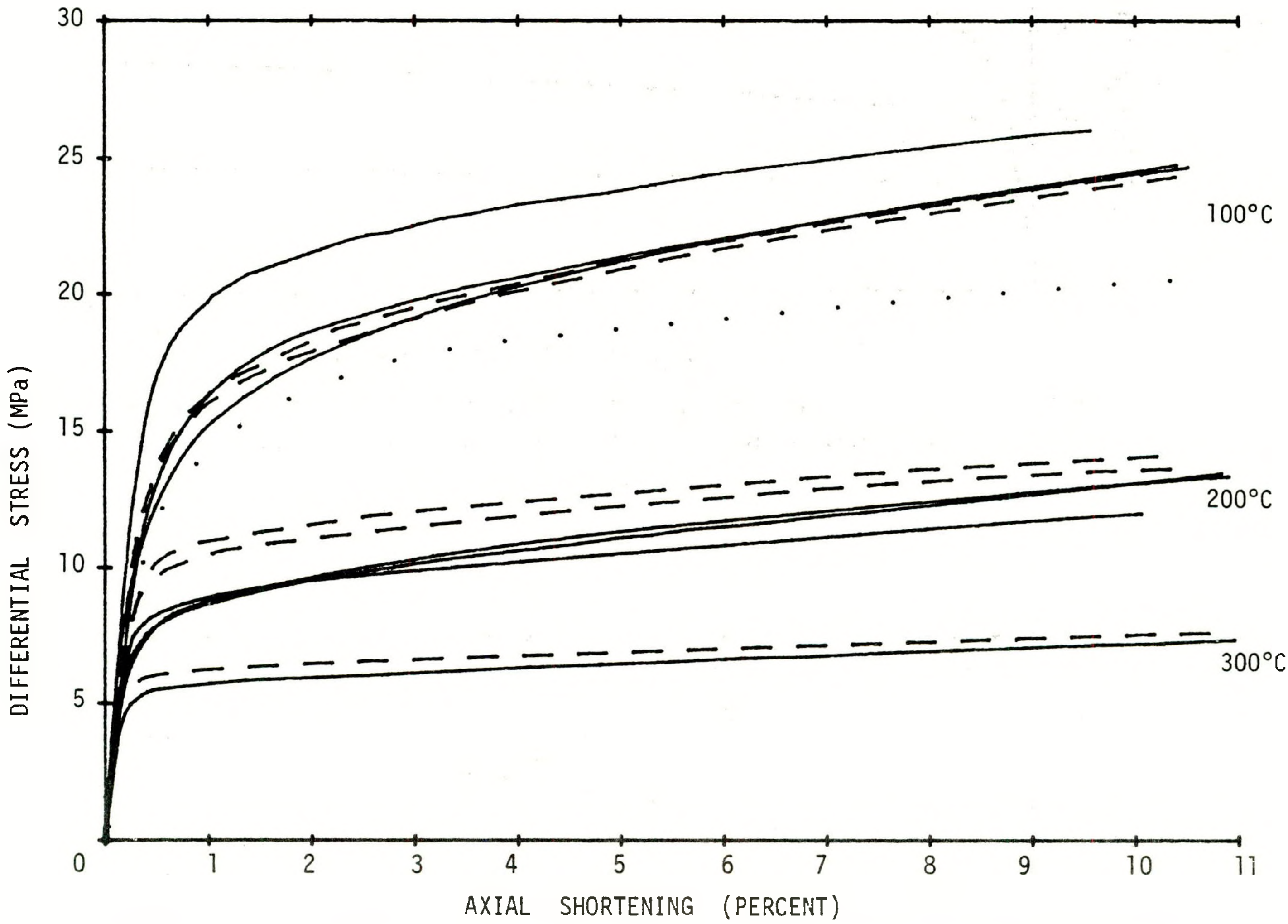


FIGURE 6. STRESS-SHORTENING CURVES FOR SYNTHETIC SPECIMENS OF PURE ROCK SALT SHOWING EFFECTS OF TEMPERATURE AND PRESSURE ON ULTIMATE STRENGTH

Six curves are given at 100 C, five at 200 C and 2 at 300 C. Dashed curves are for 200-MPa confining-pressure runs; solid curves are for those at 100 MPa; and dotted curves are for runs at 50 MPa. All data are for a strain rate of $10^{-4} sec^{-1}$.

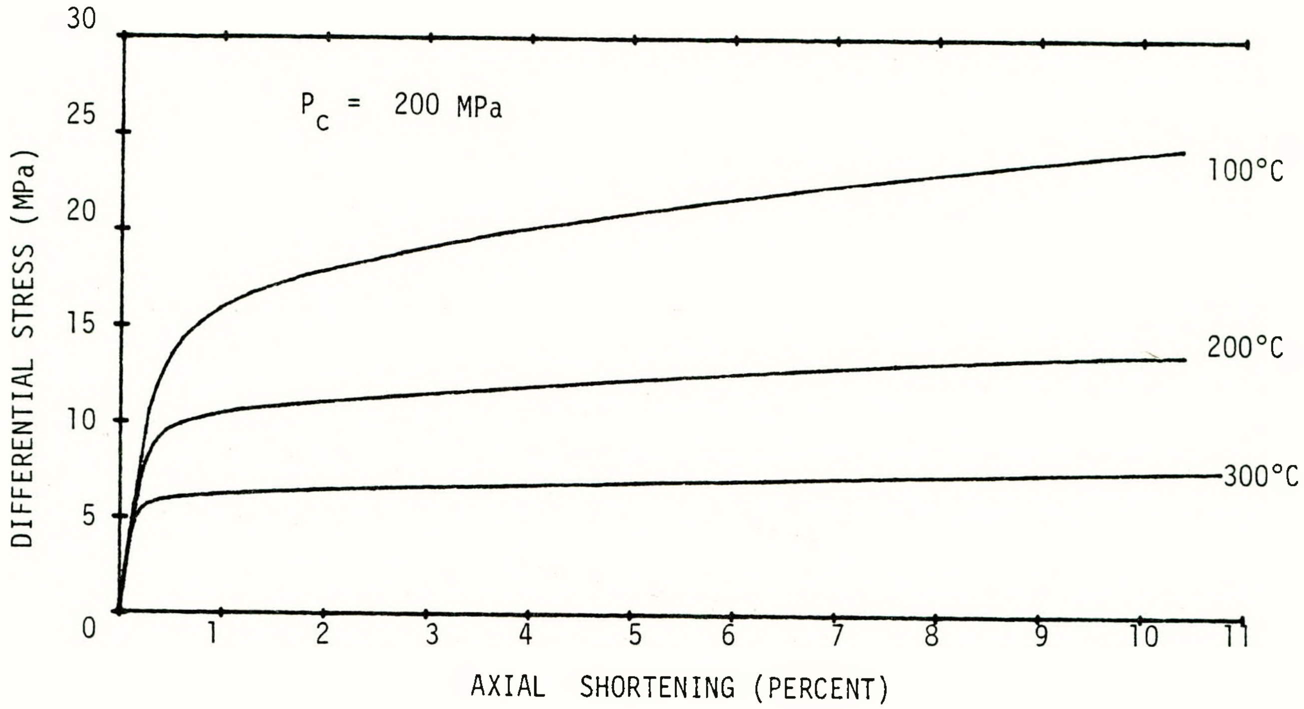


FIGURE 7. STRESS-SHORTENING CURVES SHOWING EFFECT OF TEMPERATURE AT 200-MPA CONFINING PRESSURE AND A STRAIN RATE OF $100^{-4}sec^{-1}$

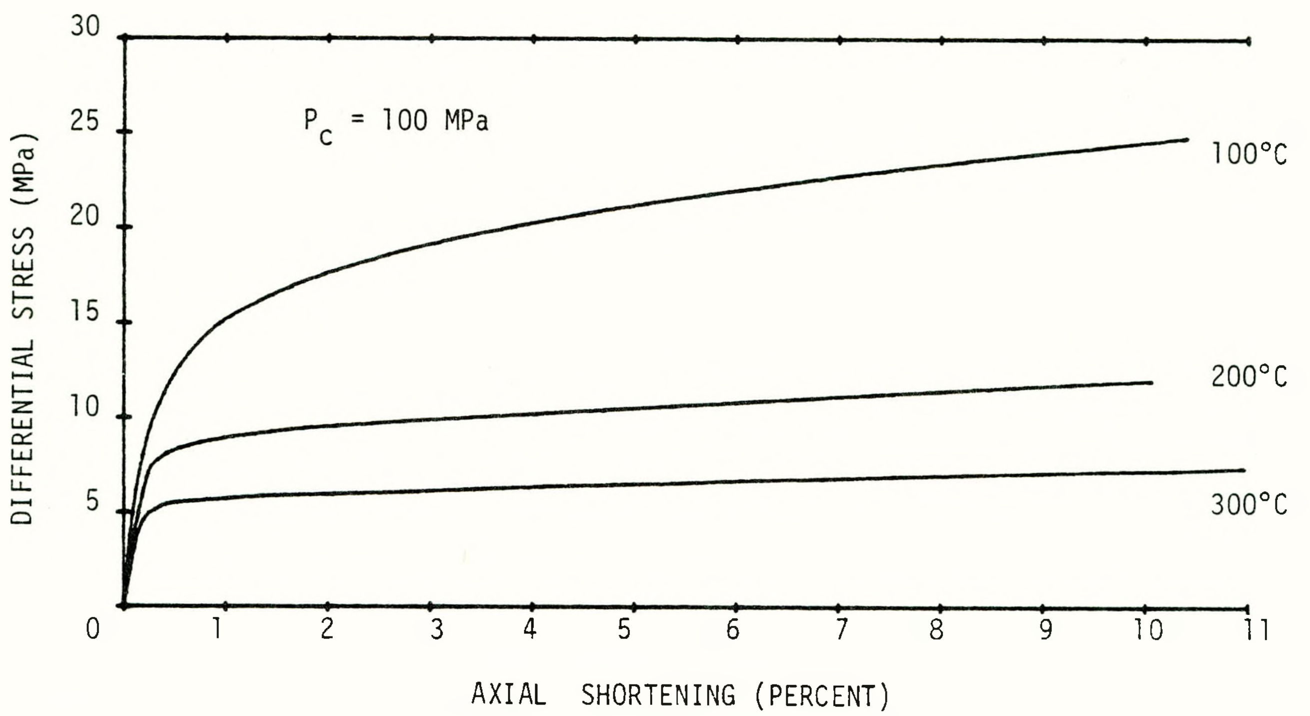


FIGURE 8. STRESS-SHORTENING CURVES SHOWING EFFECT OF TEMPERATURE AT 100-MPA CONFINING PRESSURE AND A STRAIN RATE OF $10^{-4}sec^{-1}$

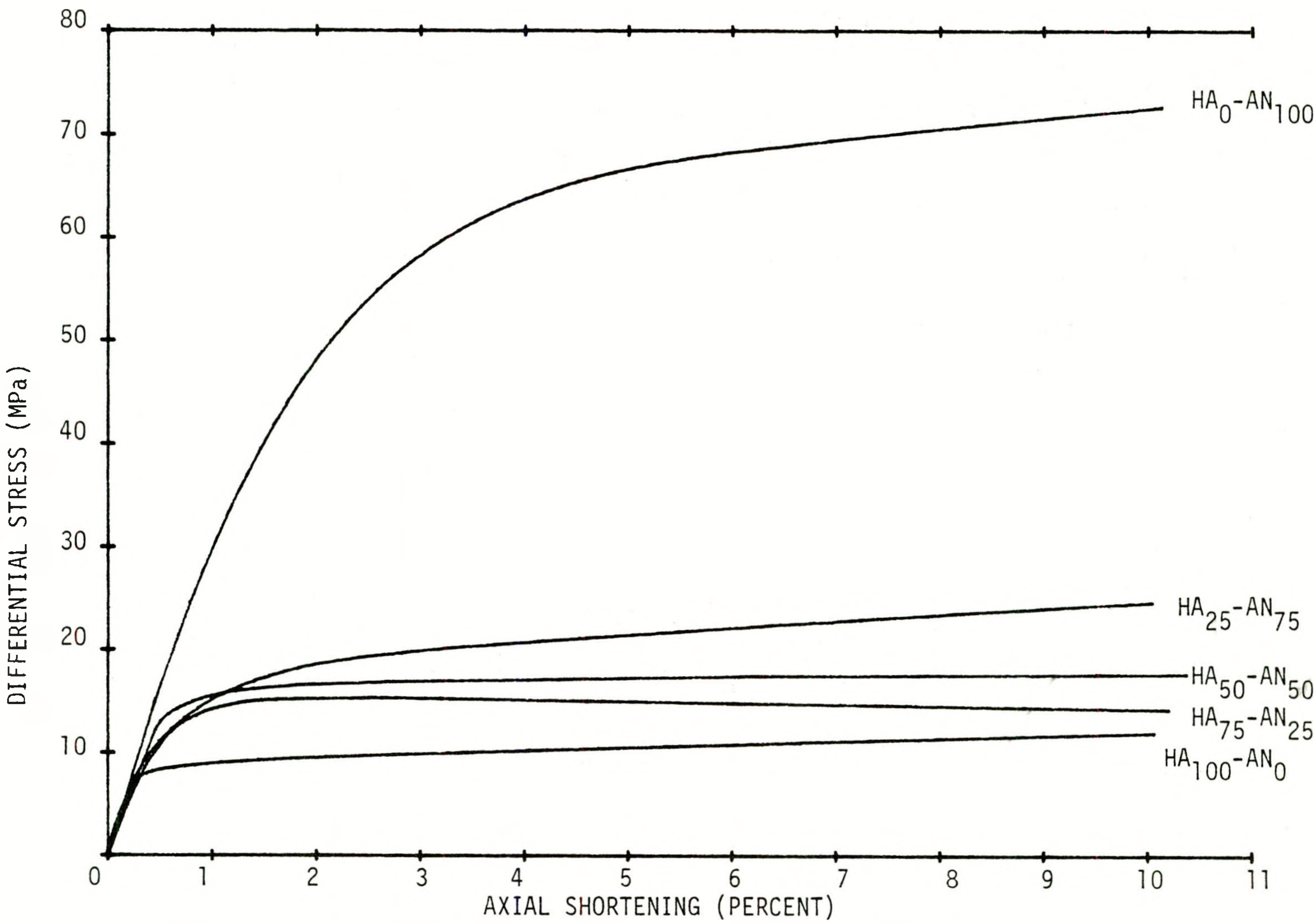


FIGURE 9. STRESS-SHORTENING CURVES FOR SPECIMENS OF VARIOUS HALITE (HA) AND ANHYDRITE (AN) COMPOSITION DEFORMED AT 100-MPA CONFINING PRESSURE, 200 C, AND A STRAIN RATE OF $10^{-4}sec^{-1}$

HA_0-AN_{100} means that the specimen is composed to 100 percent anhydrite.

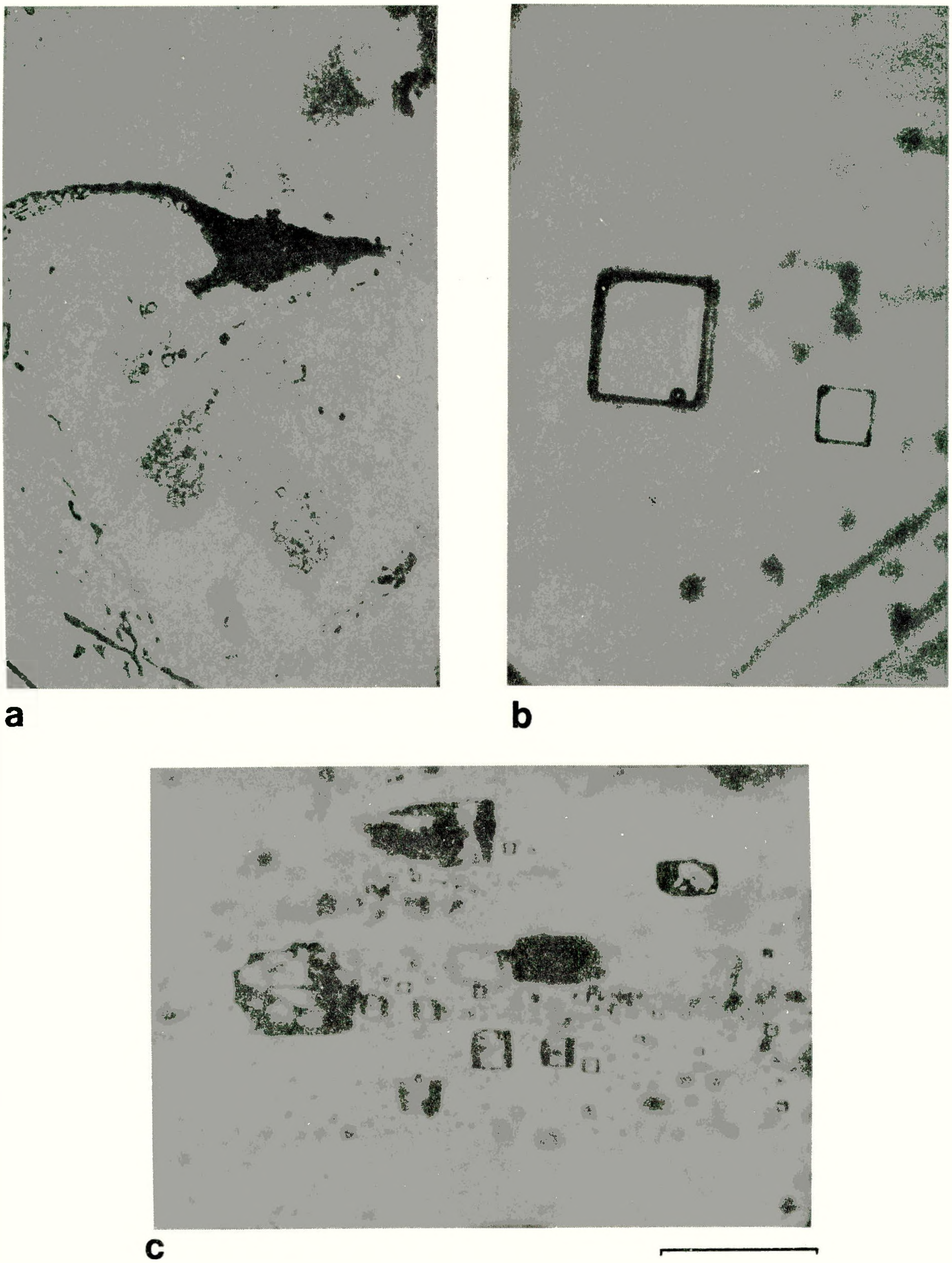
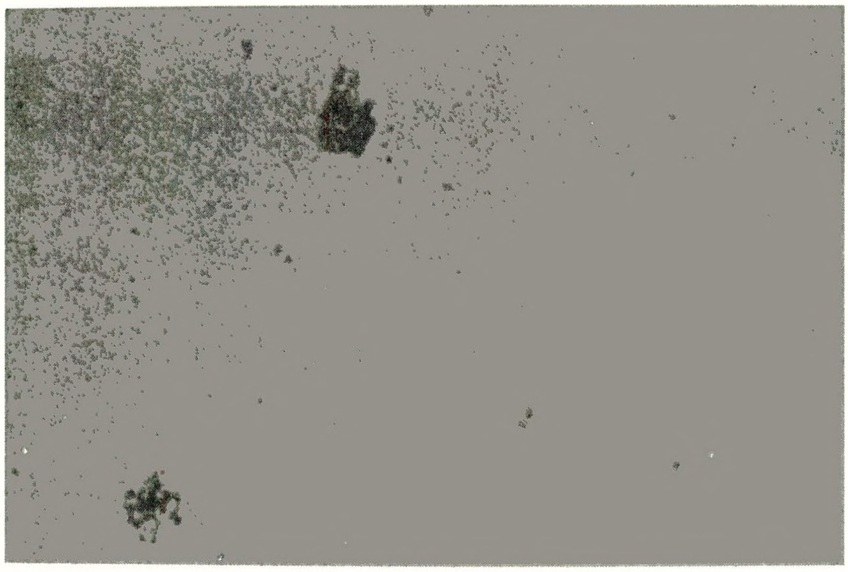
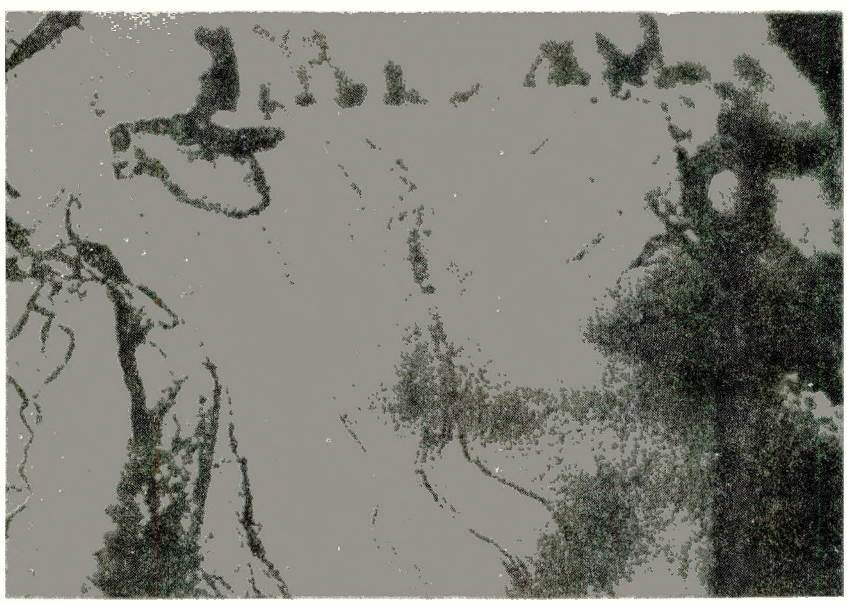


FIGURE 10. PHOTOMICROGRAPHS OF INTRAGRANULAR CUBIC INCLUSION
(Photos a and b are undeformed specimen 2671)

Photo a is an overview of inclusion development; photo b shows that each inclusion contains a small bubble of fluid. Photo c is deformed specimen 2688. Photo shows restored cubic inclusions (see text), also with internal bubbles. Scale line is 0.8 mm for a, and 0.1 mm for b and c. Plane polarized, transmitted light.



a



b

FIGURE 11. PHOTOMICROGRAPHS OF FRESHLY CLEAVED AND ETCHED SURFACES SHOWING DEVELOPMENT OF POLYGONIZATION

Photo a shows relatively rare polygonization in undeformed material, specimen 2671. Photo b shows typical polygonization development in deformed specimen 26 2668. Scale line is 0.025 mm for a and 0.25 mm for b. Plane polarized, transmitted light.

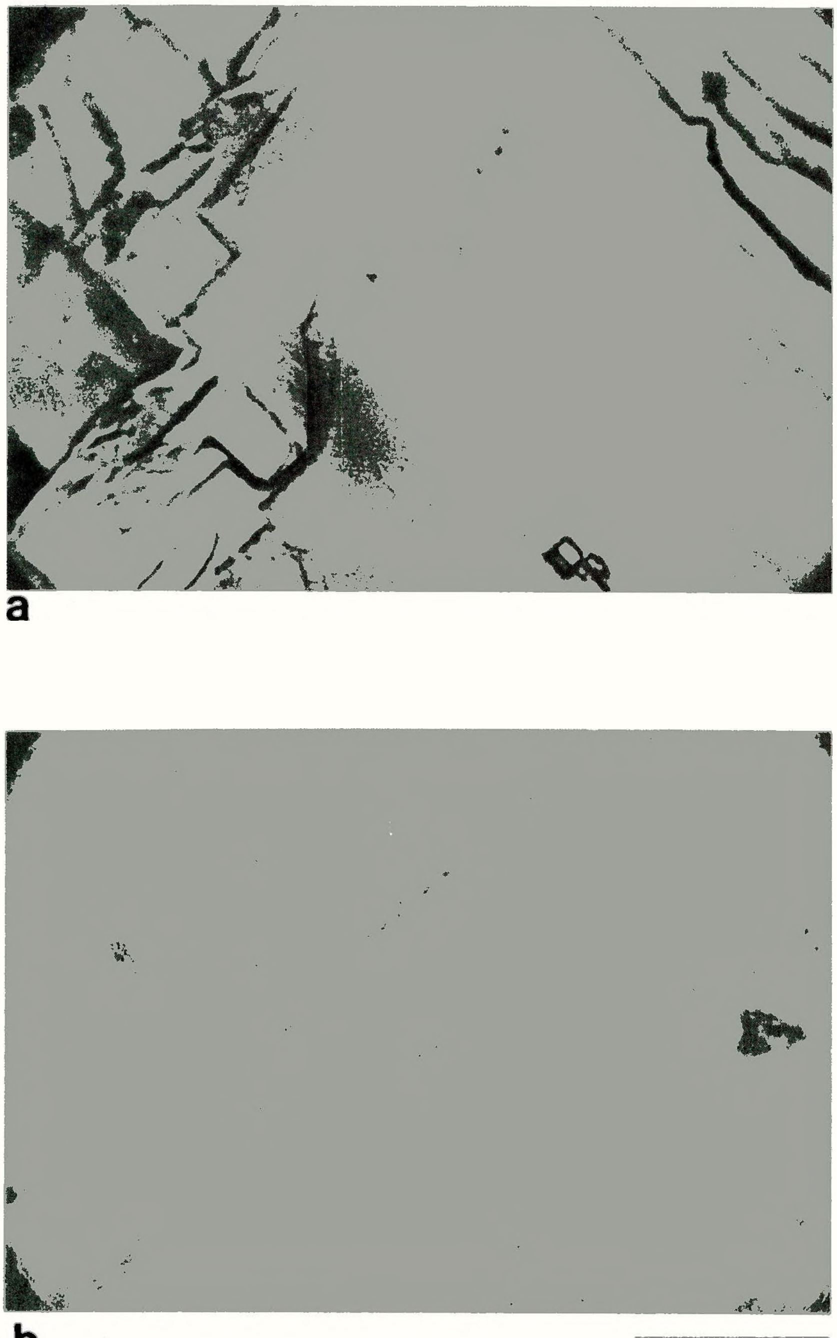


FIGURE 12. PHOTOMICROGRAPHS OF FRESHLY CLEAVED AND ETCHED SURFACES SHOWING TRACES OF $\{110\}$ $<1\bar{1}0>$ SLIP LINES IN SPECIMEN 2677

On photo a, one set of slip traces (parallel to long axis of photo) makes 45 angle to 100 cleavage (see left side of field of view). In photo b, two sets of slip lines intersect at 90. Scale line is 0.25 mm for a and 0.025 mm for b. Plane polarized, transmitted light.

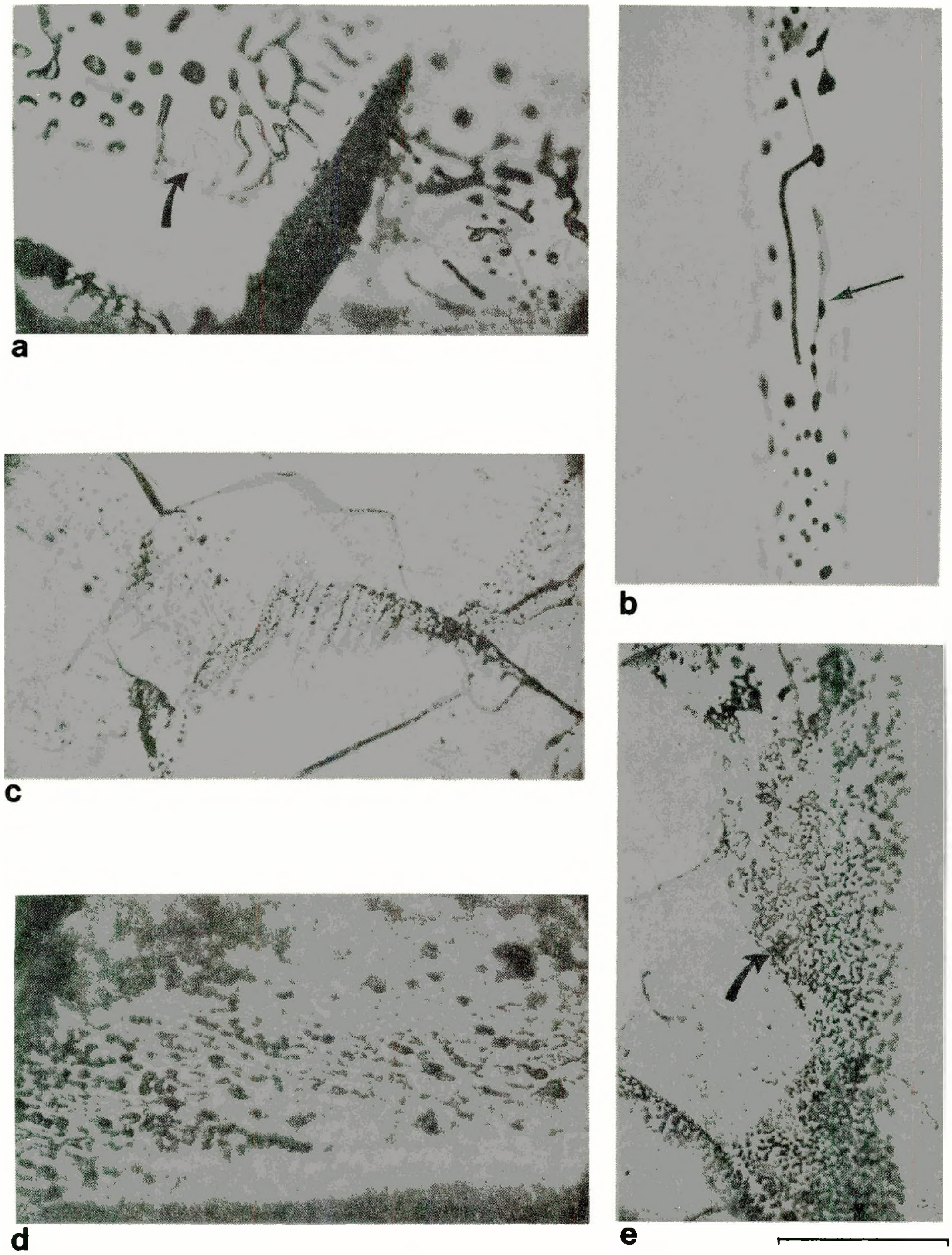


FIGURE 13. PHOTOMICROGRAPHS OF GRAIN-BOUNDARY BUBBLES AND TUBES

Photos a and b are undeformed specimen 2671. Details of the bubbles and tubes are shown, some of the latter are filled with fluid (darker ones) and some are empty (curved arrow). Note in b the meniscus within tube (straight arrow). Photo c is deformed specimen 2677. Photo shows aligned bubbles as well as randomly distributed ones along several grain boundaries. Photo d is deformed specimen 2624. Photo shows aligned, connected tube with internal segments filled with fluid (dark portions). Photo e is deformed specimen 2677. Photo shows patches of coalesced, fully connected tubes (curved arrow). Scale line is 0.1 mm for a, b, and d and 0.3 mm for c and e. Plane polarized, transmitted light.

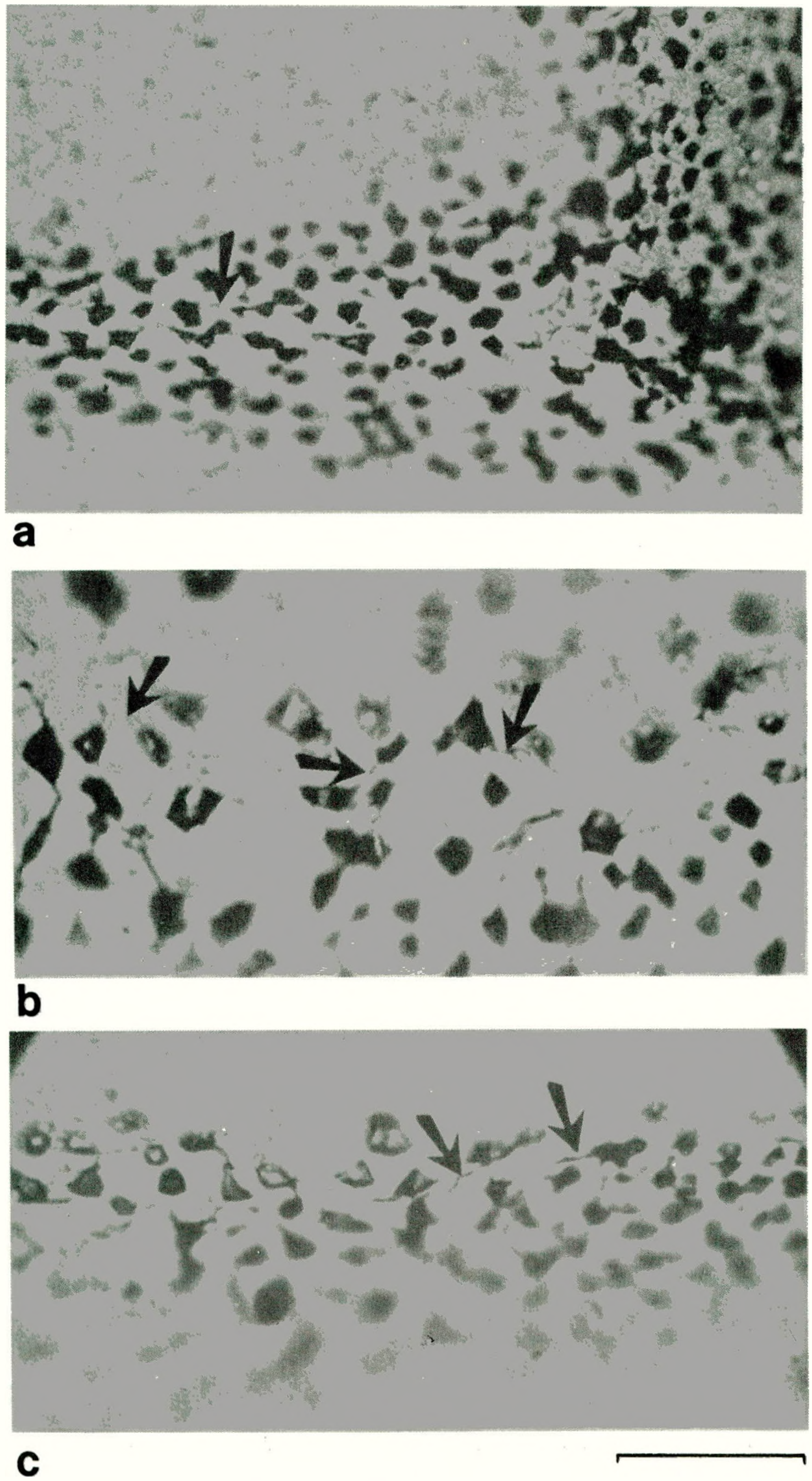


FIGURE 14. PHOTOMICROGRAPHS OF "HYDRAULICALLY FRACTURED", GRAIN-BOUNDARY BUBBLES IN EXPERIMENTALLY DEFORMED SPECIMEN 2668

Photo a is overview of grain boundary with irregularly shaped bubbles. Photos b and c details of a show bubbles are connected by thin fractures (arrows). Subsequent enlargement by solution could produce the enhanced connectivity shown in Figure 6 c and d. Scale line is 0.25 mm for a and 0.1 mm for b and c. Plane polarized, transmitted light.

(d) The intergranular cubic-fluid inclusions are decreased in number and size by the deformation. In specimens 2624 and 2677, they not only occur in fewer grains but are much smaller than in the undeformed counterpart. In specimen 2688 they are back to original size (Figure 10c). This also may reflect the recovery of this specimen.

(e) Although the grain-boundary textures do not appear very different according to the quantitative textural data (Table 2, last three columns), there are significant differences between undeformed and deformed specimens (Figure 13). These differences suggest that grain-boundary permeability may be significantly modified by deformation. This could be important relative to containment of liquid wastes. Changes due to deformation include (1) alignment of bubbles and tubes (Figure 13c, d), (2) some reduction in tube size (Table 2, last column), and (3) increased tube and bubble connectivity (Figure 13e). Changes 1 and 2 would tend to decrease grain-boundary permeability while change 3 would enhance it. Permeability measurements on selected specimens before and after experimental deformation were recommended to Sandia. Permeability changes are anticipated, but at this point it can only be speculated, rather than predicted, that deformation would decrease permeability.

(f) Changes in grain-boundary bubble and tube arrays may be produced by hydraulic fracture of the corresponding fluid inclusions (Figure 14) and subsequent enlargement of the cracks into tubes by solution.

Warm-Sintered, Synthetic Specimens. Three deformed specimens and their undeformed counterpart are being studied in thin section to characterize textural and structural changes produced by the deformation and to compare the starting material and its response to deformation with natural rock salt specimens from the WIPP site (see above). The three specimens were shortened 10 percent at 100-MPa confining pressure, at a strain rate of 10^{-4} sec^{-1}, and at temperatures of 100, 200, and 300 C (Table 3, Figure 8). Examination of data listed in Table 3 indicates the following trends:

(a) Grain sizes, grain-axial-ratio, dislocation density, and grain-boundary bubble and tube sizes do not change as a result of deformation.

(b) The number of grains, abundance, and size of the intragranular fluid inclusions decrease with increasing temperature of the deformation.

(c) The degree and number of polygonized grains increase with increasing temperature.

(d) Average polygonized subgrain size increases with increasing temperature (decreasing strength).

Possible changes in a-axis fabric are currently under study.

Comparison and Contrasts. Although the WIPP specimens were deformed in creep tests and at confining pressures, times, and temperatures very different from those used in the constant strain-rate tests on the synthetic specimens, there are some significant similarities and differences in the results, as follows.

(a) In both sets of experiments, grain size, grain-boundary bubble density, and bubble and tube sizes, and dislocation density do not change during deformation.

(b) The number of polygonized grains increases with increasing temperature of the experiment. This is consistent with the view that recovery processes are enhanced by temperature.

(c) In the synthetic specimen, the intragranular cubic inclusions are essentially annihilated by the deformation (at 300 C), while in the natural specimens they are only reduced in number and size when deformed, and tend to be reconstituted as a function of time and temperature. This contrast supports the view that the cubic inclusions are symptomatic of recovery. It is clear, however, that the recovery rate for polygonization is greater than that for the cubic inclusions (Item b).

Comparison of Natural and Synthetic Rock Salt

Structural and textural characterization of undeformed specimen 9-2671 from the WIPP site and the warm-sintered, synthetic specimen CV 85 (Tables 2 and 3, respectively) provides the opportunity to compare and contrast these materials to determine how realistic a substitute the synthetic material is. Several points seem noteworthy, as follows:

(a) The percentage of grains containing intragranular, cubic, fluid inclusions, and polygonization is about the same in each material.

(b) Grain size of the synthetic aggregate is about one order of magnitude smaller than that of the natural rock salt.

(c) Bubble and tube size in the synthetic rock salt also is smaller, but by factors of 3 and 5, respectively. Thus, although not strictly in scale, there is a general correspondence between grain size and grain-boundary features.

(d) The synthetic material has a one order of magnitude greater grain-boundary-bubble and free-dislocation density.

(e) Grain-boundary bubble and tube morphology and distribution of dislocations (etch pits) are similar in both materials. Currently under study are the a-axes fabrics of both materials.

In light of these comparisons and the similar response to deformation, it is concluded that synthetic material has sufficient textural and structural similarities to be a useful substitute for the natural rock salt at this phase of the study.

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WBS 1.1.2

Project: Material Properties Testing and Analysis

Principal Investigator: RE/SPEC Inc. (G. D. Callahan)

ONWI Project Manager: M. R. Wigley

Objective

The objectives of this program are to assess the strength and timewise deformational behavior of salt in the laboratory under applicable conditions of stress and temperature for development of consistent constitutive laws and to assess the thermomechanical behavior and constraints of repository situations in salt by analytical and numerical procedures.

Progress Reported Previously

The program was initiated on 1 October, 1978. Results and conclusions to date are highlighted below.

Preliminary analyses of data from creep experiments performed on Avery Island salt at 100 C revealed no apparent influence of confining pressure. For stress differences below 18 MPa, the steady-state strain rate, $\dot{\varepsilon}_{ss}(s^{-1})$, and axial stress difference, $\Delta\sigma$(MPa), can be described by the following equation:

$$\dot{\varepsilon}_{ss} = 2.53 \times 10^{-27} \, \Delta\sigma^{3.542}.$$

For axial stress differences above 18 MPa, the strain rate increases rapidly and cannot be predicted by the above equation. One could speculate that different micromechanisms are operable above and below 18 MPa at 100 C. However, the data are insufficient to determine what the micromechanisms may be or how many exist.

Comparison of thermal calculations and in situ field measurements performed at Avery Island, Louisiana (heater Site A), indicate that the in situ thermal conductivity may be 20 percent higher than laboratory-determined values. This discrepancy could be postulated as being due to size effects, stress relief during sampling, disturbance from sample preparation, handling and storing, in situ stresses, or instrumentation procedures.

The comparision of the vertical floor heave measured in situ at Site A with the numerical thermo/viscoelastic calculations showed reasonable agreement. The various creep formulations tended to underpredict the floor heave during early time and to bound the floor heave measurements during later time.

Numerical analyses of various pressure and temperature combinations planned for the accelerated borehole closure experiments to be performed at Avery Island, Louisiana, revealed that external pressure in range 10 to 14 MPa and temperature levels in the range ambient to 60 C would provide measurable borehole closures.

The majority of the analyses related to the Expected Repository Environments in Granite were completed last quarter. The finite element modeling in the very near field, near field, and far field simulated the thermal and thermally induced ground-water flow responses to a repository hosting commercial high-level waste, defense high-level waste, and spent fuel. In addition, related subjects such as ground-water composition, radiolysis effects, corrosion, and gas-phase pressures were investigated.

Activities During the Reporting Period

Testing

The test matrix being used for the comparison of creep of 50- and 100-mm-diameter specimens of Avery Island salt was completed. There are 49 tests in the matrix; 30 tests were performed on 50-mm-diameter specimens and the remaining 19 were performed on the larger 100-mm-diameter specimens. The test parameters included temperatures from 24 to 200 C, confining pressures from 0 to 20 MPa, and differential axial stresses from 10 to 30 MPa.

Creep tests on 100-mm-diameter specimens from Avery Island are in progress to determine the stress dependence of steady-state strain rate as well as to produce specimens for petrofabric analyses. The objective of these analyses is to determine the influence of stress and temperature on dislocation density and subgrain size at steady state. This study will provide information on how stresses and temperature control and steady state structure and, in turn, how this structure influences the steady state strain rate.

Data Analysis

Statistical analysis of the creep data from 50- and 100-mm-diameter specimens of Avery Island salt has been halted temporarily while the computer used for data storage and handling is replaced. The new computer should be operational during the second week of July, and the analysis should be completed by the end of July.

Data have been added to the plot of steady-state strain rate, $\dot{\varepsilon}_{ss}$, as a function of axial stress difference $\Delta\sigma$. Updated plots are presented in Figures 1 and 2. Two new points are plotted and a new fit has been made to the data. The exponent on stress increased by about 7 percent to 3.77; however, it is still substantially less than the value of 5 expected if the mechanism controlling creep is dislocation climb. The deformation map for salt given by Munson (1979) indicates that dislocation climb is the rate-controlling mechanism for 100 C and the range of stresses employed in these experiments. Present test conditions do, however, lie very near the (postulated) boundary between the regions where dislocation climb is the rate-controlling mechanism and where some undefined mechanism(s) controls creep. If the addition of subsequent data does not increase the stress exponent substantially, it must be concluded that dislocation climb is not the rate-controlling mechanism at 100 C and stress differences in the range $\Delta\sigma = 10^{-3}\ \mu$, where μ is the shear modulus.

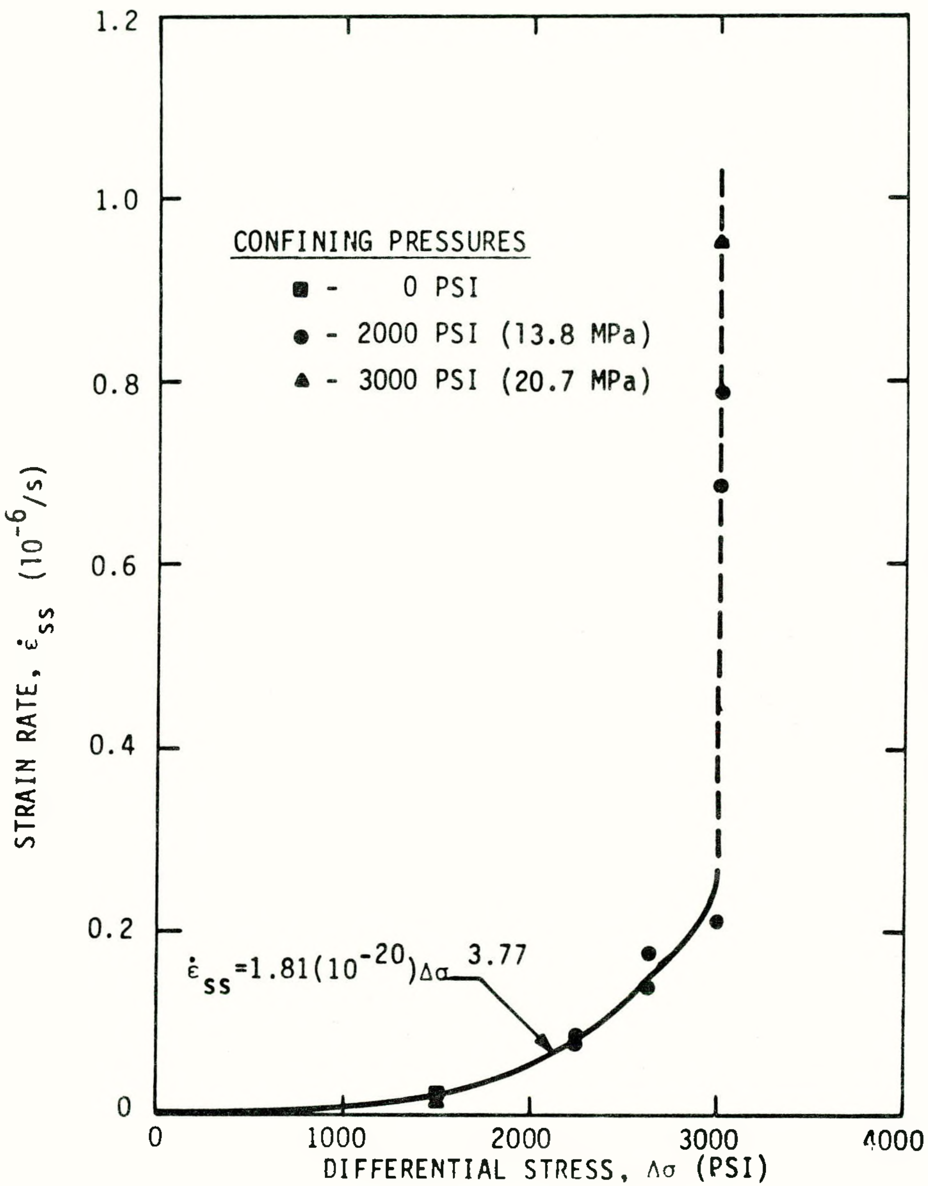


FIGURE 1. STEADY STATE STRAIN RATE AS A FUNCTION OF DIFFERENTIAL STRESS AT 100 C FOR AVERY ISLAND SALT

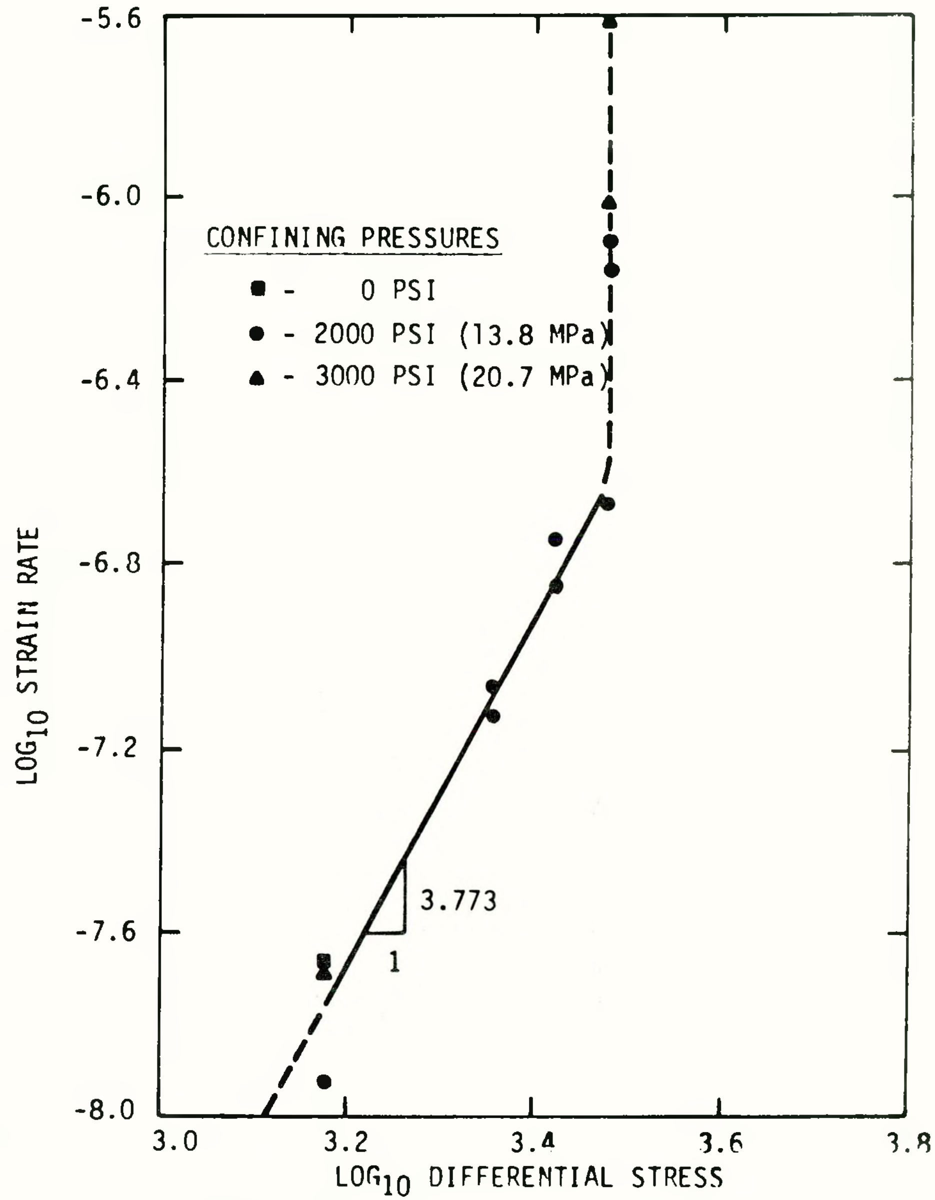


FIGURE 2. LOG_{10} STEADY STATE STRAIN RATE AS A FUNCTION OF LOG_{10} DIFFERENTIAL STRESS AT 100 C FOR AVERY ISLAND SALT

IN SITU HEATER TEST SUPPORT

Objective

Thermomechanical simulations of the planned accelerated borehole closure experiments to be executed at Avery Island, Louisiana, were performed. Comparison of the simulation results and the field data will provide a means for assessing the validity of constitutive relations and material properties determined in the laboratory and applied to field situations.

Procedure

Briefly, the accelerated borehole closure experiments involve 0.2-meter boreholes overcored 1.0-meter in diameter. The overcoring produces a 0.02-meter annulus which will house flatjacks with internal heaters. Four experiments are planned. One will represent a reference borehole at ambient conditions with no overcoring. The other three experiments will consist of flatjack pressures/temperatures of 14.84 MPa/60 C, 14.84 MPa/27 C, and 10.6 MPa/60 C. The primary measurements in the experiment will be borehole deformation measurements along the quarter points of the 1-meter-long borehole.

A schematic of the finite element model used in the thermomechanical simulation of the borehole closure experiments is shown in Figure 3. The section shown represents an axisymmetric model about the center of the borehole. Placement of the boundaries was determined by preliminary analyses such that they would not influence the thermal or mechanical results.

The thermal properties used in the simulation are given in Table 1.

TABLE 1. SALT THERMAL PROPERTIES USED FOR BOREHOLE CLOSURE SIMULATION

Thermal Conductivity[(a)], W/m-K	Specific Heat, J/kg-K	Density, kg/m^3
4.5-0.11T	871	2162

(a) T represents temperature in C.

The salt thermal properties were taken from Morgan (1979). The linear, temperature-dependent thermal conductivity expression represents a fit to Morgan's data for temperatures less than 100 C. A convective film coefficient of 3.97 W/m^2-K suggested by Cheverton and Turner (1972) was used to represent the mine ventilation along the surface of the model.

The mechanical properties of the salt used in the simulation are given in Table 2.

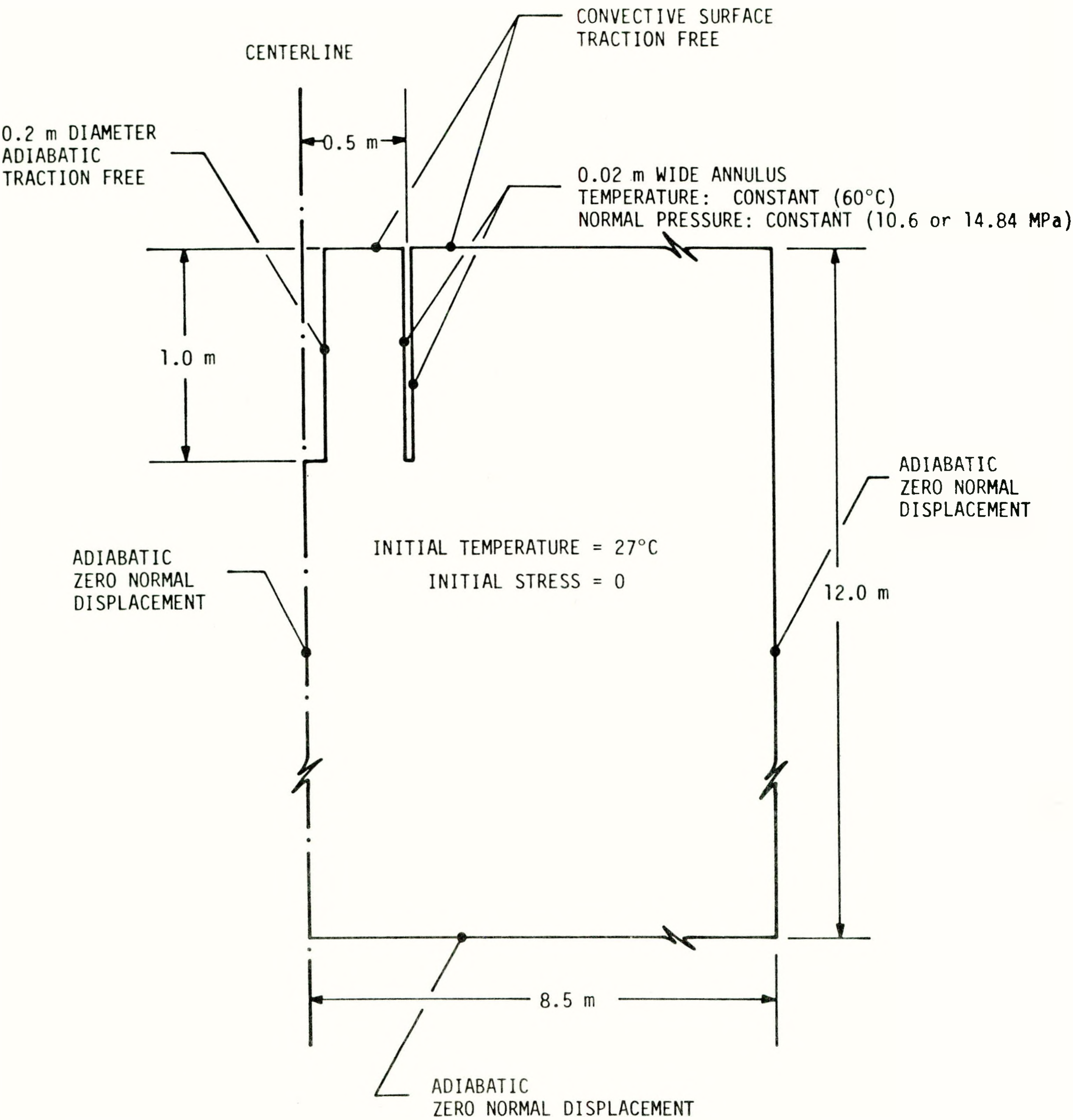


FIGURE 3. SCHEMATIC OF THE AXISYMMETRIC FINITE ELEMENT SIMULATION MODEL

TABLE 2. SALT MECHANICAL PROPERTIES

Young's Modulus, MPa	Poisson's Ratio	Thermal Expansion Coefficient, K^{-1}
1380	0.4	39.6

The empirical transient creep power law used to describe the viscous behavior has been reported by Hansen and Mellegard (1980). The creep strain, ε^c_{ij}, is given by:

$$\varepsilon^c_{ij} = 7.23 \times 10^{-36} \sigma_e^{2.28} S_{ij} t^{0.45} T^{11.45}$$

where

$\sigma_e = \sqrt{3J_2}$

J_2 = second invariant of deviator stress, MPa^2

S_{ij} = deviatoric stress, MPa

t = time, hr

T = temperature, K.

Preliminary analyses were performed to determine the effect of the initial in situ stress field on the borehole model. An initial lithostatic stress field due to the overburden (about 3.2 MPa) was assumed. Subsequently, excavation of the borehole and the flatjack annulus was simulated. The resulting effective stresses were less than 3 percent of the smaller applied traction (10.6 MPa). Thus, the in situ stress was considered to have a negligible influence on the core and was assumed to be zero.

Preliminary elastic analyses indicated tensile stresses at the base of the flatjack annulus as expected. Their magnitude was similar to the applied flatjack pressures. Since the tensile strength of salt (about 2 MPa) is almost an order of magnitude less than the generated tensile stresses, fractures will most likely emanate from the base of the flatjack annulus and relieve these stresses. To relieve the tensile stresses, a plasticity analysis was performed prior to the initiation of the thermo/viscoelastic analysis. The resulting stress field from the plastic analysis relieved the tensile stresses at the base of the flatjack annulus, but had a negligible influence on the stress field in the core—the area of interest.

Results and Conclusions

Figure 4 illustrates the temperature-rise contours about the isolated cylinder after 100 days of heating. The cylinder reaches steady conditions after approximately 5 days of heating, with the temperature level at all points being within 5 C of the desired 60 C temperature level. The other accelerated borehole closure experiments are planned at ambient (27 C) conditions.

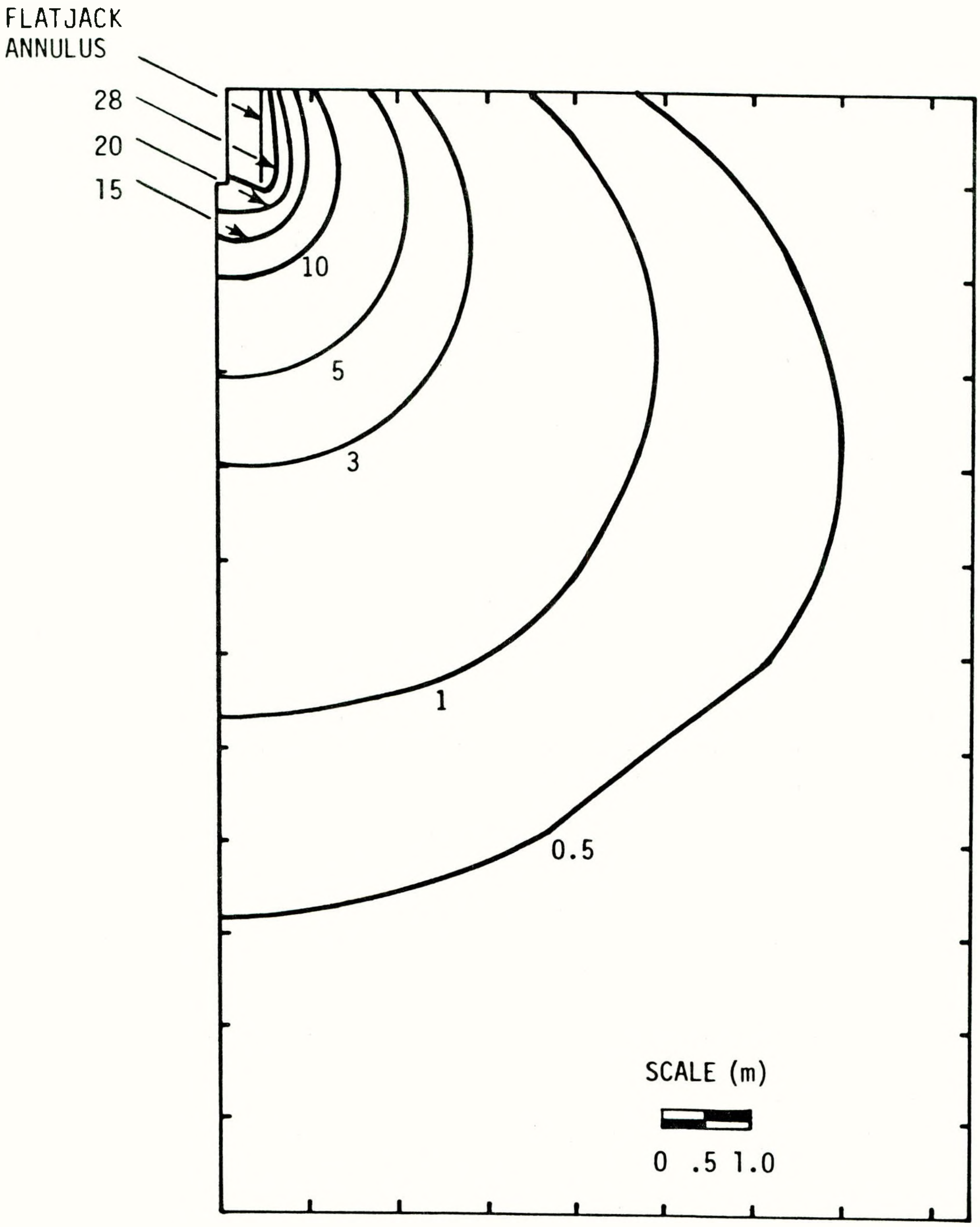


FIGURE 4. TEMPERATURE RISE ISOTHERMS (K) AFTER 100 DAYS OF HEATING

Figure 5 illustrates the displacement profiles for the elevated-temperature situation and flatjack pressures of 10.6 MPa and 14.84 MPa after 100 days of heating. The cylinder has a noticeable elongation and the borehole displaces the most near midheight. This is more evident in Figures 6 and 7, which show the transient behavior of the borehole for the 10.6 MPa and 14.84 MPa flatjack pressures, respectively. Figures 6 and 7 also compare the current results with those from the experimental planning analyses. The planning analyses performed assumed a constant temperature field and investigated a section of the cylinder under plane strain conditions. Thus, the results are in closest agreement near the midheight, as one would expect. The difference in the early displacements can be attributed to the thermal transients in the current analysis, whereas the scoping analyses assumed constant temperature fields.

After the field experiments are completed, these simulation results will be compared with the field results. The results of the comparisons will allow an assessment of the laboratory-determined constitutive relation and material properties and the modeling procedures.

TECHNICAL ASSISTANCE ON SPECIAL REPOSITORY PROBLEMS

Introduction

Several items were included within this task during the past quarter, including the ESTP Rock Mechanics Subgroup activities, salt core preparation, and far-field calculations for purposes of comparison with those of the University of Minnesota.

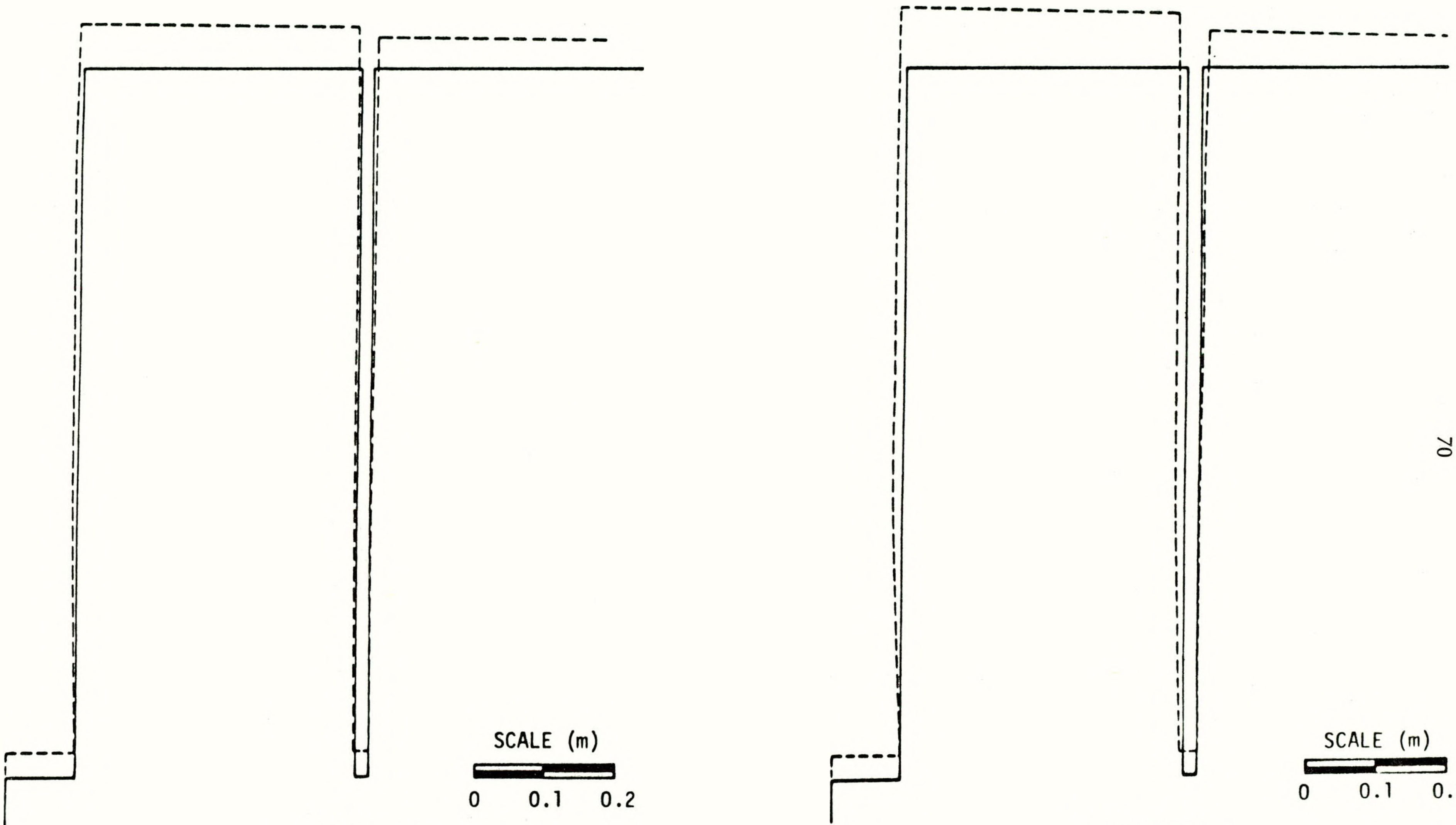
The ESTP Rock Mechanics Subgroup activities have been related solely to the preparation and issuance of a (draft) final report. These activities commenced on 1-2 April, 1980, with a review of a draft report. On the basis of comments and suggestions received from the reviewers, the draft report was extensively rewritten.

Twenty 100-mm-diameter salt specimens of Avery Island domal salt were prepared for the testing program at Texas A&M. These specimens were obtained from the same location at Avery Island and are the same size as the samples RE/SPEC has tested in the laboratory. Use of the same specimens should make correlation and interpretation of the two sets of data simpler.

A far-field model is being analyzed by RE/SPEC using the finite element method for comparison with the University of Minnesota's boundary element techniques. To date, the thermal analysis has been completed and compared with a near-field model. The following sections describe the far-field problem and the results obtained.

Procedure

The far-field problem involves a salt repository at a depth of 610-meters, with 20 rooms and 18 pillars symmetrically located about a 180-meter barrier pillar. The geometry and boundary conditions of the problem are shown in Figure 8. The effective thermal load for the repository section is 14.83 W/m^2, resulting from spent fuel 10 years out of pressurized water reactor. The salt thermal properties are given in Table 3.



a. 10.6 MPa

b. 14.84 MPa

FIGURE 5. DISPLACEMENT PROFILE AT 100 DAYS FOR FLATJACK PRESSURES OF 10.6 AND 14.84 MPa

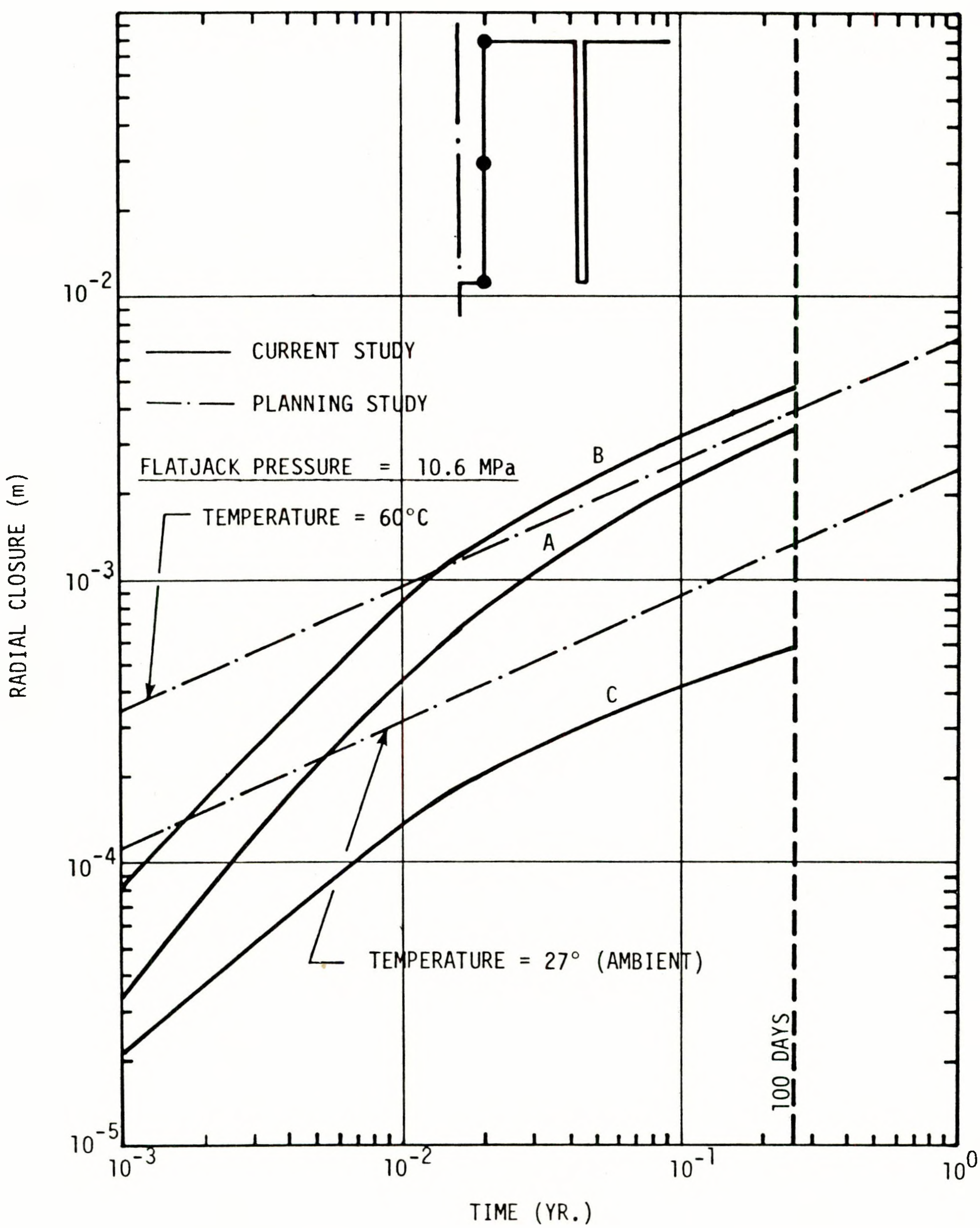


FIGURE 6. RADIAL DEFORMATION AT THE BOREHOLE SURFACE FOR A FLATJACK PRESSURE OF 14.84 MPa

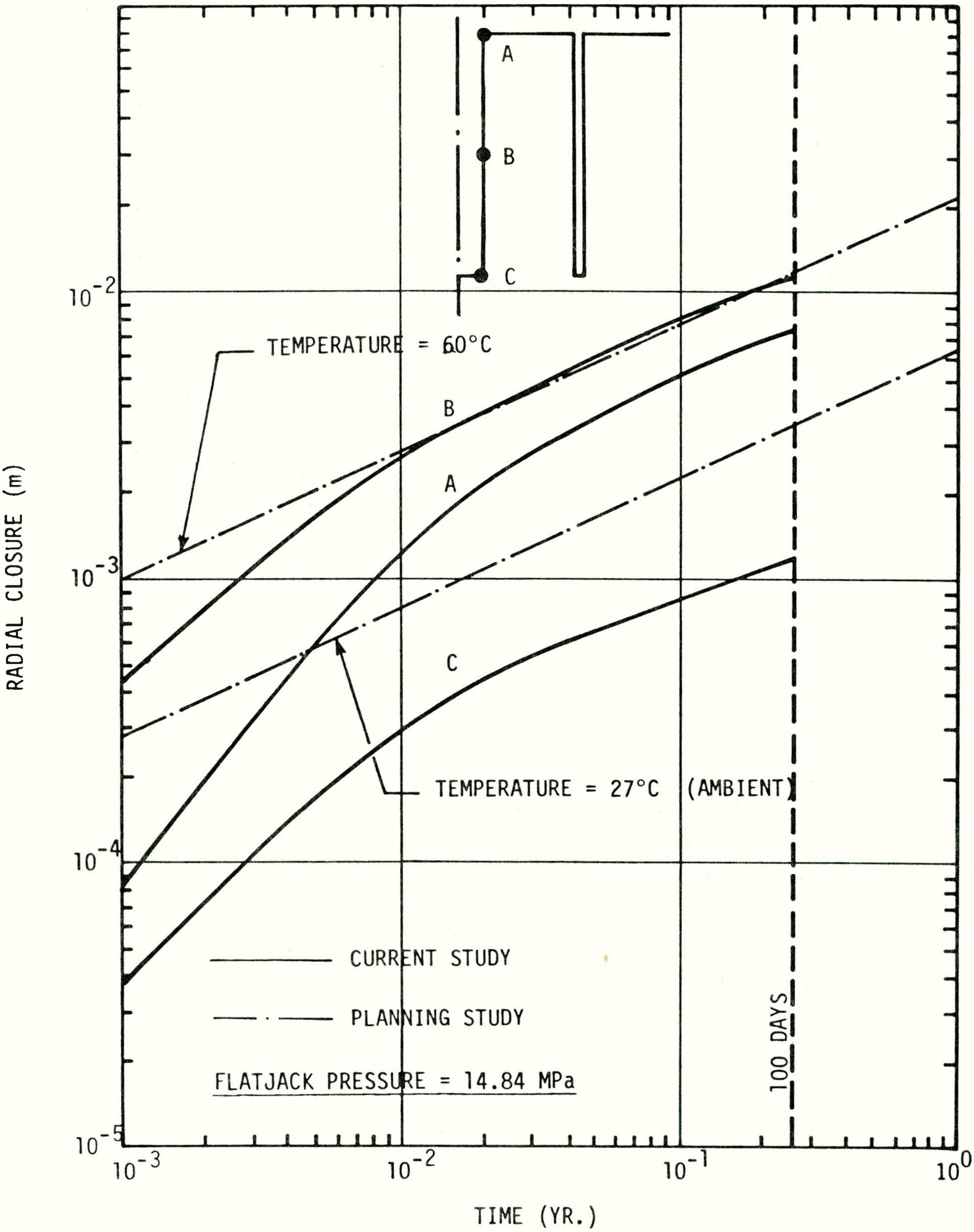


FIGURE 7. RADIAL DEFORMATION AT THE BOREHOLE SURFACE FOR A FLATJACK PRESSURE OF 14.84 MPa

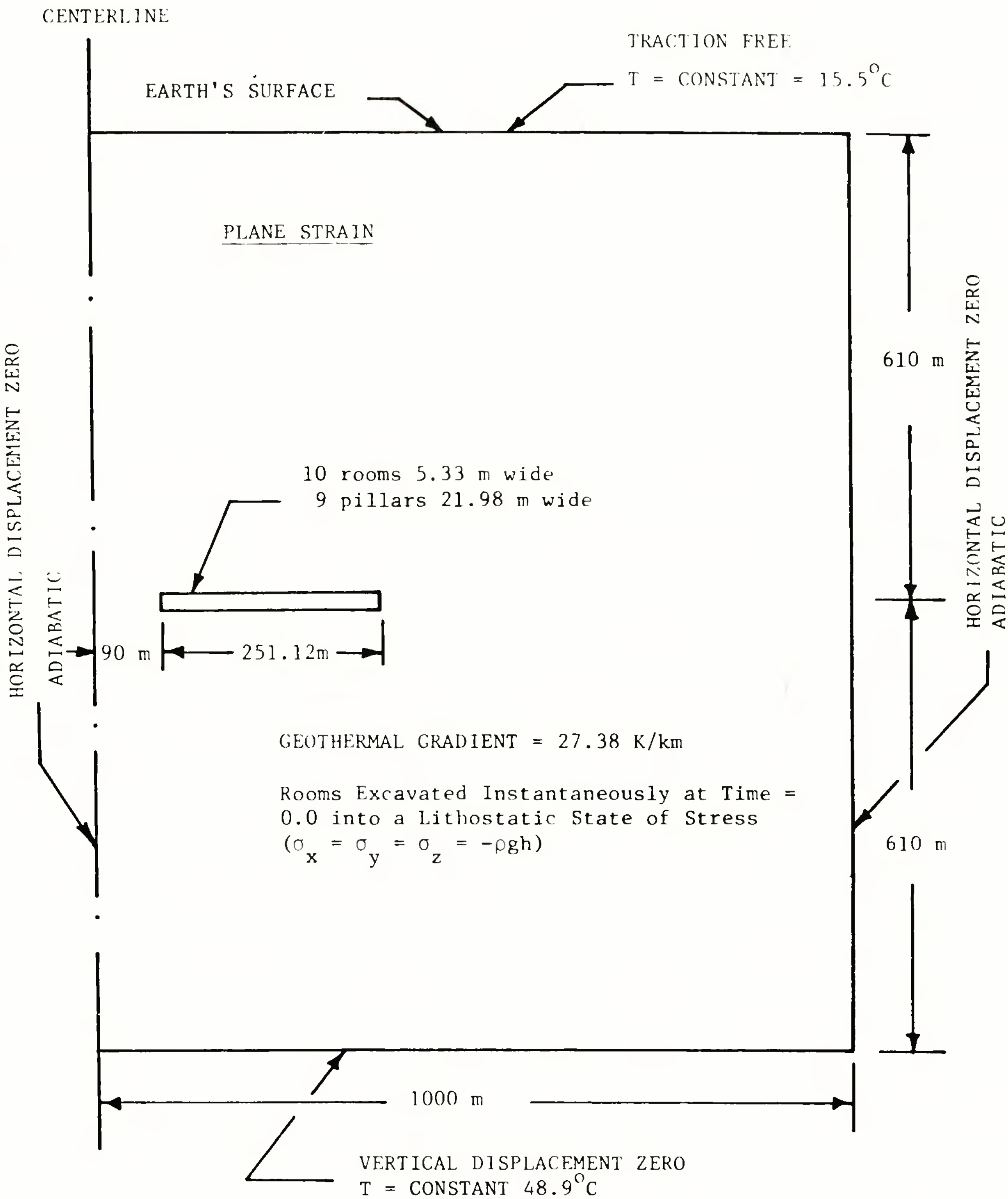


FIGURE 8. PROBLEM GEOMETRY AND BOUNDARY CONDITIONS

TABLE 3. THERMAL PROPERTIES USED IN FAR-FIELD ANALYSIS

Density, kg/m^3	Specific Heat, J/kg-K	Thermal Conductivity, W/m-K
2100	920	4.76

A near-field analysis, representing one-half of a room and one-half of a pillar from the central portion of the far-field model, was also simulated. The relative finite element mesh gradations used in the near-field and far-field models are shown in Figure 9.

Results and Conclusions

Figure 10 compares the temperature rises at three locations for the near-field and far-field models. The far-field results presented were taken from the central pillar and rooms. Even with the coarseness of the far-field model, the results compare remarkably well. The largest discrepancy is noted at the floor of the room. This can be attributed to the areas in each model over which the heat-generating waste is assumed to reside. In the far-field model the waste was modeled in the element beneath the floor (see Figure 9); in the near-field model the waste was modeled in the third element below the center of the room. Thus, the near-field model has a locally higher thermal density near the center of the room.

Figures 11 and 12 illustrate the growth of the temperature contours about the repository rooms. The elliptical contours are skewed downward because of the temperature rise with depth dictated by the geothermal gradient. Progressing through time, the repository end effects become quite vivid. At 40 years, the end repository rooms temperature levels are approximately 15 C lower than the centrally located rooms. At 30 years, one can just begin to see the effect of the smaller, centrally located, barrier pillar as compared with that of the larger outside barrier pillar.

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Hansen, F. D., and K. D. Mellegard, 1980. "Creep Behavior of Domal Salt from Avery Island, Louisiana", *Topical Report RSI-0118,* Prepared for the Office of Nuclear Waste Isolation under Subcontract No. E512-02300 with Battelle Memorial Institute, May (ONWI-104).

Morgan, M. T. 1979. "Thermal Conductivity of Rock Salt from Louisiana Salt Domes", ORNL/TM-6809, June.

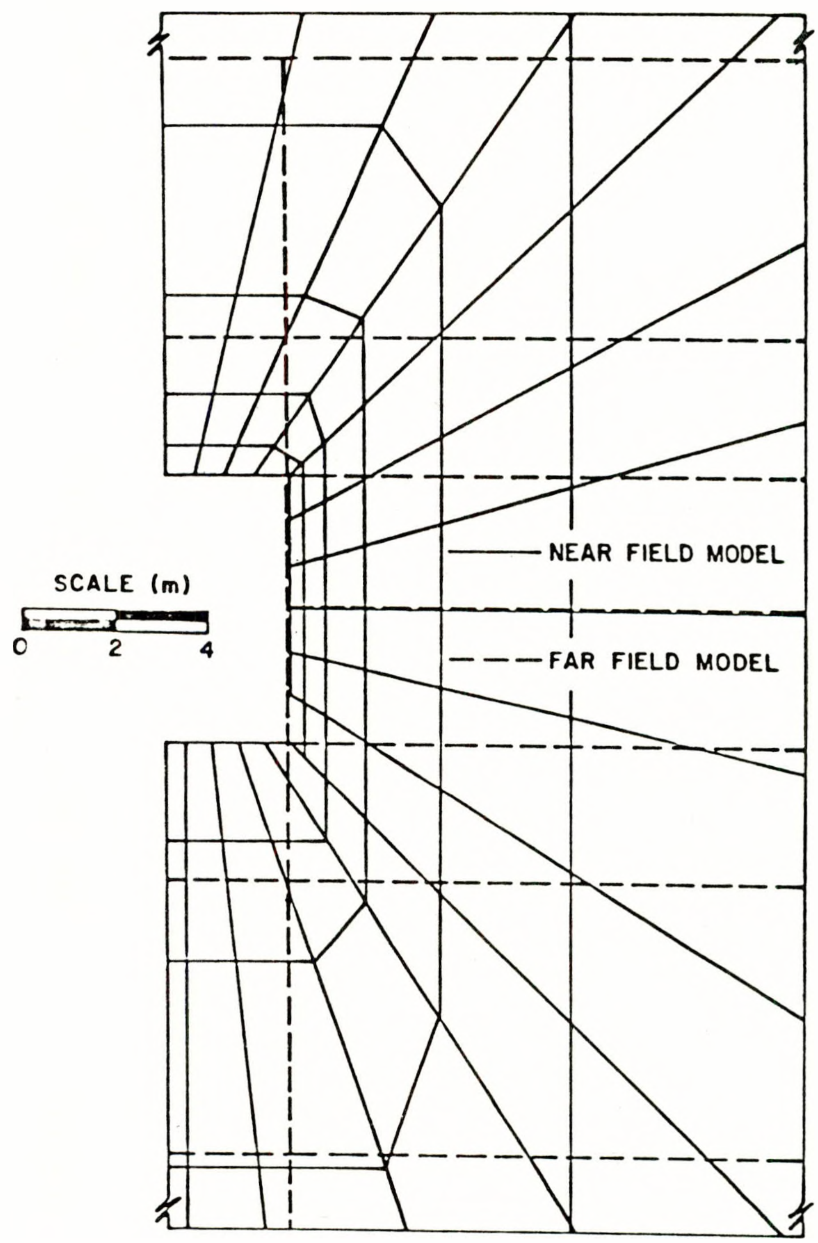


FIGURE 9. COMPARISON OF FAR-FIELD AND NEAR-FIELD FINITE ELEMENT MESHES

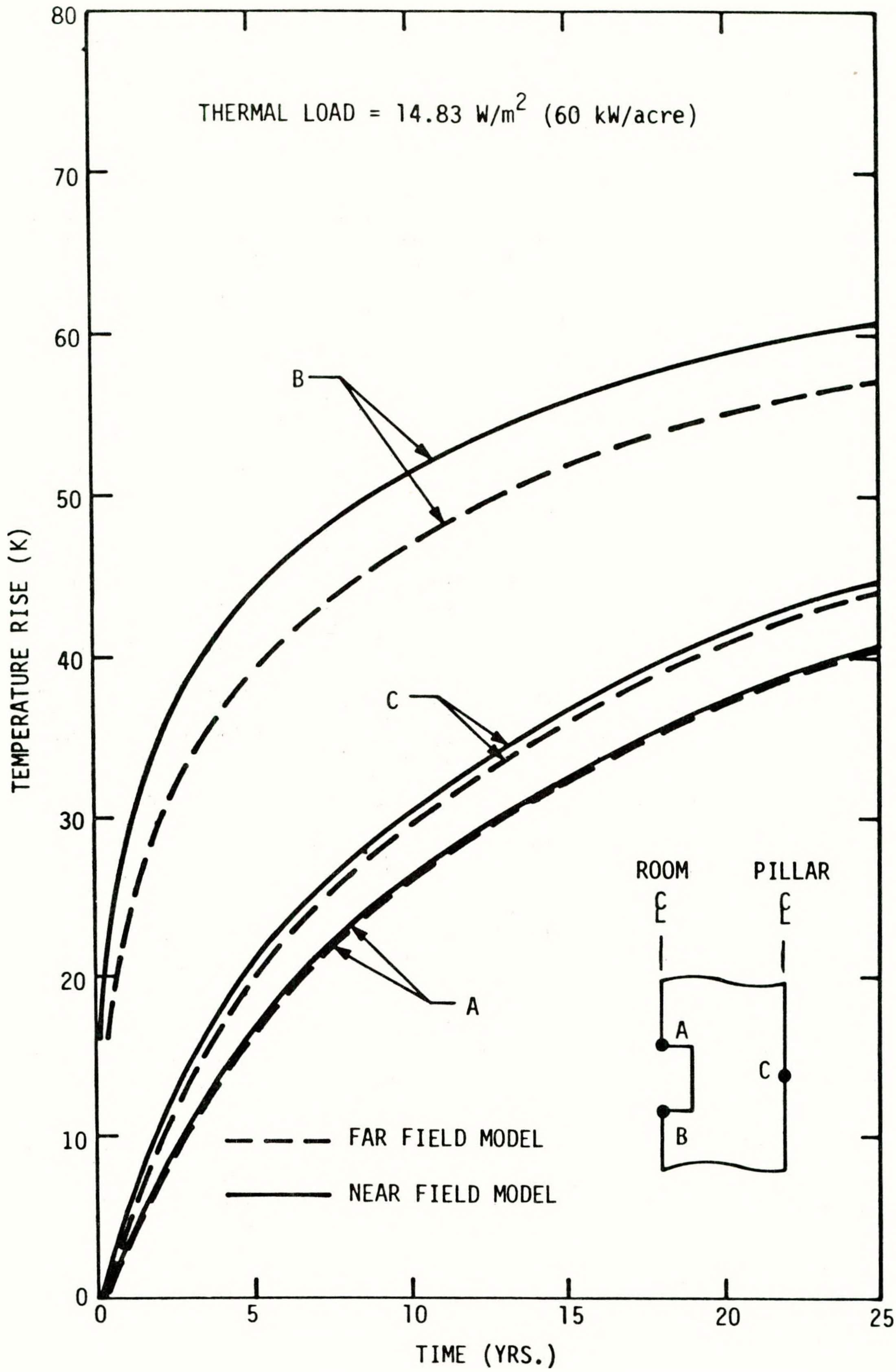


FIGURE 10. COMPARISON OF THERMAL RESULTS FROM NEAR-FIELD AND FAR-FIELD MODELS

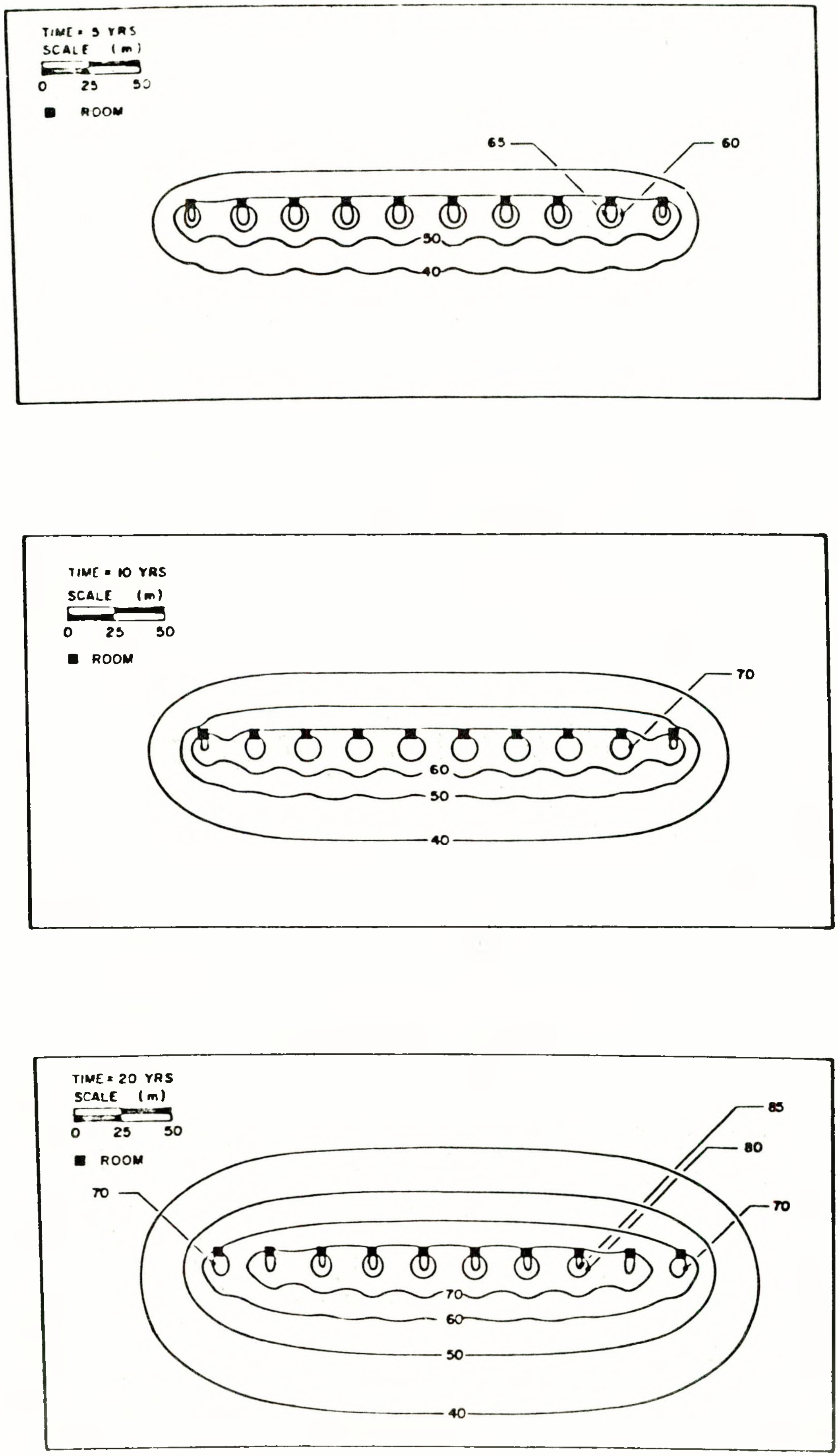


FIGURE 11. TEMPERATURE CONTOURS FOR THE FAR-FIELD MODEL TO 20 YEARS

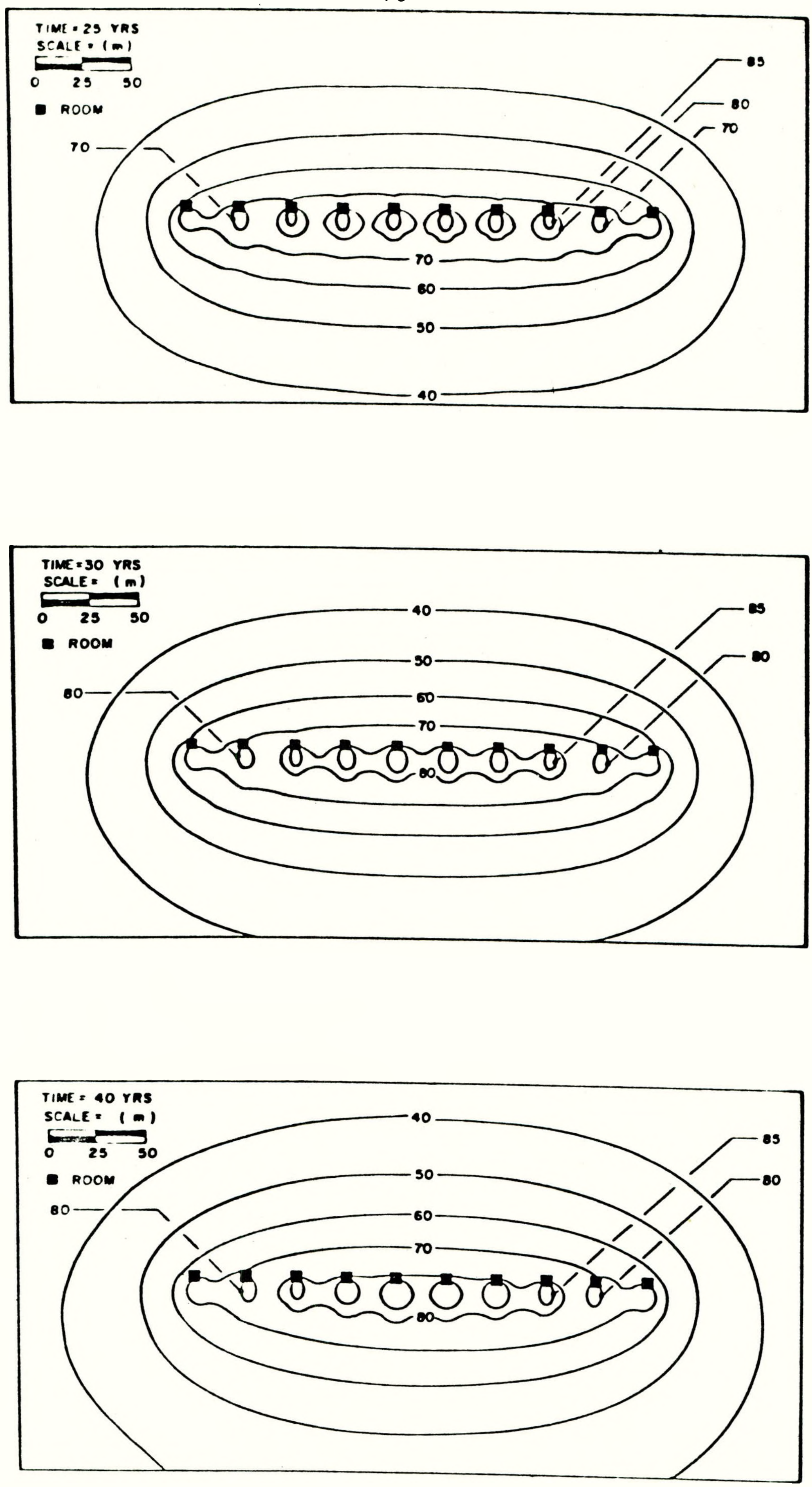


FIGURE 12. TEMPERATURE CONTOURS FOR THE FAR-FIELD MODEL TO 40 YEARS

Munson, D. E. 1979. "Preliminary Deformation-Mechanism Map for Salt (with Application to WIPP)", Report SAND-79-0076, Sandia Laboratories, Albuquerque, New Mexico.

Wagner, R. A. 1978. "Parametric Study Involving Thermo/Viscoelastic Analysis of a Room and Pillar Configuration", *Technical Memorandum Report RSI-0070,* Prepared for the Office of Nuclear Waste Isolation under Subcontract No. E512-02300 with Battelle Memorial Institute, November 23 (ONWI/SUB-78/E512-02300/1).

WBS 1.1.2

Project: Numerical Modeling of Radioactive Waste Disposal Sites in Bedded Salt

Principal Investigator: University of Minnesota (C. M. St. John, S. L. Crouch, K. Sinha)

ONWI Project Manager: J. Monsees

Objective

There are two major objectives of this work. The first concerns development and application of a group of computer models based on boundary element techniques. The second is a laboratory investigation of the inelastic behavior of salt under varying loading conditions.

The computer models are largely based on a technique called the Displacement Discontinuity Method that has been developed for the analysis of stresses and displacements around underground excavations. The models used in this investigation incorporate thermal loading as well as permitting creep of the material on the excavation horizon. The objectives of the current work are to complete development of all models to the extent that they are available for design studies, and to establish the scope of their applicability by comparison with computer models based on different numerical procedures.

The laboratory investigation was initiated as a direct consequence of questions raised regarding the appropriate constitutive model for salt. In particular, a program to investigate the path dependence of salt deformation with respect to changes in stress, temperature, and strain rate is being developed.

Progress Reported Previously

A benchmark study involving a comparison between the two-dimensional displacement-discontinuity code SALTY, and a finite-element code from RE/SPEC, Inc. was initiated. The benchmark study was to consist of an analysis on a repository scale of a simplified configuration to test the applicability of displacement discontinuity codes in the far-field. Initial results from SALTY indicated considerable stress-arching between the barrier pillar and the abutment zones beyond the panels. This arching has direct consequence on the pillar loads and conditions around disposal rooms.

In the laboratory phase of the program, design acquisition and construction of equipment continued. Fabrication of the triaxial pressure chambers was near completion, and the construction of loading frames and retaining structure had been initiated.

Activities During the Reporting Period

The current work consists of three Tasks. Activities under each of these Tasks will be summarized below.

Task I — Repository Design Studies

Following cessation of general design studies until successful completion of the benchmark exercise, activities within the Task have been restricted. Discussions have led to definition of a benchmark problem consisting of two waste disposal panels separated by a barrier pillar. Preliminary analyses have been completed so that the problem is adequately defined before comparative analyses by SALTY and a finite-element model are completed. However, the geometry for the displacement-discontinuity code SALTY has been modified to accommodate an existing finite-element grid setup available to RE/SPEC, Inc. The new geometry, shown in Figure 1, was reevaluated to complete this phase of the comparison. The parameters for the comparison are listed in Table 1. The minor changes have not resulted in any revisions of conclusions reported earlier, and complete, revised results will be available shortly.

Task II Code Development

As part of the benchmark study, SALTY is being modified to incorporate both time-hardening and strain-hardening creep laws. This work is still in progress. Planned developments allowing treatment of anisotropy and inhomogeneity have been delayed until successful completion of the benchmark study.

Task III Laboratory Investigation

During the reporting period, the major progress in this task has been in equipment acquisition. Fabrication of the three triaxial chambers ordered in December was completed in June and the units have arrived. The key components for the automatic remote acquisition system (the Apple II microcomputer and the Kaye Digistrip II Logger) have also been received and installed in the laboratory. Various other components such as the Linear Variable Displacement Transducers (LVDTs), load cells, strain indicators, etc. have been acquired. The pressure intensifier required for the program is not yet available and must be manufactured. Also, the proper pressure actuator must be acquired.

Since the last quarterly report, design of the system progressed and has been modified to a minor degree. As presently conceived, the load frame will consist of a four-rod support design with exterior alignment sleeves as shown in Figure 2. Supported by this frame, each load train (Figure 3) will contain a triaxial chamber, load cell, and pressure actuator, together with appropriate connectors. The system will have an LVDT holder mounted on the load piston to monitor axial deformation.

Axial and lateral pressure, axial and lateral deformations, and temperature will be monitored during all phases of testing, employing the monitoring system shown in Figure 4. Seismic monitoring equipment will be included with one chamber.

Construction of the load frames was finalized and the retaining frame which holds the three load frames is near completion.

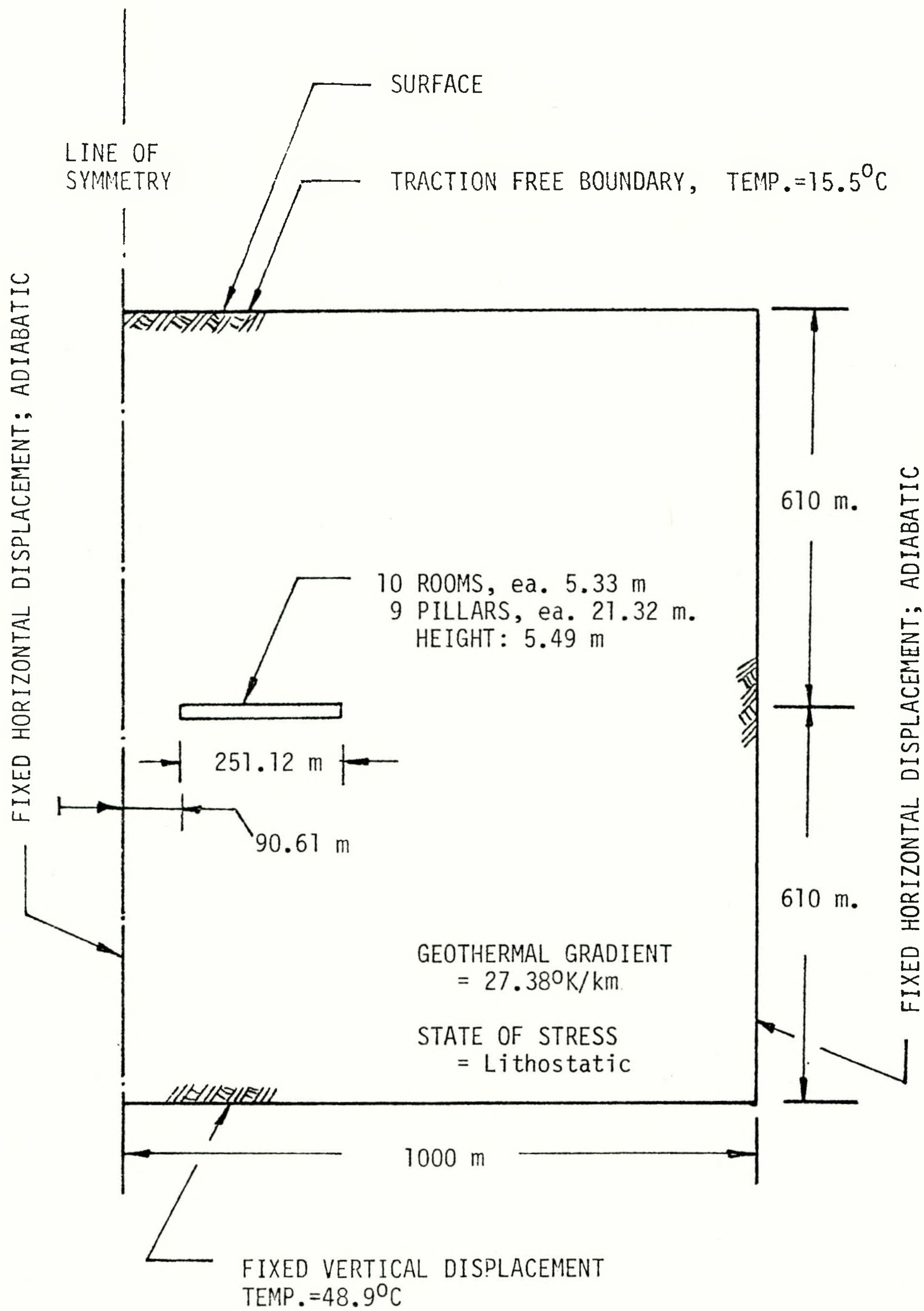


FIGURE 1. GEOMETRY FOR BENCHMARK STUDY – TASK I COMPARISON

Plane strain model with instantaneous room excavation.

TABLE 1. STUDY PARAMETERS

Parameter	Units	Value
Young's Modulus	GPa	13.79
Poisson's Ratio	(None)	0.40
Density	kg/m^3	2162.
Heat Capacity	J/kg-K	920.
Thermal Diffusivity	m^2/s	2.46×10^{-6}
Coefficient of Thermal Expansion	k^{-1}	3.96×10^{-5}
Thermal Conductivity	W/m-K	4.76
Unconfined Compressive Strength	MPa	2.2
Uniaxial Tensile Strength	MPa	2.2
Creep Equation	—	$E = A\theta^a t^b \sigma^c$
Creep Coefficient (A)	$Pa^{-c} hr^{-b}\ K^{-a}$	4.18×10^{-49}
Creep Temperature Exponent (a)	(None)	9.5
Creep Time Exponent (b)	(None)	0.4
Creep Stress Exponent (c)	(None)	3.0
Initial Temperature of Repository	K	305.2
Repository Depth	m	610
Room Width	m	5.33
Room Height	m	5.49
Pillar Width	m	21.98
Extraction Ratio	%	19.52
Geothermal Gradient	K/km	27.38
Surface Temperature	K	288.5
Base Temperature at 1220 m	K	321.9
Thermal Loading	W/m^2	14.83

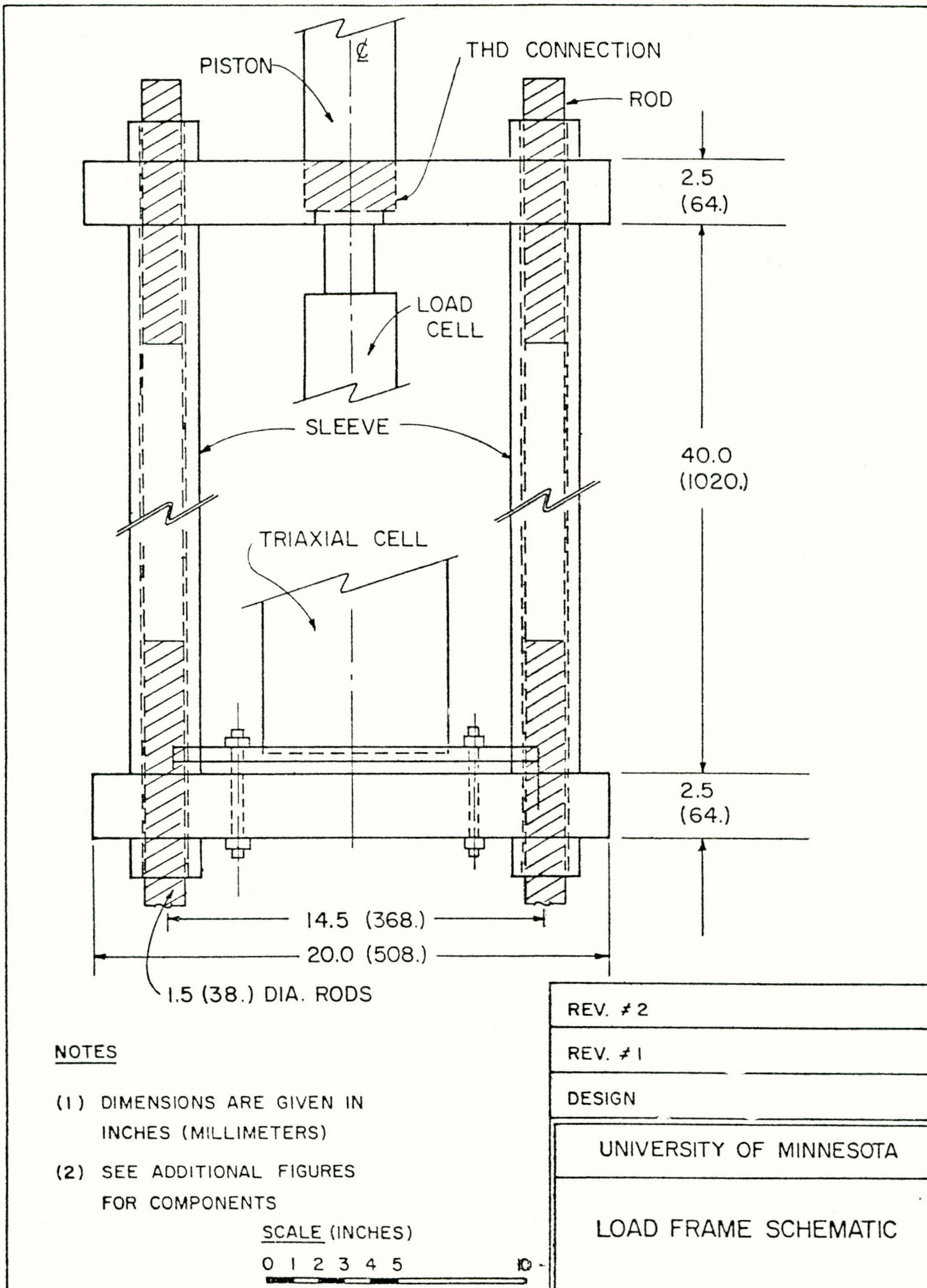


FIGURE 2. REVISED LOAD FRAME DESIGN

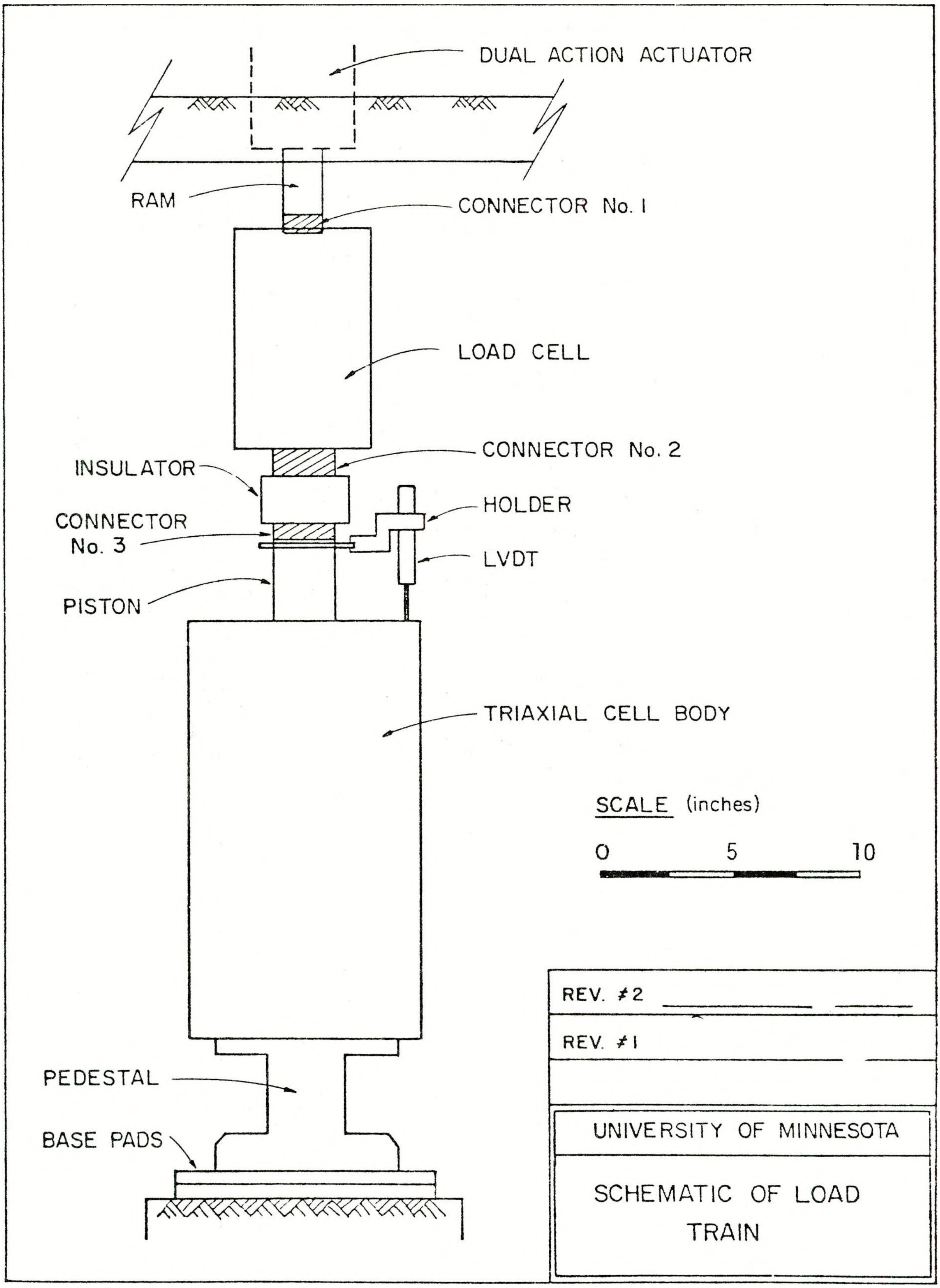


FIGURE 3. LOAD TRAIN DIAGRAM FOR TRIAXIAL CELL

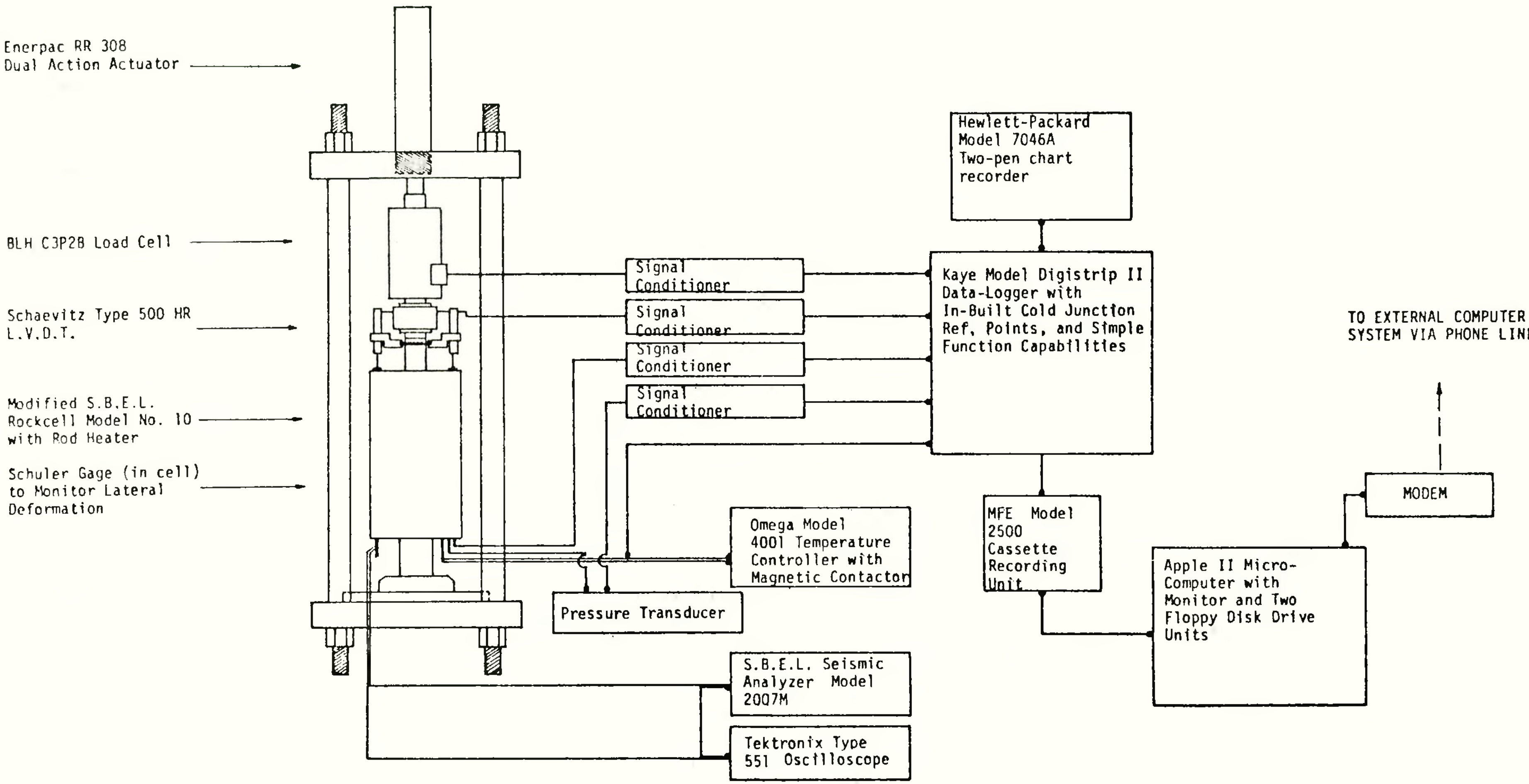


FIGURE 4. BLOCK DIAGRAM OF DATA MONITORING SYSTEM

WBS 1.1.2

Project: Rock Behavior Under Elevated Pressure and Temperature

Principal Investigator: Lawrence Livermore Laboratory (H. C. Heard)

ONWI Project Manager: M. M. Lemcoe

Objective

The overall objective of the program is to develop an understanding of rock behavior under elevated pressure and temperature such that the response in space and time of a mined cavity in these rocks can be predicted. In order to do this, measurements are made in the laboratory at simulated, deep in situ conditions. It is expected that these data will be correlated with field observations.

For Thermal Properties of Rocks, the objective is to determine the thermal conductivity, thermal diffusivity, and thermal expansion of candidate waste repository rocks at in situ conditions of temperature, pressure, and fluid content.

For Water Transport: Permeability and Related Measurements, the objective is to make systematic measurements of the permeability of sound and fractured rock as a function of confining pressure, pore pressure, and deviatoric stress. In order to extend the usefulness of the data, simultaneous measurements of strain, electrical conductivity, and acoustic velocity will also be carried out.

For Pressure and Temperature Dependence of Rock Elastic Constants, the objective is to determine the elastic moduli of a suite of candidate repository rocks as a function of temperature and pressure. These measurements, including Young's modulus, bulk modulus, and thermal expansion, are necessary to understand and predict repository behavior after emplacement of the waste.

Progress Reported Previously

Thermal Properties of Rocks

This task started in August, 1977. Making measurements under the conditions of temperature (to 300 C) and pressure (to 200 MPa) in the presence of pore fluid required an advance in measurement state of the art for rocks. Therefore, an apparatus was designed, fabricated, assembled, and debugged. In the course of debugging, a run was made on an unjacketed aluminum sample. This run showed the basic design to be viable.

Results on the first sample of Avery Island salt indicated that hydrostatic pressure has little effect on the thermal conductivity, diffusivity, and linear expansion. At room temperature and effective confining pressure increasing from 10 to 50 MPa, thermal conductivity and diffusivity are constant at roughly 7W/mK and 3.6×10^{-6} m^2/s, respectively. At 50 MPa and temperature increasing from 300 to 573 K, both conductivity and diffusivity drop by a factor of 2. Thermal linear expansion at 0 MPa matches that at 50 MPa, increasing from roughly 4.2×10^{-5}/K at 300 K to 5.5 x 10^{-5} at 573 K. Simple models of microcracking suggest that among common geological materials the lack of pressure dependence is unique to rock salt.

Preparation of two samples of Climax quartz monzonite for the next sequence of runs was begun. A fused silica sample was ordered in the exact configuration of a typical rock sample to be used as a standard reference for our measurements at pressure and temperature. The core seals around the electrical feedthroughs of the main pressure plug were remade to make them more reliable and less sensitive to temperature fluctuations. The new plug demonstrated better leak tightness than the old design. The electrical feedthroughs were now made of the same steel as the plug itself, so the seals should be less prone to working loose because of thermal expansion mismatches.

Water Transport: Permeability and Related Measurements

This task started in June, 1976. A summary of progress through March 1980 includes the following major items:

- Design, construction and placement into operation of two complete sets of apparatus to determine permeabilities of large rock samples (15 cm diameter by 28 cm long) in the range of 10^{-11} to 10^{-24} m^2. These data are taken simultaneously with the principal imposed stresses and strains, acoustic velocities and pulse amplitudes, electrical conductances, and displacement of a fracture (if present). A microprocessor system controls the test and records the data.

- Measurements of the above type were completed on intact samples of Westerly granite, White Lake gneissic granite and Creighton gabbro, and on fractured Westerly granite and Creighton gabbro.

- Failure envelope data were completed on unfractured Westerly granite, White Lake gneissic granite, Creighton gabbro, and Montello granite. Two samples of Stripa granite and one of Montello granite have been prepared. One of each type of granite was fractured. The fractured Stripa sample was jacketed and placed into the vessel for measurement.

- Some effort was spent on sample preparation, debugging, and testing of a new multiple-sample permeability apparatus for high-temperature permeability measurements. A limited number of tests was planned for the Climax quartz monzonite and Stripa granite at room temperature in this apparatus, and these samples had been prepared and jacketed.

- The capacitance bridge which is used for the conductance measurements was interfaced with our LSI-11 microprocessor and fully automated.

- Two topical reports were initiated. The first dealt with a complete description of the existing permeability apparatus, the second examined the transient method of permeability determination. Five topical reports, three abstracts, and two extended summaries had been issued as a direct outgrowth of this project.

Pressure-Temperature Dependence of Rock Elastic Constants

This task started in June, 1979. A summary of progress through March, 1980 includes the following major items:

- Determination of the thermal expansion characteristics of Climax quartz monzonite to pressure of 27.6 MPa and 300 C. Results of this study on expansion and its relationship to in situ permeability are to be published soon.

- Multiple test samples of Stripa and Westerly granites, Creighton gabbro, and Climax quartz monzonite had been prepared for testing to 55 MPa and 350 C. This involves three samples of each rock cored in each of three orthogonal directions.

- All measurements had been completed on three samples each in the three orthogonal directions of the Stripa granite. About two thirds of the data had been reduced. Analysis of the thermal expansion (α) results indicate α ranges from 5 to $8 \cdot 10^{-6}$ C^{-1} at 40 C (T) to 12 to $15 \cdot 10^{-6}$ C^{-1} at 325 C. The values for α are not linearly related to either T or P. The compressibility (β) of Stripa granite ranges from 1 to $9 \cdot 10^{-11}$ Pa at 19 C to 4 to $22 \cdot 10^{-11}$ Pa at 350 C, depending on P. The maximum sensitivity of β to P occurs at the lower pressures. Data on Young's modulus had not yet been completely evaluated.

Activities During the Reporting Period

Thermal Properties of Rocks

The run on the last Avery Island salt sample was completed during the quarter, as were preparations for the first run on Climax Stock Quartz Monzonite (CSQM).

The salt run produced a complete set of thermal properties data in a test matrix ranging to 50 MPa and 165 C. Good agreement with existing data, where overlap existed, and excellent reproducibility indicate the high quality of the new data. The thermal behavior of Avery Island salt is summarized below.

Conductivity in the range 300 K to 440 K drops in approximately linear fashion at a rate of $-2.6 \pm 0.3 \times 10^{-2}$ W/mK/K at fixed pressure. In the range 440 to 573 K and at fixed pressure of 50 MPa (the only pressure tested in this range) the decrease can also be approximated by a linear rate of $-1.4 \pm 0.7 \times 10^{-2}$ W/mK/K. The conductivity of untested material at 300 K is independent of pressure and has been fixed by other workers at 7 ± 1 W/mK. In the range of confining pressure 20 to 50 MPa, conductivity is pressure independent at all temperatures tested. However, above 340 K, a pressure decrease from 20 to 10 MPa causes conductivity to drop by roughly 0.6 W/mK. Diffusivity from 300 to 440 K decreases at a rate of $-0.75 \pm 0.2 \times 10^{-8}$ m^2/s/K at fixed pressure. The decrease continues, with much poorer precision, to 573 K. The starting value at 300 K is fixed by other workers at $3 \pm 0.5 \times 10^{-6}$ m^2/s. The data show pressure independence above 30 MPa and an increase in diffusivity of roughly 0.5×10^{-6} m^2/s in dropping pressure from 30 to 10 MPa. The pressure effect is suspected to be an artifact (still unexplained) because it is in opposition to that expected from reasonable physical models on the basis of the conductivity measurement. Linear expansivity is independent of pressure and increases with increasing temperature from 4.6×10^{-5}/K at 340 K to 5.4×10^{-5}/K at 550 K.

The only unanticipated result of the latest run was the pressure dependence of the thermal conductivity below 20 MPa. However, such behavior in a polycrystalline material at elevated temperatures is consistent with a model of thermally induced microfractures that would interface with thermal conductance when open below a certain pressure. A sharp knee in the conductivity versus pressure curve, if it is real and if it is caused by the behavior of microfractures, would indicate a narrow range of crack aspect ratios in the material. This also is roughly consistent with what one observes in salt, with fractures tending to be confined to cleavage fracturing traversing the length of a given grain.

Preparation of the new CSQM sample went smoothly and it was successfully electron-beam welded into its jacket at the close of the quarter. The new sample jacket incorporates improvements based on experience with the last salt sample. Three sets of sample end caps have been made to allow for simultaneous preparation of several samples. CSQM is anticipated to have one-half to one-third the conductivity of Avery Island salt, so the "insulators" immediately at either end of the sample (formerly pyrophyllite) are now made of very-low-conductivity Pyrex.

Experience with the two very successful runs on salt have provided the groundwork for a number of minor design changes aimed at speeding and facilitating the experimental assembly and disassembly, and at improving data accuracy and precision. These changes have been made in anticipation of the first CSQM sample. For example, all thermocouple connections within the vessel are now of the quick-disconnect variety; brazing and spot welding have been eliminated. Also, a positive location mechanism on the internal heaters has been added. The heater positions will now be very well defined (to a few thousandths of an inch) and the effect on the data of controlled shifts in heater positions can now be measured.

Water Transport: Permeability and Related Measurements

During this quarter, two fractured Stripa granite samples were prepared, jacketed, and tested. However, only one of these tests was completely successful. The permeability, electrical conductance, compressional velocity, compressional wave amplitude and fracture width data are now being analyzed. Effective pressures for this test varied up to 25 MPa and the end loading ranged to 0.63 of the fracture stress.

A fractured sample of Climax quartz monzonite has been prepared and jacketing procedures are about 40 percent complete.

Preliminary permeability results on 5-cm-diameter by 11-cm-long samples of intact Stripa granite and Climax quartz monzonite have been obtained. Data were taken at 10 MPa only (no axial loading). Both rocks were found to have permeabilities of about 10^{-20} m^2 (10^{-8} D)—about the same value as intact Westerly granite. Further work is planned.

Pressure and Temperature Dependence of Rock Elastic Constants

During this quarter all necessary analysis for the linear thermal expansion (α) and compressibility (β) of the Stripa granite was completed. Also completed were all measurements necessary for the determination of α, β, and Young's modulus (E) of Westerly granite. Three samples each were tested in three mutually orthogonal directions at pressures (P) to 55 MPa and temperatures (T) to 300 C. In the same manner as the Climax quartz monzonite and Stripa granites previously reported, α and β of Westerly granite are neither constant nor a simple function of T or P. Both α and β seem consistent with available literature data at comparable conditions. E is yet to be evaluated for the latter two rocks.

Summary of Measurement Status Through June 1980

Under the task on the thermal properties of rock, all measurements have been completed on duplicate samples of Avery Island salt. A sample of Climax quartz monzonite has been prepared and jacketed. Testing on the monzonite should begin shortly.

For the task on permeability, Table 1 summarizes the measurement status.

TABLE 1. MEASUREMENTS FOR PERMEABILITY

Rock	Unfractured	Fractured	Comments
Westerly granite	X (F)	X	R
Montello granite	J (F)	P	
White Lake gneissic granite	X (F)		R
Creighton gabbro	X (F)	X	R
Stripa granite	P,X_p (F)	X	
Climax quartz monzonite	P,J,X_p	P	

Legend: X — Measurements complete
X_p — Preliminary data only
P — Samples prepared
J — Samples jacketed and instrumented
R — Report issued
(F) — Failure envelopes completed.

For the task on pressure and temperature dependence of rock elastic constants, the status of measurements is shown in Table 2.

TABLE 2. MEASUREMENTS ON PRESSURE AND TEMPERATURE DEPENDENCE OF ROCK ELASTIC CONSTANTS

Rock	Status	Comments
Climax quartz monzonite	X_α	R
	P_β	
	P_E	
Westerly granite	$X_{\alpha,\beta,E}$	Data analysis continuing for E
Stripa granite	$X_{\alpha,\beta,E}$	Data analysis continuing for E
Creighton gabbro	$P_{\alpha,\beta,E}$	

Legend: R — Report issued
P — Samples prepared
X — Measurements complete.

WBS 1.1.2

Project: Fractured Rock Studies Program

Principal Investigator: Lawrence Berkeley Laboratory (W. Stromdahl)

ONWI Project Manager: M. R. Wigley

TESTING FACILITIES FOR ULTRA-LARGE ROCK CORES

Objective

The ability to accurately define the in situ conditions and properties of the subsurface media is essential to the design of underground facilities for nuclear waste isolation. Of particular importance are the hydrological properties of joints and faults as a function of rock type and the states of stress, fluid pressure, and temperature. To study these issues, it is necessary to make measurements in rock subject to a wide range of well-defined and well-controlled states of stress, deformation, fluid pressure, and temperature. Traditionally this has been attempted in laboratory tests on specimens of rock with dimensions of several centimeters. However, the hydrological behavior of rock is size-dependent. Thus, it is important to obtain measurements on rock samples much closer to that of practical concern, namely meters rather than centimeters.

To provide the capability to conduct experiments using ultra-large samples, Lawrence Berkeley Laboratory is managing, operating and modernizing a large-scale testing facility at the Richmond Field Station, University of California. The facility includes a triaxial testing machine and associated plant and equipment capable of handling rock cores up to approximately 1 meter in diameter and 2 meters axial length. In the present configurations, cores can be tested in triaxial compression at confining pressures up to 750 psi and axial loads up to 4×10^6 lbf. The testing facility will be available to support nuclear waste isolation program testing research, including the Swedish-American Cooperative (SAC) Waste Storage Program. Independent of other NWI Programs, LBL is conducting a fundamental investigation of the effects of sample size on the measured hydrological properties of rock and rock fissures.

The test facility will be operated and maintained throughout FY 80. Experimentation during the first half of the year will be for the SAC program using the ultra-large Stripa core.

A program of size-effect studies will be initiated using a 0.91-meter-diameter by 1.83-meter-high naturally fractured ultra-large core of charcoal black granite. The sample will have a fracture at the mid-height normal to the long axis. A series of tests will be performed in which several cycles of increasing and decreasing normal stress will be applied to the fracture to investigate the stress-flow relationship. These experiments will be repeated on the same sample after the diameter has been reduced. Four increments of diameter reduction will likely be made until it is reduced to approximately 45 centimeters.

Sample instrumentation will include measurement of fracture aperture, hydraulic gradient, and flow rate. Data from the tests will be analyzed to study the validity of the parallel plate analogy and the cubic law of flow in fractures. By the end of FY 80, two series of tests at two different diameters should be well advanced.

Activities During the Reporting Period

During the reporting period, LBL staff visited quarries at several sites and identified massive samples of fractured granite suitable for forming into ultra-large cylindrical cores. Based on the field work, orders have been placed for two cylindrical samples of charcoal black granite and one sample of Lake Placid green granite. Delivery of the samples to the test facility is scheduled for September, 1980.

Preparation of the charcoal black sample to be used in the size-effect test program was advanced during the reporting period. The fractures and inclusions in the rock have been mapped; the core upended, centered and cemented to a base plate; and a 3-inch-diameter hole drilled through the long axis. Falling-head permeability tests designed to investigate approximate hydraulic characteristics of the sample were completed in June, 1980. Preliminary analysis of the data from these tests shows that flow through the fracture that intersects the mid-plane of the sample is about 2.0 cc/min under a head of some 28 kPa (4.0 psi). The instrumentation matrix for this sample has been designed and drilling of support mountings is scheduled for the first week of July, 1980. Nine LVDTs will be placed vertically across the fracture around the periphery of the sample. A total of 20 strain gages will be used to investigate stress distribution across the sample and in proximity to the principal fracture. Two additional LVDTs will be mounted across secondary fractures present in the sample.

THERMOMECHANICAL-HYDROLOGICAL MODEL DEVELOPMENT

Objective

During FY 79 about 20 existing numerical models were selected for detailed study. This evaluation is to be completed in early FY 80 with a draft report.

In the later half of FY 80, efforts will concentrate on the improvement of the LBL model, ROCMAS. This model includes thermal effects, which makes it a potentially useful tool in the study of thermally induced, coupled stress, and fluid-flow phenomena. The model will be improved, validated, and eventually applied to generic studies as a means of illuminating some of the key problems in understanding the thermo-mechanical-hydrological process.

Activities During the Reporting Period

The development of the numerical model ROCMAS was initiated during this quarter. The flow-stress part of the program has been validated against a number of fracture flow problems for plane two-dimensional and axisymmetric systems. The program has been revised to produce a clarified version for easy usage and development. An initial thermal portion has also been incorporated into the program. Various validation studies are being planned. The temperature dependence of the fluid properties will be implemented shortly in the program to improve its capability of modeling thermal, flow, and stress fields.

Three papers were prepared based on studies with ROCMAS. The first is a paper entitled "Numerical Modeling of Thermohydrological Flow in Fractured Rock masses", prepared for publication in the Proceedings of the Fracture Hydrology Workshop. The paper summarizes the efforts of the past few years that have culminated in the development of the coupled stress-fluid flow analysis code ROCMAS. The overall theoretical basis of the stress flow analysis for plane two-dimensional and axisymmetric cases are introduced and the results of modeling the problem of a deep asymmetric reservoir with a fracture at the center are presented and discussed in the paper.

The other two papers give more detailed discussions of the background and rationale of the program. The title of one is "A Finite Element Method for Stress and Fluid Flow Analysis in a Fractured Rock Mass, Part I: Formulation and Verification". The other paper is "A Finite Element Method for Stress and Fluid Flow Analysis in a Fractured Rock Mass, Part II: Generalization and Application to a Deep Axisymmetric Confined Reservoir with a Horizontal Fracture at the Center".

IN-SITU TESTING FACILITY IN CRYSTALLINE ROCK

Objective

The objective of this task is to complete a feasibility study for a possible in situ test facility in crystalline rock in the United States.

Activities During the Reporting Period

A final report will be published during the final quarter of FY 80 for this project.

LARGE TRIAXIAL CELL SITE USAGE AND SAFETY INVESTIGATION

Objective

The objective of this task is the resolution of the crucial site usage and safety questions connected with the construction of a new high-pressure/high-temperature triaxial testing cell for ultra-large rock cores at the Richmond Field Station.

Activities During the Reporting Period

During the quarter, plans for the new high-pressure/high-temperature triaxial cell test facility were reviewed with various safety and regulatory institutions. In most cases, the key requirement seems to be that the pressure vessel carry an official stamp of compliance with the ASME Boiler Code. Potential vendors for the triaxial cell component are capable of supplying the ASME stamp.

In the absence of specific personnel safety requirements imposed from outside LBL, an obligation to assess operational hazards in a rigorous, objective manner, and to provide appropriate safeguards is recognized. The independent evaluation of at least one qualified outside specialist will be obtained as part of this process.

STRIPA IN SITU STRESS MEASUREMENT

Objective

The Stripa in situ stress measurement program began 1 May, 1980. The primary goal for the program for FY 80 is to measure the stress in a 400-meter vertical hole drilled from the surface about 1 mile north of the mine. The purpose of the measurements is to determine the far-field stress prior to underground measurements within the mine itself near the test facility.

Two stress measurement techniques are being used. The first is the Leeman triaxial cell, a strain gage device which is overcored. While this technique is commonly used in short (<30-meter) holes, only the Swedish Power Board has been able to successfully adapt it to holes of greater depth. Details of the method are presented in Hiltscher, Martna, and Strindell (1980).

The second technique is hydraulic fracturing (Haimson, 1978), which is the only technique which has been routinely applied to deep holes.

Activities During the Reporting Period

Previously, a system for hydraulic fracturing was built at LBL, including two innovations—a downhole assembly for measuring packer pressure and injection pressure with simultaneous surface readout, and a wireline impression packer for obtaining fracture orientation. The former of these devices is a high-pressure modification for instruments used in the Stripa hydrology program. The entire fracturing system was assembled and tested in a 100-foot borehole. The rock was granite, and the site was chosen to simulate the rock and borehole conditions expected at Stripa. The tests were performed during three field sessions in May and June, and the tested system is being readied for shipment to Sweden in mid-July.

During May, plans were made for drilling a 400-meter borehole at Stripa, Sweden and performing four sets of three measurements each using the Leeman cell. The measurements are to be done at 100, 200, 300, and 400 meters. The Stripa mine test facility is at a depth of 343 meters.

Drilling began in Sweden on 25 June. The first 100 meters was completed 8 July, and the first set of overcoring measurements was completed 14 July. On the present schedule, drilling will be completed between 11 August and 22 August, at which time the hydraulic fracturing will be performed.

Hydrologic tests for permeability and pore pressure are routinely done during drilling. The decline in water level after drilling is monitored nightly and pressure permeability measurements using a simple packer and downhole pressure are made over each weekend on the zone drilled the previous week. The hole is continuously cored and core-logged for use in locating the subsequent hydrofracture tests.

POST HEATER DRILL-BACK INVESTIGATION

Objective

The objective of this task is the investigation of the effects of the now complete heating/cooling cycle on the Stripa H-10 heater borehole and adjacent granite rock mass. This is to be accomplished by the drilling and TV logging of two new boreholes intersecting the heater location. Core samples will be shipped to Berkeley for laboratory examination.

Activities During the Reporting Period

Two 76-mm-diameter holes, approximately 12 meters long, were drilled horizontally from the extensometer drift into, through, and approximately 2 meters beyond the H-10 heater hole. The holes were spaced 1 meter apart vertically and bracketed the position of the central plane of the heater. Core recovery was essentially 100 percent. The lithology and orientation and spacing of fractures were logged and the core was packed and shipped to Berkeley for subsequent petrographic and geochemical examinations and geomechanical tests.

REFERENCES

Haimson, B. C. 1978. "The Hydrofracturing Stress Measuring Method and Recent Field Results", *Int. Jour. Rock Mech. Min. Sci.*, 15:167-178.

Hiltscher, J., F. Martna, and L. Strindell. 1979. "The Measurement of Triaxial Rock Stress in Deep Boreholes in the Design and Construction of Rock Openings", *Proc. 4th Cong. Int. Soc. Rock Mech.*, Montreaux, Switz., Vol. 1, pp. 227-234.

WBS 1.1.2

Project: Stripa Test Program

Principal Investigator: Lawrence Berkeley Laboratory (LBL)

ONWI Project Manager: R. A. Robinson

Objective

LBL, in conjunction with the Swedish Nuclear Fuel Safety Board (KBS), is to conduct in situ heater tests, hydrologic tests, and fracture system characterization studies in granite in an iron ore mine at Stripa, Sweden.

Activities During the Reporting Period

GEOPHYSICAL ASSESSMENT

During the first part of the quarter, work progressed on the analysis of the gamma ray logs and the cross-hole ultrasonic and acoustic emission data collected around the H9 heater experiment. Calibration checks were run on the gamma ray probe at Stripa, and in Berkeley a laboratory system was set up for measuring attenuation and velocity of ultrasonic propagation in stressed samples.

In June, final cross-hole ultrasonic measurements were made on the cooled-down H9 heater area at Stripa. By comparing the measurements with those made before heater turn-on, it should be possible to assess the change in rock properties resulting from the thermal cycling of the rock around H9.

A report on the acoustic emissions monitoring of H9 and H10 cool-down is nearing completion. One interesting occurrence noted in the acoustic emission data for H9 was a renewed burst in acoustic emission activity at a time well after heater turn-off, and at a time in which the number of events was expected to be small. This increase in acoustic emission activity was preceded by a sudden drop of the P-wave velocity. Though this phenomenon is not completely understood, it may signify the opening of a fracture.

STRIPA ULTRA-LARGE CORE STUDY

Objectives

The permeability of the core will be investigated under varying states of axial stress. This will be achieved by injecting water into (or possibly withdrawing water from) a borehole drilled through the long axis of the core while the core is subjected to axial loading in the ultra-large triaxial testing machine. Several cycles of increasing-decreasing axial stress will be applied to study the effects of load-history on permeability and deformation modulus. The tests will be designed to study the overall permeability of the core and the conductivity of selected principal fissures. The core will be instrumented to gain insight into the stress-deformation behavior of the principal fracture and its relationship to fracture conductivity. Measurement of total axial strain will yield information regarding the deformation modulus of fissured Stripa granite. Data of this type, obtained from a sample of dimensions closer to those of practical significance than has previously been available, is important to the rational interpretation of the in situ hydrological and geotechnical results gathered from the Stripa experiments.

Activities During the Reporting Period

Testing of the ultra-large Stripa core was completed on 20 March, 1980. The principal effort during the current reporting period has involved the extensive task of reducing the raw data gathered from the test instrumentation. The first objective of this work is to produce an edited raw data base expressed in transducer output voltages, annotated with pertinent test log summaries. Next, a similar data base will be produced, but in calibrated engineering units. These files will be produced in hard copy and magnetic tape form, supported by our guides. Except for cursory checks, data analysis will begin after the engineering-units data base is complete. Draft versions of these raw data and engineering units files have been prepared during the reporting period and editing is approximately 90 percent complete. The data analysis effort has been initiated and is concerned with study of the consistency of data gathered from the various instrumentation systems. Comparison of deformations measured by linear variable displacement transducers (LVDTs) mounted across fractures and anchored at the top and bottom of the sample, and strains measured with the strain gages is in progress. Early results indicate that the deformation or "elastic" modulus of the sample was on the order of 20 GPa during loading, and 37 GPa during unloading. This compares with moduli of some 50 to 55 GPa found for the 5.2-cm-diameter samples of Stripa granite tested during preliminary work for this project.

SMALL-CORE TEST FACILITY

Objectives

The objectives are to develop a facility for testing small rock cores, and to complete testing of a preliminary series of rock samples from the Stripa mine experiments. Specifically, data will be produced on the rock moduli and coefficient of thermal expansion as a function of confining pressure and temperature. These data are needed to provide a better understanding of the constitutive behavior of the Stripa rock mass and a broader data base for the numerical modeling effort. Continued testing of a large number of rock samples will provide a significant data base for determining rock property values to be used in various modeling programs.

Activities During the Reporting Period

A computer Data Acquisition System (DAS) has been assembled and software has been written for automated data recording. Components for a servo-control system to be tied into the DAS computer have been designed and ordered. This will allow faster, more precise testing than the original manual control mode, and also offers a potential for more automated test cycling in the future.

During May, a system calibration sequence was successfully run on an aluminum dummy sample of known properties. The effort in June was directed at sample preparation and initial testing of a rock specimen. A 62-mm-diameter intact sample was prepared with six strain gages and one temperature sensor mounted to it. Four 1/2-inch gages, two mounted axially and two mounted circumferentially, were used. Additionally, two 3/4-inch gages were mounted axially. This was done to determine whether the difference in gage length and gage area affected measured strain. The sample was jacketed using heat-shrinkable Teflon tubing and placed in a test cell. The first test consisted of increasing all-around confining pressure to 55 MPa and then applying a maximum axial load of 260 MPa.

Continuing progress has been made on the final design of the electro-servo-control system for the test machine. The servo motors have been received and tested to verify adequate start-up torque to overcome static friction in the system. Once this was done, the corresponding electrical power supply units were ordered. All components of the system should be available for assembly and fine-tuning during August and September.

WBS 1.1.2

Project: Thermomechanical Simulations

Principal Investigator: Science Applications, Incorporated (R. Hofmann, D. E. Maxwell)

ONWI Project Manager: M. R. Wigley

Objective

Objectives of this program are as follows:

(1) Validation of the STEALTH 2D and 3D explicit finite-difference computer codes as analytic predictive and licensing tools relative to the generic design of nuclear waste repositories in various geologic strata.

(2) Development of constitutive models for various nuclear waste repository geologies.

(3) General technical support and assistance to help ONWI assess constitutive models and data, numerical techniques, and physical mechanisms related to generic nuclear waste repository designs.

(4) Development of a hydrology model for STEALTH 2D.

Activities During the Reporting Period

No progress report was submitted for the period.

WBS 1.1.2

Project: Convective Heat Transfer in Room and Pillar Geometries

Principal Investigator: Ohio State University (R. Christensen)

ONWI Project Manager: G. Raines

Objective

The objective is the determination of local and average convective heat transfer coefficients on the surfaces of the repository mine drift, and measurement of local temperature distribution in the drift.

Activities During the Reporting Period

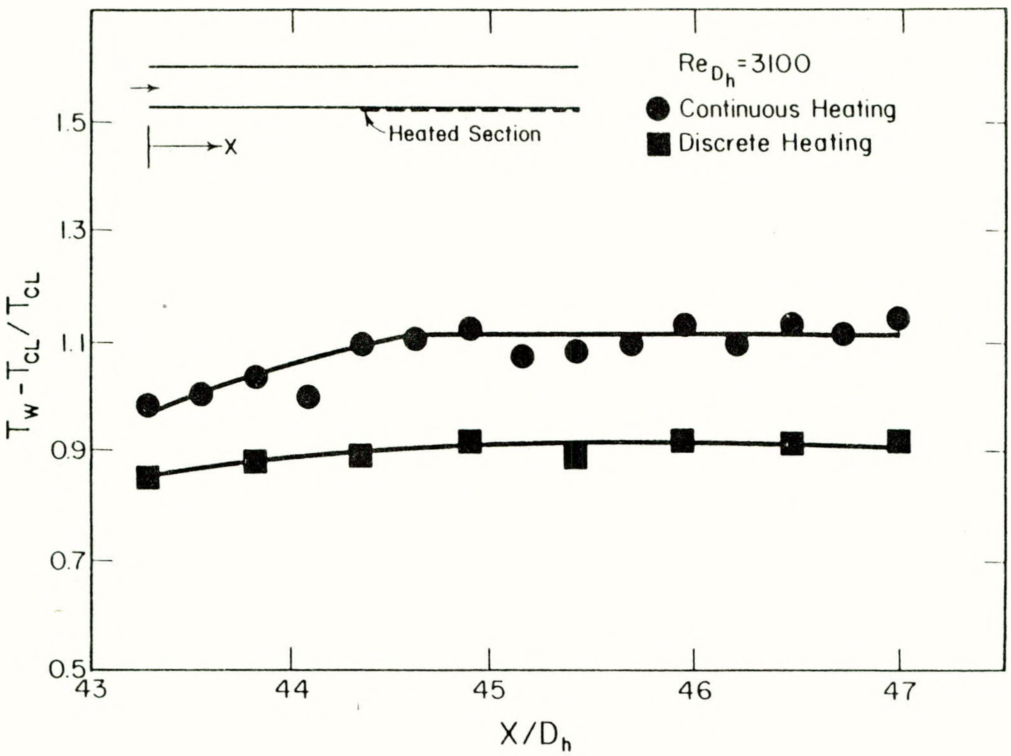
Temperature Measurements

The experimental apparatus was run at Reynolds numbers ranging from 3,000 to 30,000. For these runs, the Reynolds number was defined in terms of the hydraulic diameter of the flow channel, and the kinematic viscosity was evaluated at the average centerline temperature, $T_{CL,avg}$. The average centerline temperature was taken as the arithmetic mean of the centerline temperatures upstream and just downstream of the heated portion of the channel. The maximum variation between T_i and T_e was about 2.5 F, which is within the accuracy limits of the instrumentation.

For each heater that was activated in these runs, the temperature above and below it and the temperature of the surface of the channel floor, T_W, were measured. Heater power was also continuously monitored to maintain it at a constant value of 5 watts.

At each Reynolds number, 16 heaters were used. In one set of runs, the heaters were activated sequentially, giving the effects of continuous heating on the floor of the channel over progressively greater lengths of the floor. This modeled a typical loading sequence for waste canisters. In another set of runs, heaters were alternately activated. (Only eight heaters were used.) Plots of the dimensionless wall temperature at the center of each heater $(T_W - T_{CL})/T_{CL}$ versus the dimensionless channel length, x/D_h, measured from the inlet (i.e., at the blower upstream of the heated section), are presented in Figure 1a through 1e. Figure 1a contains a diagram further defining the coordinate system. Both continuous and discrete heating are represented in these figures.

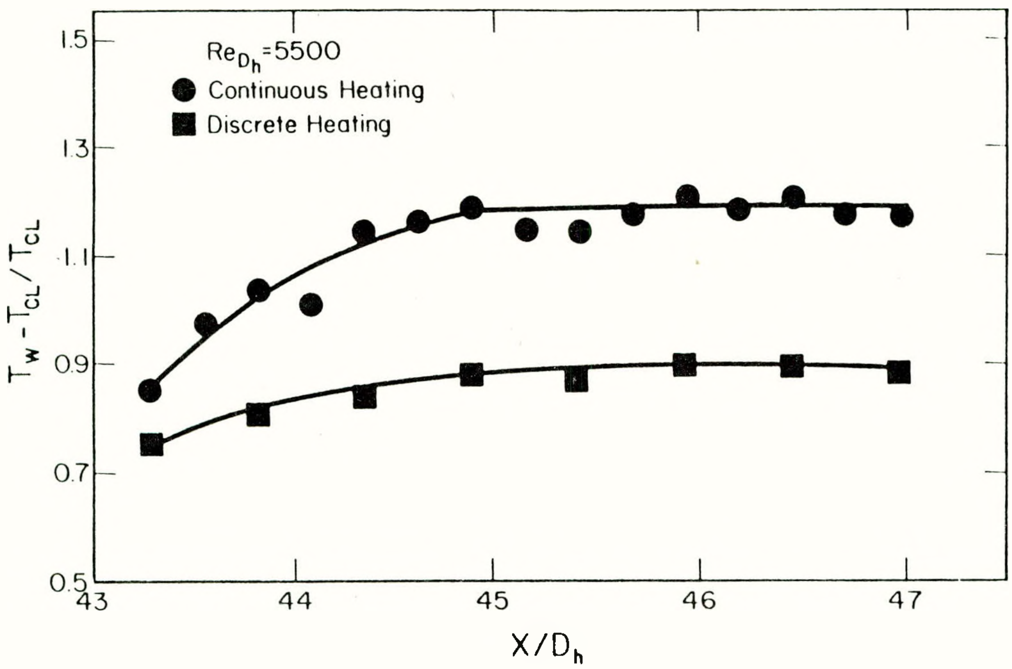
In each of the five runs, the dimensionless wall temperature increases monotonically with distance over the initial portion of the heated length. The fourth heater ($x/D_h \simeq 44.12$) is an exception to the general trend since its temperature is low in all cases. A defective thermocouple is suspected as the cause of this low reading. With increasing distance in the heated section, it appears that an asymptotic value for dimensionless wall temperature is reached for both continuous and discrete heating. These trends indicate the approach to a fully developed heat-transfer coefficient on the channel floor.



a.

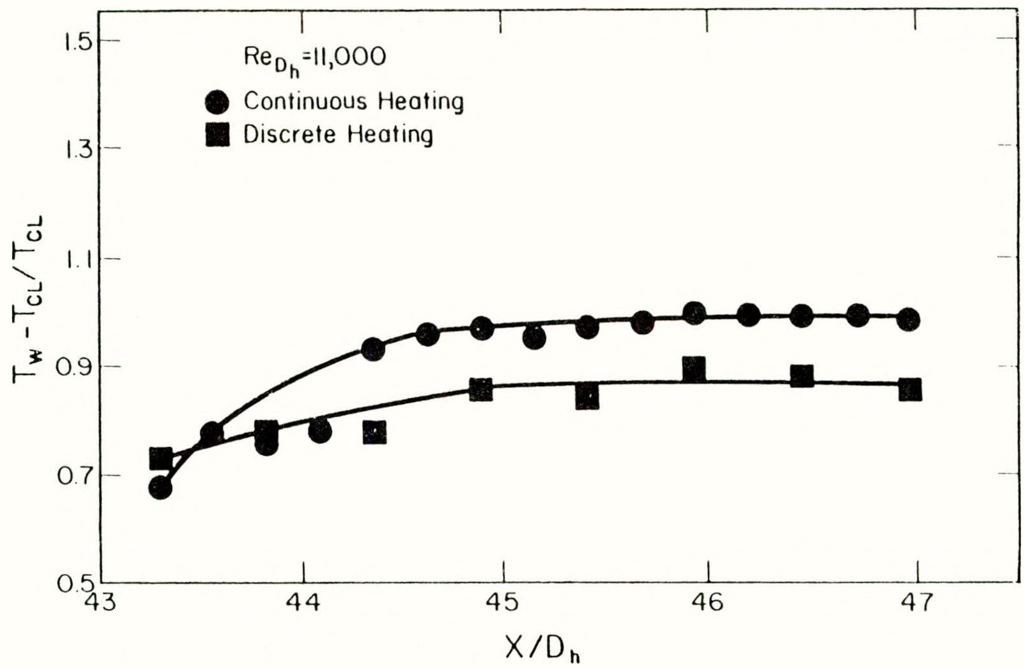
FIGURE 1. DIMENSIONLESS WALL TEMPERATURE VERSUS DISTANCE FROM CHANNEL INLET

Power is 5 watts per heater.



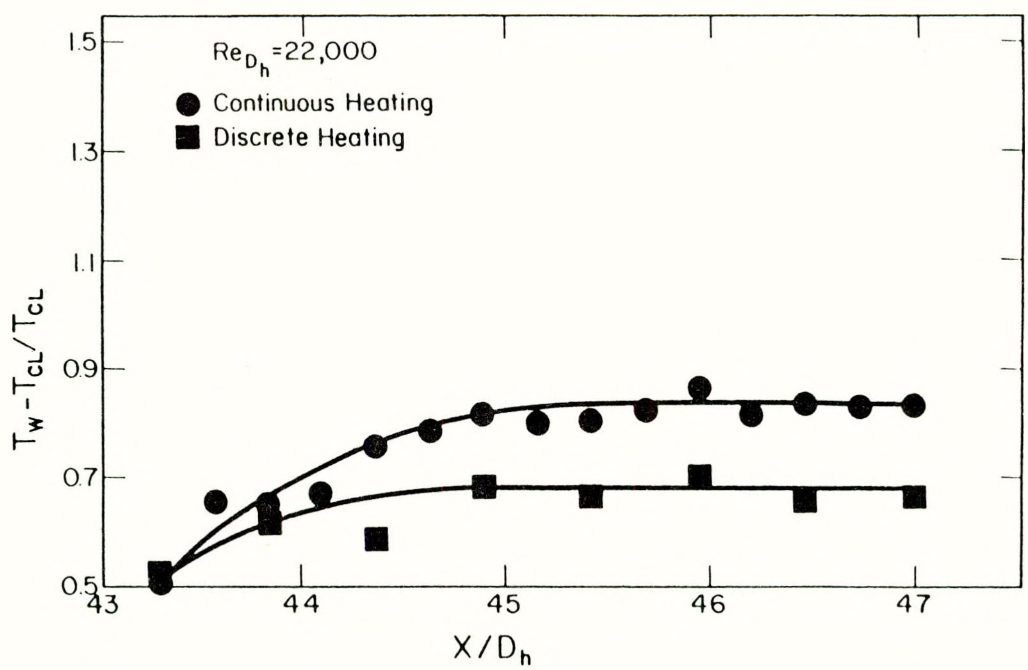
b.

FIGURE 1. (CONTINUED)



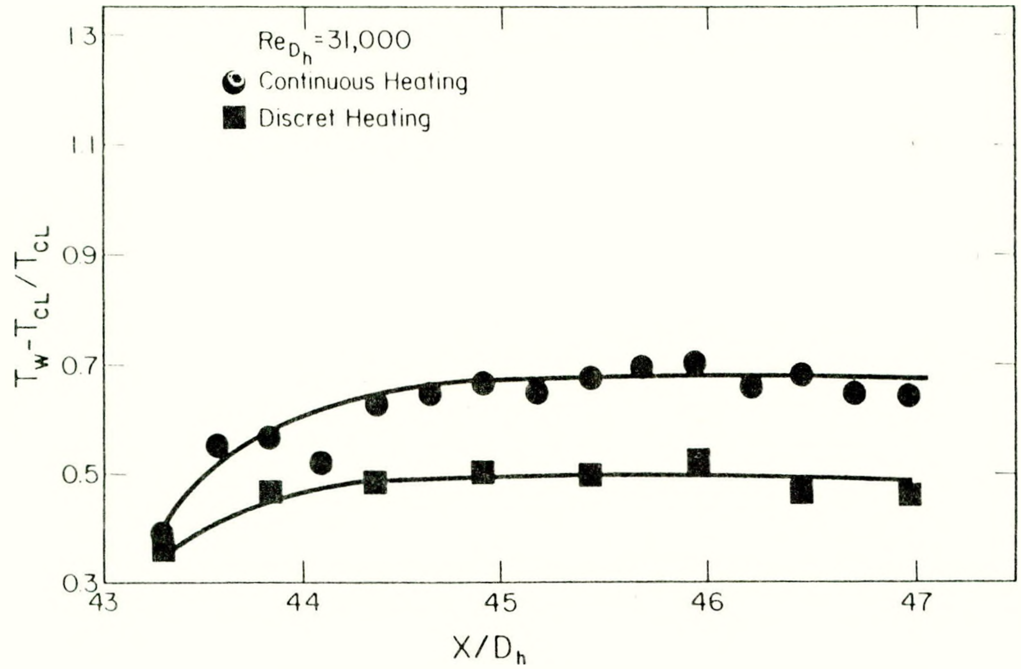
c.

FIGURE 1. (CONTINUED)



d.

FIGURE 1. (CONTINUED)



e.

FIGURE 1. (CONTINUED)

Heat-Transfer Coefficient

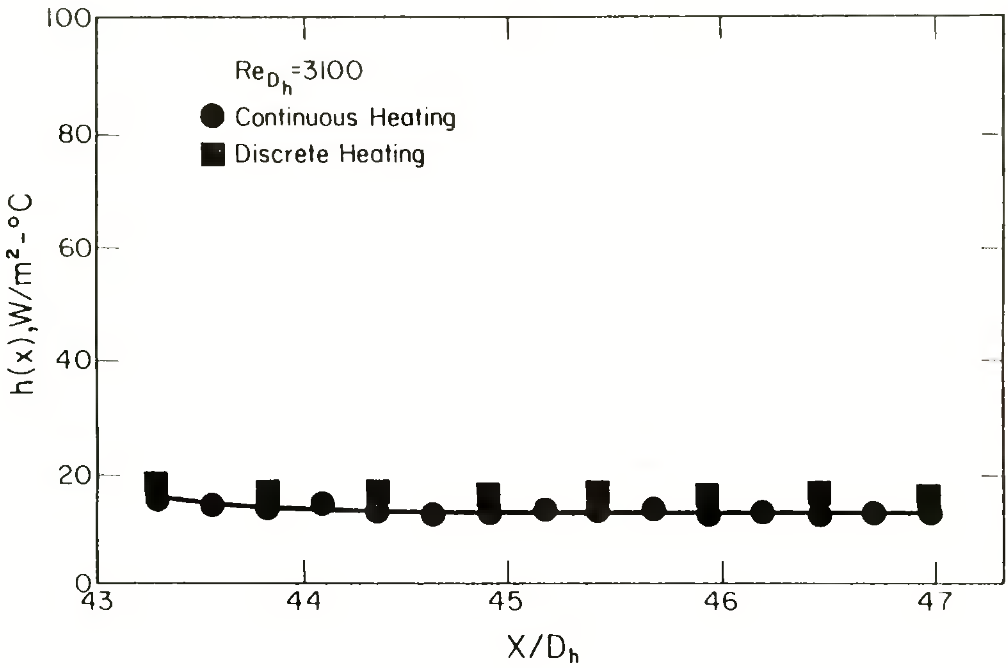
For the experimental data presented in Figures 1a through 1e, the local heat-transfer coefficient was calculated in terms of the heat flux through the floor of the channel and the local temperature difference between the wall and the centerline of the channel. Thus,

$$h = Q/A_p\Delta T, \tag{1}$$

where A_p is the area of the heater.

The experimental data have shown that the heat-transfer rate through the floor into the channel is 99 percent of the heater power. This has been taken into account in the heat-transfer-coefficients calculations. However, the area of the heater, A_p, is not the exact area for heat transfer due to axial conduction, nor is the temperature profile above the heater a constant at T_w. These effects will cause some error and/or uncertainty in the heat-transfer coefficients calculated with Equation 1. A subsequent report will contain an error analysis that will put a numerical bound on the total uncertainty in the heat-transfer coefficients. It may be expected, nevertheless, that the trends in local heat-transfer coefficients will not be significantly changed when the error analysis is completed.

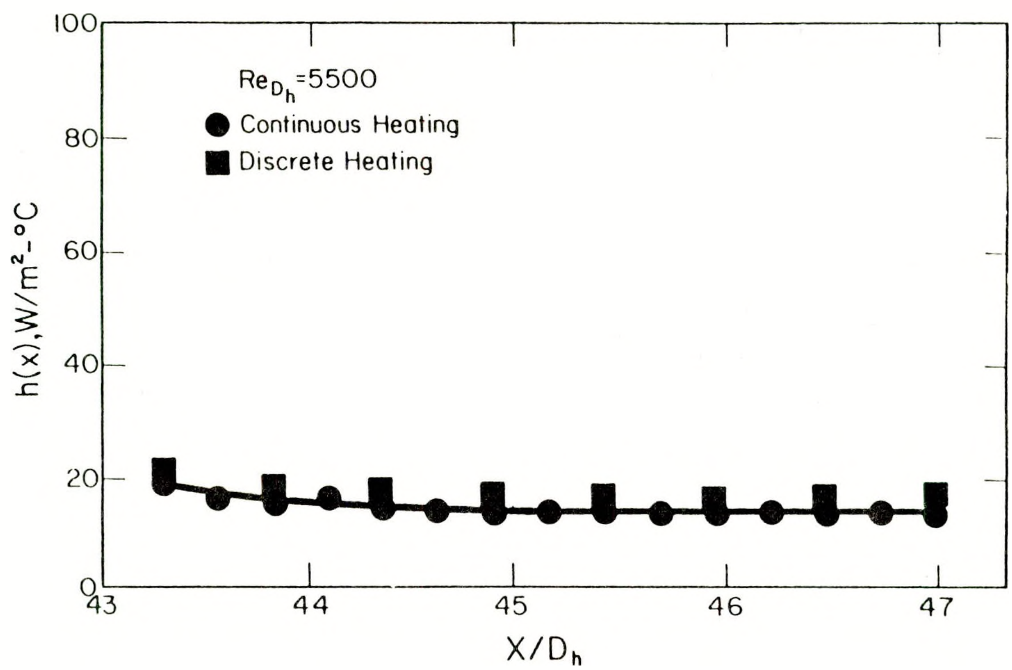
In Figures 2a through 2e the heat-transfer coefficients are plotted as a function of dimensionless distance in the fully developed turbulent flow regime for continuous and discrete heating. In all cases, the heat-transfer coefficient decreases with increasing distance from the leading edge of the heated section. A nearly constant heat-transfer coefficient is obtained after approximately four heaters from the leading edge for continuous and discrete heating. Owing to axial conduction and the location of wall thermocouples at the approximate center of the heater, the present data will not show an infinite heat coefficient at either the leading edge of the heated section or at the first heater. This, of course, will be the case in a repository since axial conduction will always be present in the walls.



a.

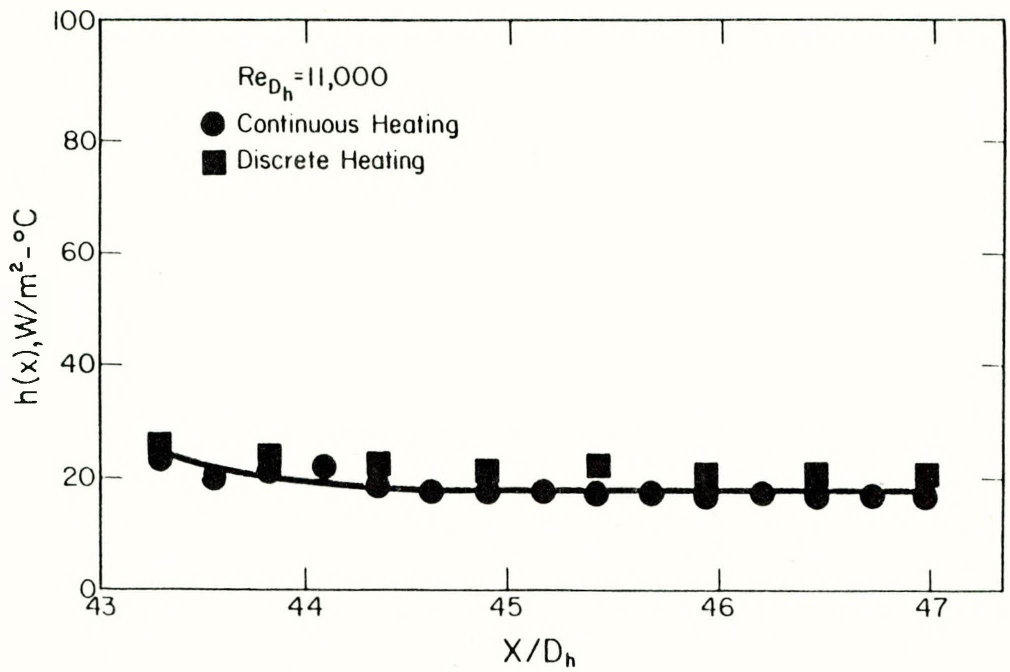
FIGURE 2. LOCAL HEAT-TRANSFER COEFFICIENTS VERSUS DISTANCE FROM CHANNEL INLET

Power is 5 watts per heater.



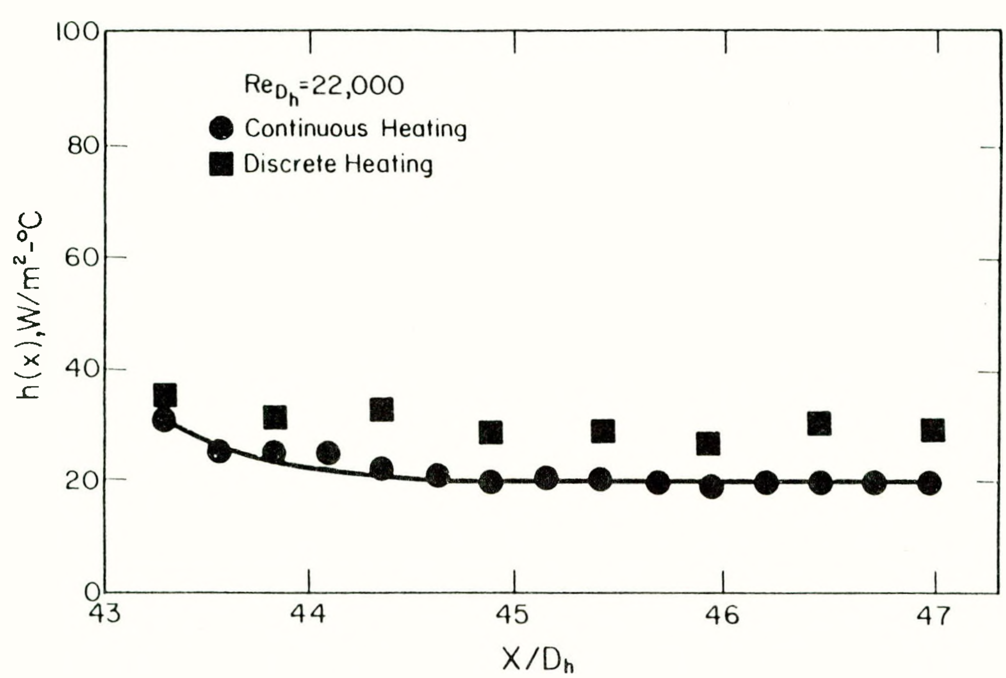
b.

FIGURE 2. (CONTINUED)



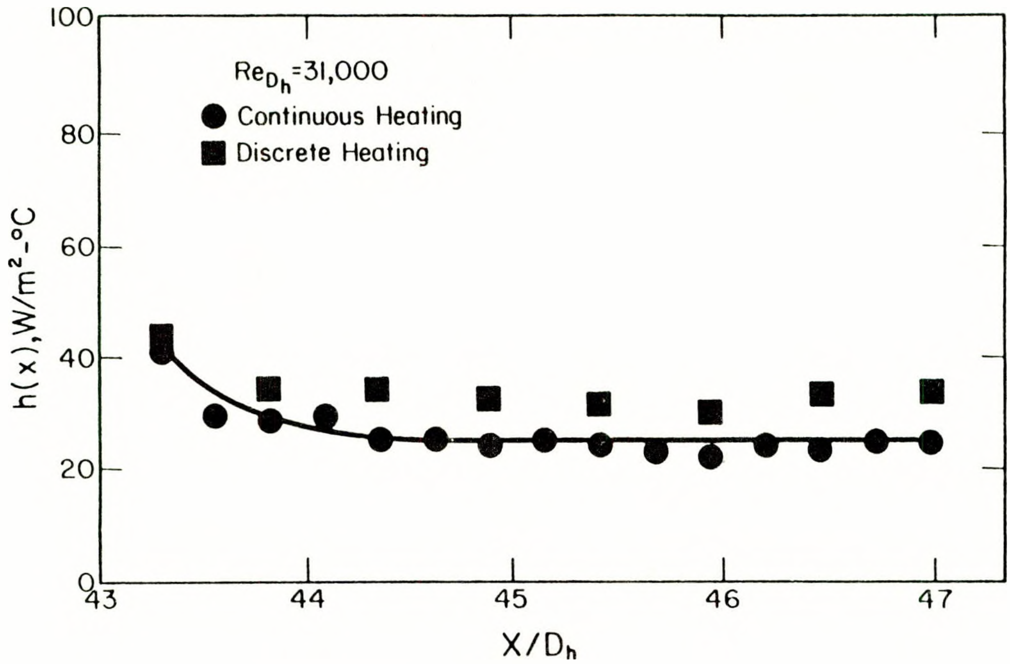
c.

FIGURE 2. (CONTINUED)



d.

FIGURE 2. (CONTINUED)



e.

FIGURE 2. (CONTINUED)

Asymptotic values of the local heat-transfer coefficients plotted as a function of Reynolds number are presented in Figure 3.

Nusselt numbers for the present runs have been calculated in terms of the hydraulic diameter, D_h, as the characteristic length scale. The thermal conductivity of the fluid (air) was evaluated at the average centerline temperature, $T_{CL,avg}$. Local Nusselt numbers as a function of dimensionless distance are presented in Figures 4a through 4e. In all cases, the local Nusselt numbers follow trends established by local heat-transfer coefficients. Asymptotic values of Nu(x) are plotted in Figure 5 as a function of Reynolds number and are compared with values for pipe flows developed by Gnielinski (1976).

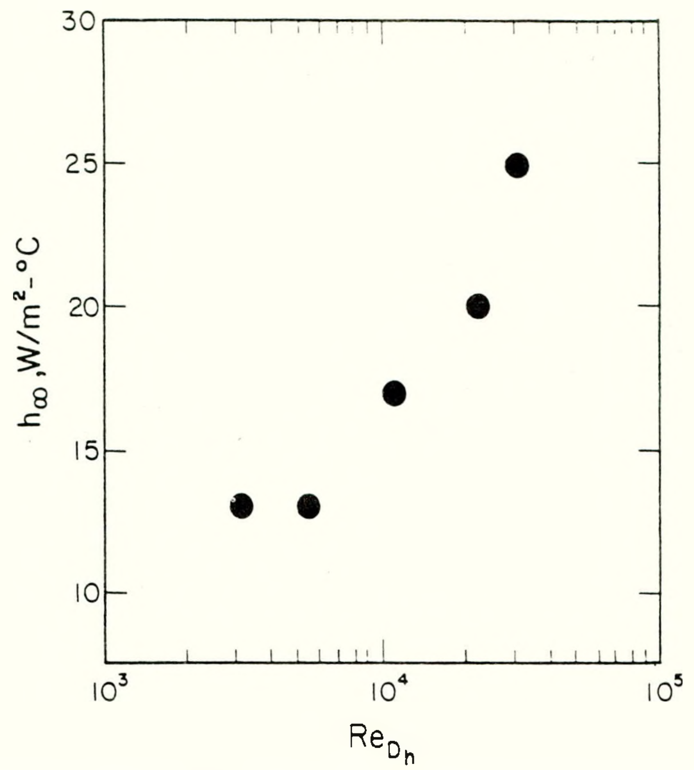
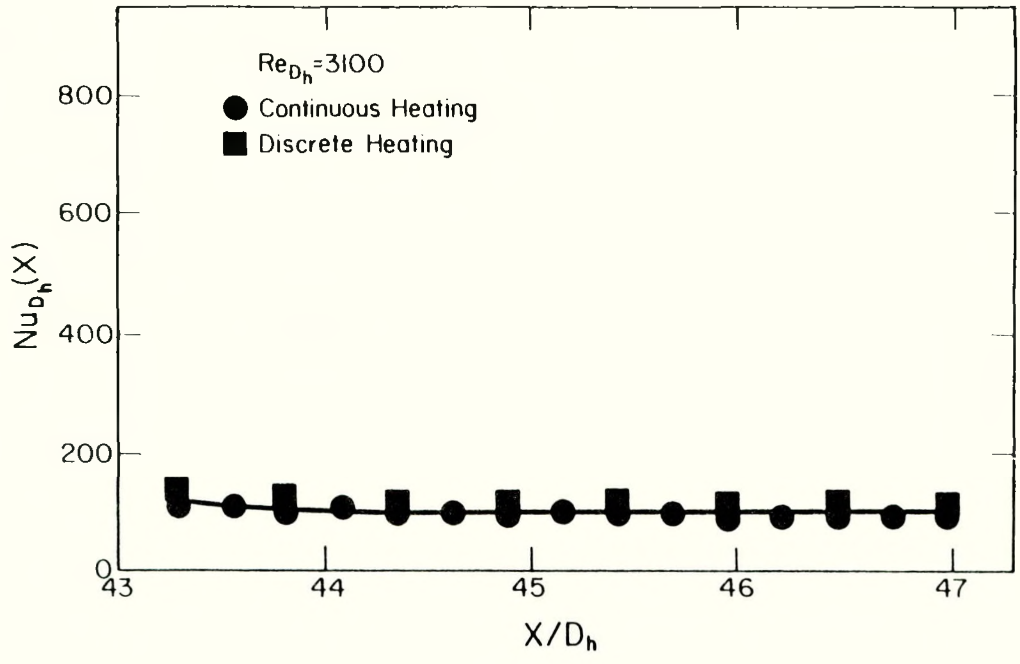


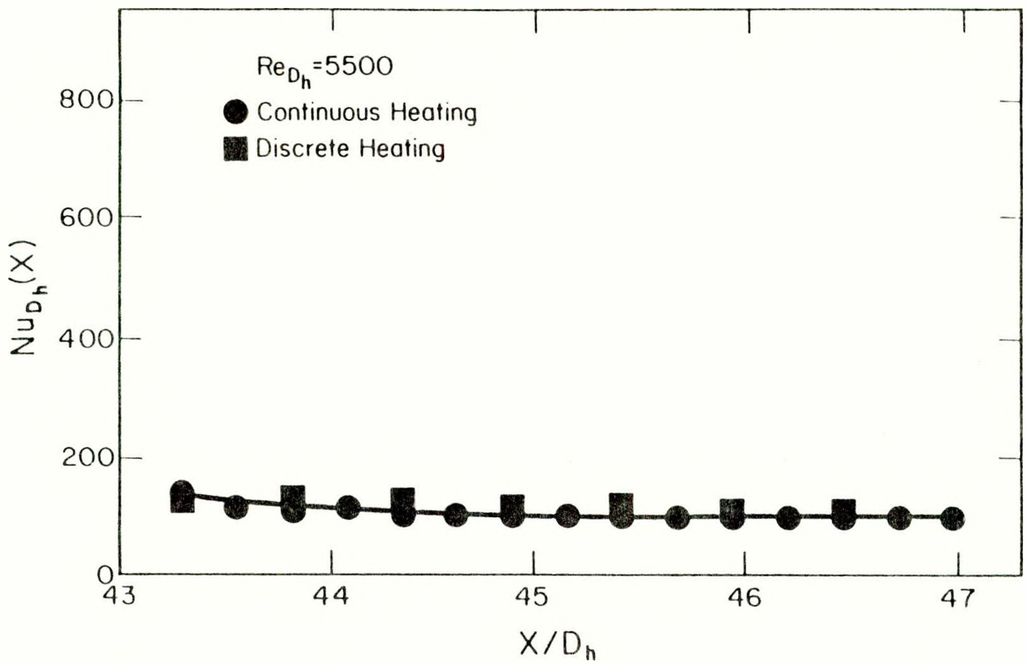
FIGURE 3. ASYMPTOTIC HEAT-TRANSFER COEFFICIENTS FOR CONTINUOUS HEATING



a.

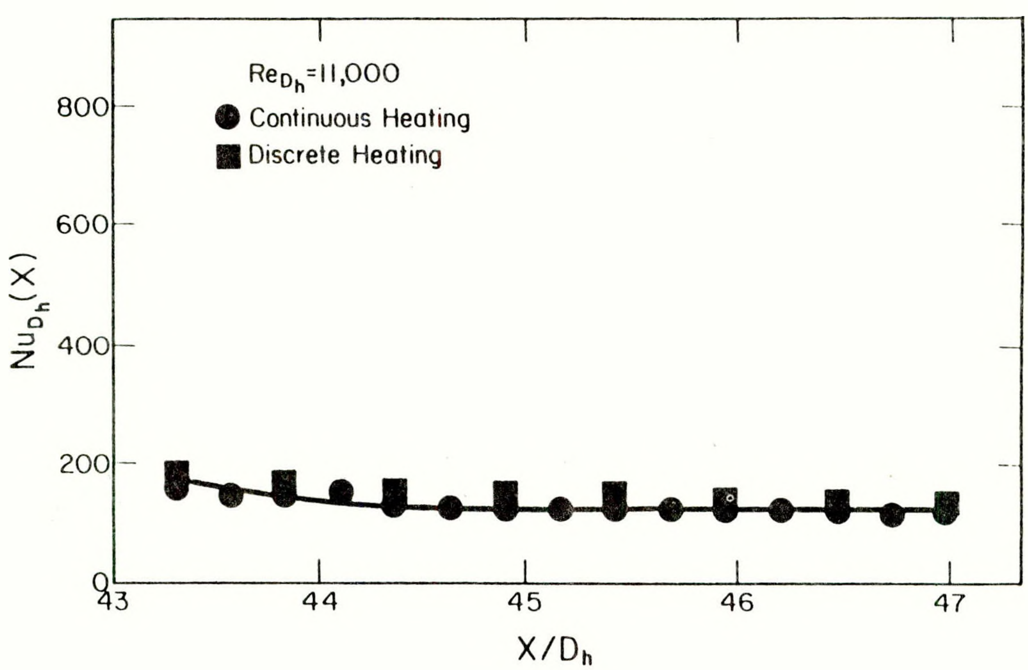
FIGURE 4. LOCAL NUSSELT NUMBER VERSUS DISTANCE FROM CHANNEL INLET

Power is 5 watts per heater



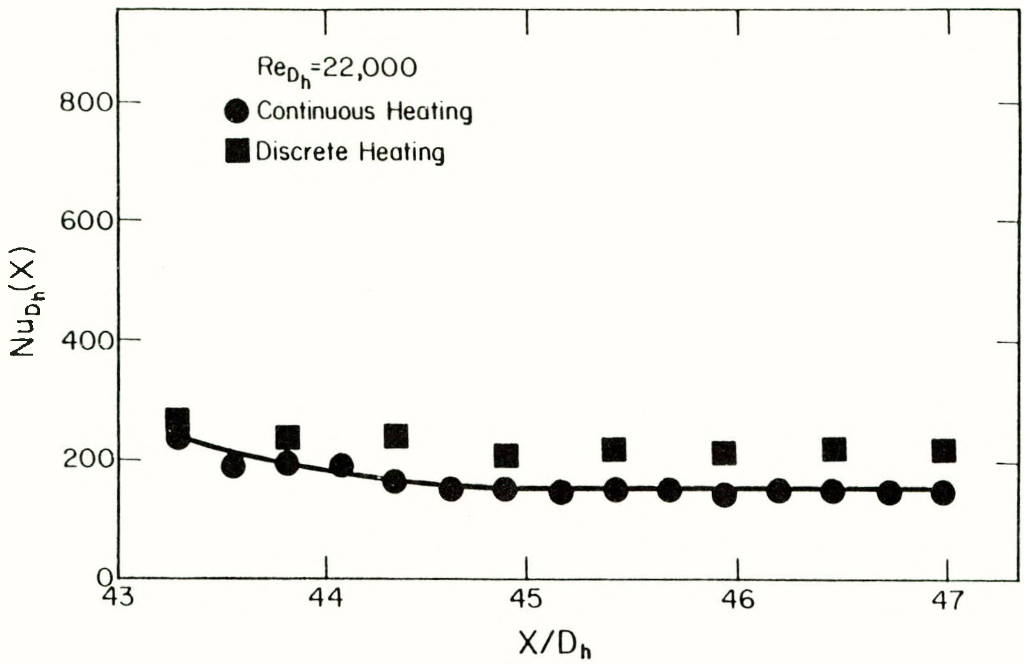
b.

FIGURE 4. (CONTINUED)



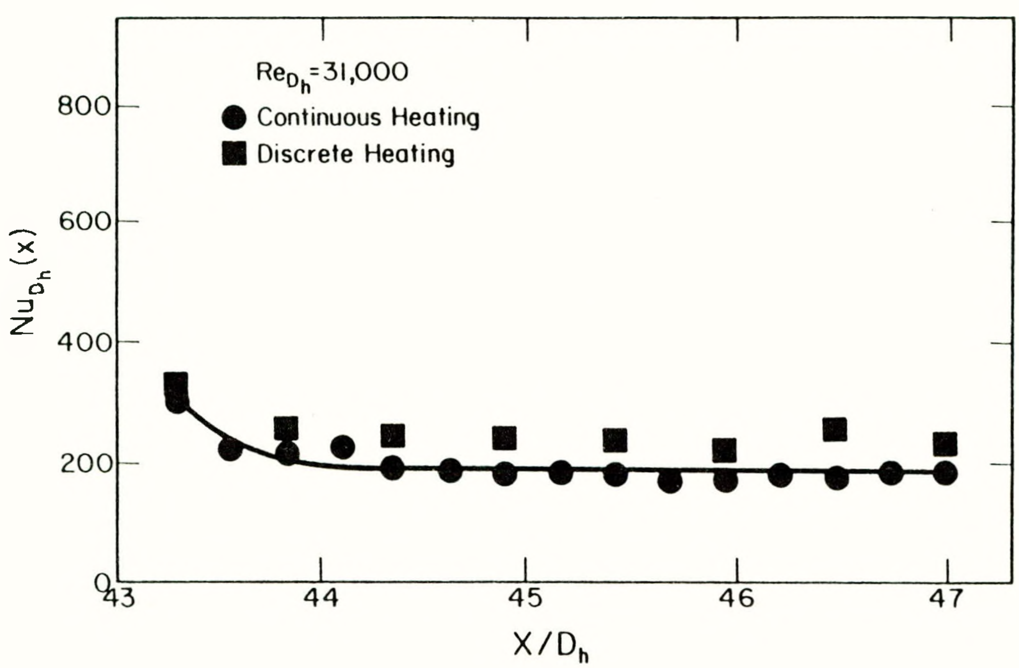
c.

FIGURE 4. (CONTINUED)



d.

FIGURE 4. (CONTINUED)



e.

FIGURE 4. (CONTINUED)

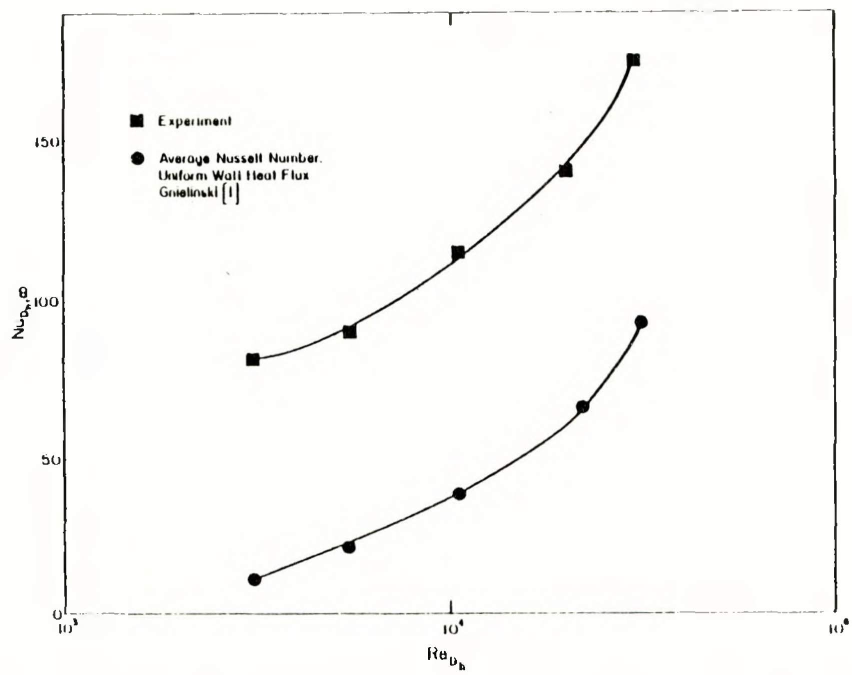


FIGURE 5. ASYMPTOTIC NUSSELT NUMBERS FOR CONTINUOUS HEATING

NOMENCLATURE

A_c	Cross-sectional area of channel, m^2
A_p	Heater pass area, m^2
D_h	Hydraulic diameter, $4A_c/P_w$/m
h	Heat-transfer coefficient, W/m^2-C
k	Thermal conductivity of fluid, W/m-C
Nu	Nusselt number, hD_h/k
P_w	Channel perimeter, meters
Q	Heat-transfer rate, watts
Re_{Dh}	Reynolds number, VD_h/ν
$T_{CL,avg}$	Average centerline temperature, $(T_i+T_e)/2$, C
T_e	Channel centerline air temperature at exit, C
T_i	Channel centerline inlet air temperature, C
T_w	Channel floor surface temperature, C
ΔT	$T_w - T_{CL}$, C
V	Average channel velocity, m/sec
x	Distance from blower along channel, meters
ν	Kinematic viscosity, m^2/sec

REFERENCE

Gnielinski, V. 1976. "New Equations for Heat and Mass Transfer in Turbulent Pipe and Channel Flow", *International Chemical Engineering*, 16 (2):359-368.

WBS 1.1.2

Project: Convective Heat Transfer Within Spent Fuel Canisters

Principal Investigator: Ohio State University (F. A. Kulacki)

ONWI Project Manager: G. Raines

Objective

The objective is the determination of local and average convective heat transfer coefficients at the inside surface of a spent fuel canister, the local temperature distribution of the canister, and the axial variation of rod temperatures within the assembly. Owing to the complex nature of the flow created by the fuel rods and their support plates, the problem must be treated experimentally.

Activities During the Reporting Period

Experimental Results

The experimental runs were conducted in the following manner for each power level at the central rod. First a run was conducted with the system at atmospheric pressure to obtain heat transfer via combined convection and thermal radiation. The system was then evacuated to approximately 15 mm Hg. Heat-transfer data at the same power level were then obtained and these were subsequently used to determine the overall conductance for thermal radiation between the two cylinders. This quantity was calculated from the following relation:

$$C_r = \frac{q}{\sigma\,(T_i^4 - T_o^4)\ \text{vacuum}} \tag{1}$$

where C_r is defined by

$$C_r = \frac{1}{\dfrac{1}{\varepsilon_i} - 1 + \dfrac{1}{F_{i-o}} + \left(\dfrac{A_i}{A_o}\right)\left(\dfrac{1}{\varepsilon_o} - 1\right)} \tag{2}$$

Once the value of C_r is obtained, it can be used to determine the equivalent heat-transfer coefficient for thermal radiation. This quantity is given by

$$h_r = C_r \sigma (T_i^2 + T_o^2)(T_i + T_o). \tag{3}$$

The temperatures used to find h_r are taken from measurements at atmospheric pressure. The radiation heat-transfer coefficient is then subtracted from the total heat-transfer coefficient, which is the ratio of the total heat flux to the temperature difference across the annulus. The final value of the heat-transfer coefficient is the corrected value for free convection.

Figures 1 and 2 show the temperature distribution along the rod with power input as a parameter. The data in Figure 1 were obtained at atmospheric pressure, while those in Figure 2 were obtained at 15.2 mm Hg. It is evident that a reduction in pressure corresponds to a sharp increase in temperature.

The temperature along the surface of the outer cylinder is kept constant to an acceptable level by thermostatically controlled water circulating through a copper coil attached to the outside of the cylinder. Figure 3 shows the typical temperature distribution along the cylinder. The mean temperature for these particular data is 24.8 C with a standard deviation of 0.3 C.

The mean temperatures on the rod and cylinder surfaces at pressures of 760 and 15.2 mm Hg are given in Tables 1 and 2, respectively. Thermal conductance values for each run are also given in Table 2.

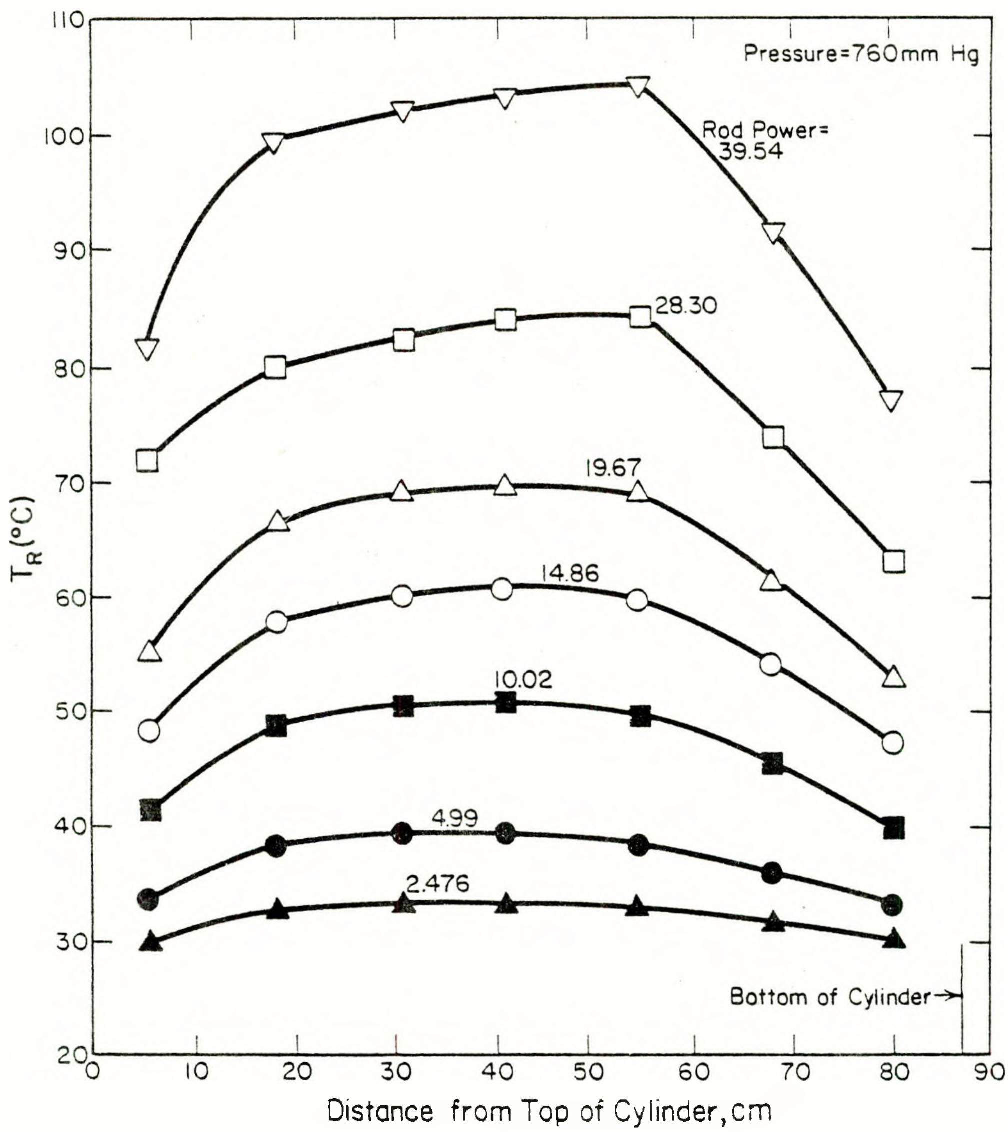


FIGURE 1. ROD SURFACE TEMPERATURE AS A FUNCTION OF DISTANCE FROM TOP OF ROD AT P = 760 mm Hg

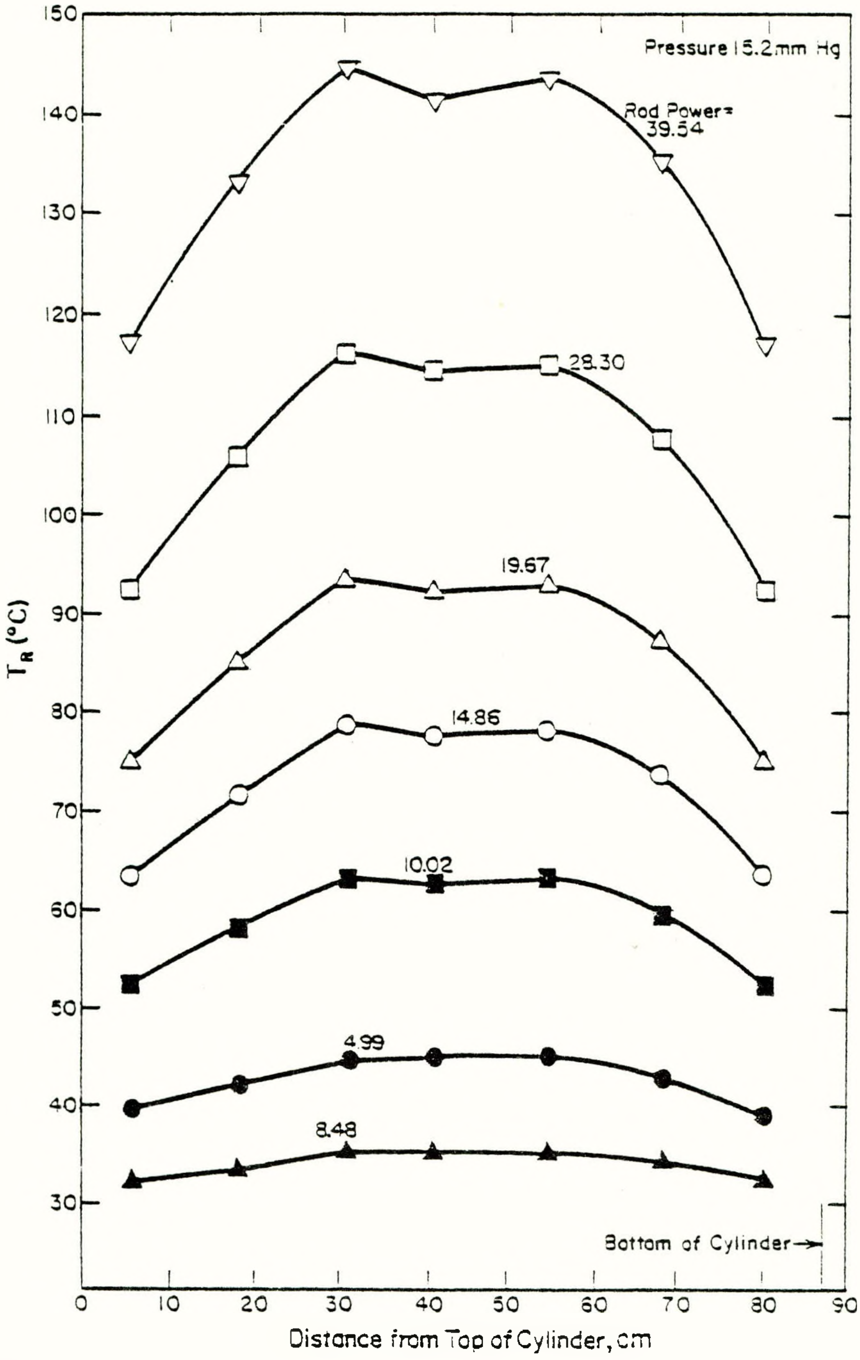


FIGURE 2. ROD SURFACE TEMPERATURE AS A FUNCTION OF DISTANCE FROM TOP OF ROD AT P = 15.2 mm Hg

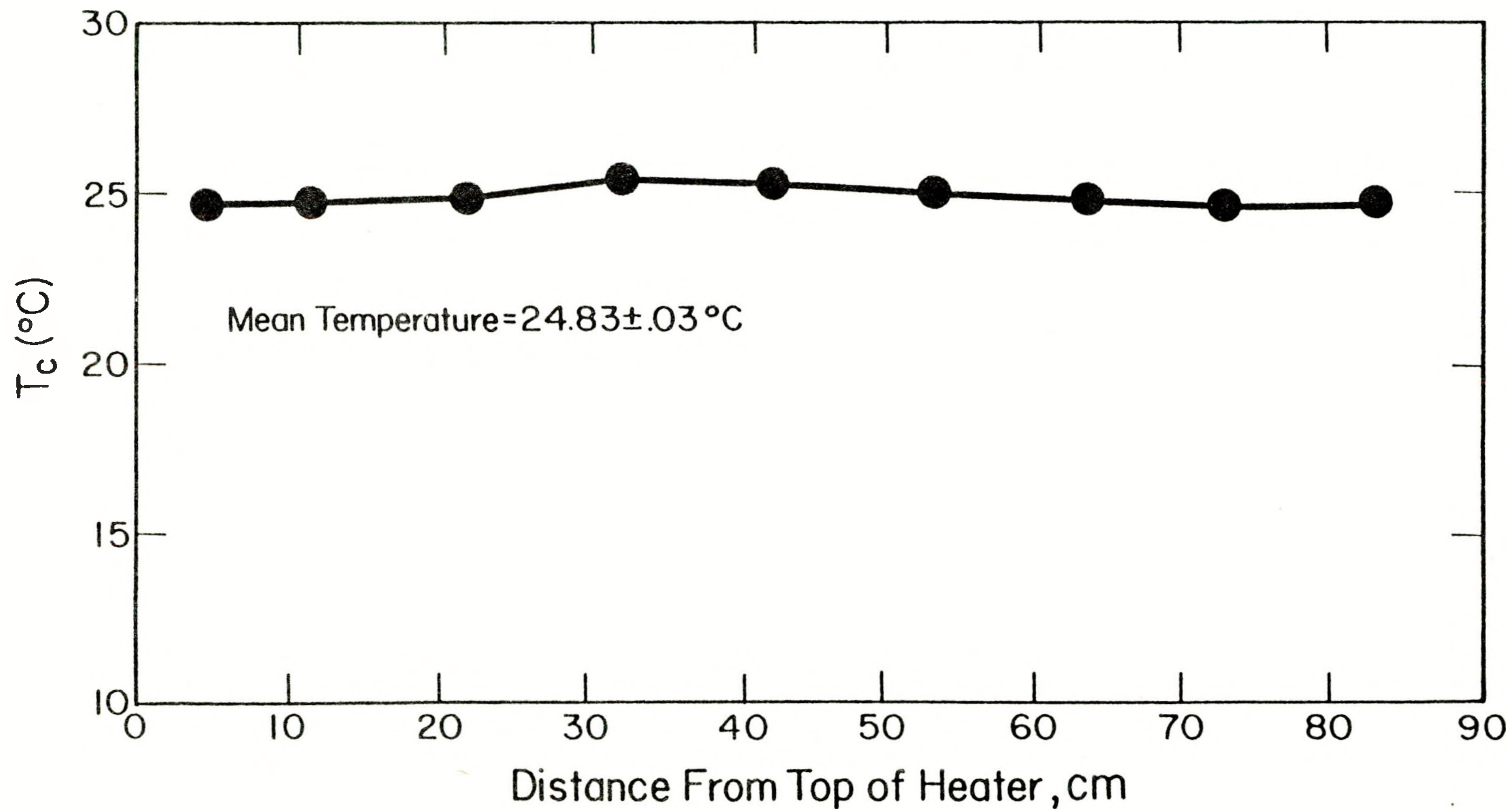


FIGURE 3. SURFACE TEMPERATURE OF CYLINDER AS A FUNCTION OF DISTANCE FROM TOP OF APPARATUS

TABLE 1. MEAN TEMPERATURES OF ROD AND CYLINDER AT P = 760 mm Hg

Rod Power,	Rod Temp, C		Cylinder Temp, C		ΔT,
W	T_{mR}	Std. Dev.	T_{mc}	Std. Dev.	C
2.476	31.94	1.44	24.51	0.10	7.43
4.99	36.94	2.61	24.44	0.08	12.5
10.02	46.67	4.42	24.7	0.15	21.97
14.86	55.55	5.67	24.84	0.47	30.71
19.67	63.22	7.00	24.56	0.30	38.66
28.3	77.22	7.78	24.87	0.47	52.35
39.54	94.17	11.1	25.18	0.54	68.99

TABLE 2. MEAN TEMPERATURES OF ROD AND CYLINDER AT P = 15.2 mm Hg

Rod Power,	Rod Temp, C		Cylinder Temp, C			
W	T_{mR}	Std. Dev.	T_{mc}	Std. Dev.	T, C	C_r
2.476	33.83	1.28	24.64	0.14	9.19	0.815
4.99	42.22	2.72	24.44	0.08	17.78	0.818
10.02	58.78	4.89	24.68	0.13	34.10	0.820
14.86	72.50	6.61	24.75	0.23	47.75	0.811
19.67	85.78	7.94	24.83	0.30	60.95	0.764
28.3	106.11	10.16	24.59	0.28	81.52	0.769
39.54	133.39	11.83	24.85	0.44	108.54	0.682

The reduced data in terms of Rayleigh Number, Grashof Number, and the Nusselt Numbers obtained from the numerical correlation of Thomas and de Vahl Davis (1970) are given in Table 3. The measured and predicted Nusselt Numbers are in good agreement. The percentage of heat transferred by natural convection is also given in Table 3 for each Rayleigh number. As rod power is increased, a larger fraction of the energy is transferred by natural convection. Additional experiments are required in order to determine whether this trend in the data will persist at higher power levels.

Figure 4 presents a graphical comparison of the present experimental data with the results of Thomas and de Vahl Davis (1970). Work is in progress to obtain Nusselt Numbers at higher and lower Rayleigh Numbers to complete this "baseline" case in the total plan of experiments.

The percent increase in temperature of the rod surface versus the power input as the pressure is reduced to 15.2 mm Mg is given in Table 4. Mean rod and surface temperatures as a function of power input with pressure as a parameter are given in Figure 5. The mean rod surface temperature exhibits a nonlinear dependence on power input at both pressures. Further experiments are needed to verify the functional relation between temperature and power.

TABLE 3. EXPERIMENTAL NUSSELT NUMBERS COMPARED WITH NUMERICAL VALUES OF THOMAS AND DE VAHL DAVIS (1970)

Rod Power, W	Ra	Gr	Nu (Exp.)	Nu	Percent by Convection
4.99	3.43×10^4	4.77×10^4	2.914	3.466	31.5
10.02	5.59×10^4	7.76×10^4	3.943	4.0	37.5
14.86	7.88×10^4	1.09×10^5	4.268	4.24	38.6
19.67	9.40×10^4	1.3×10^5	4.97	4.75	43.2
28.30	1.17×10^5	1.62×10^5	4.98	5.03	41.7
39.54	1.42×10^5	1.97×10^5	5.829	5.28	47.0

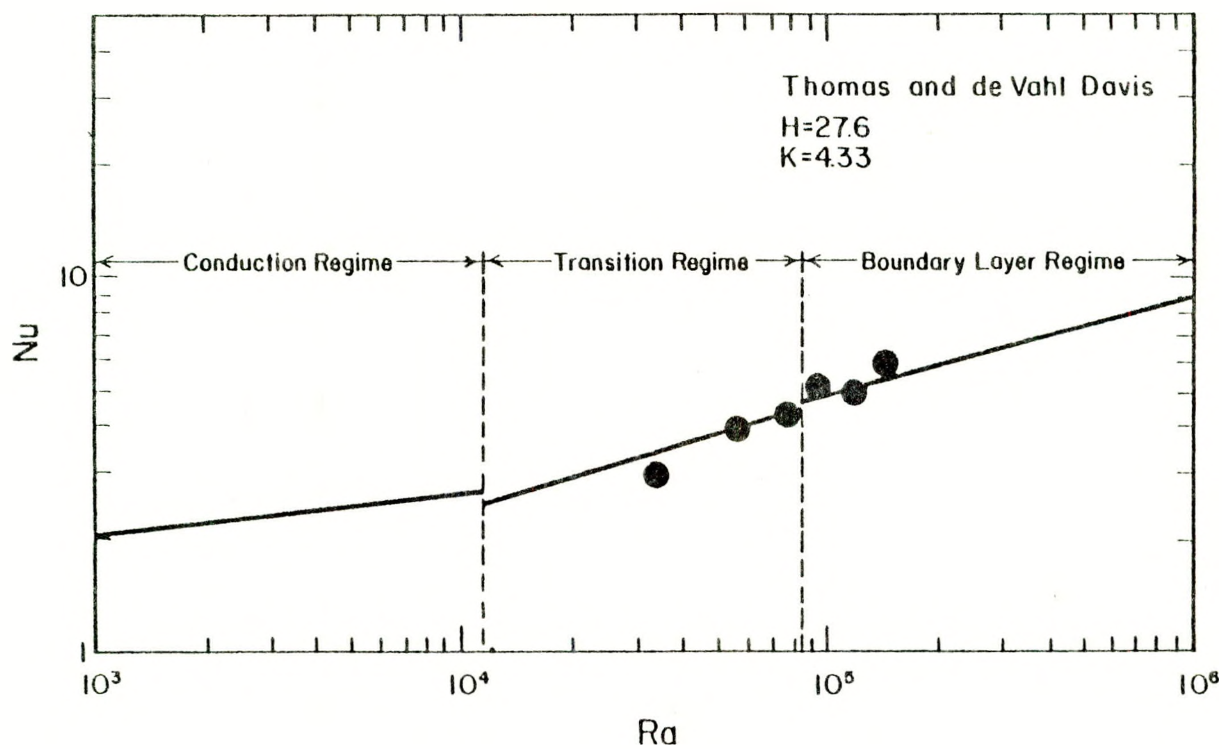


FIGURE 4. AVERAGE NUSSELT NUMBER AS A FUNCTION OF RAYLEIGH NUMBER

TABLE 4. PERCENT INCREASE IN TEMPERATURE OF ROD AS PRESSURE IS REDUCED FROM 760 mm Hg TO 15.2 mm Hg

Rod Power, W	2.476	4.99	10.0	14.9	19.7	28.3	39.6
Percent Increase	5.9	14.3	25.9	30.5	35.7	37.4	41.6

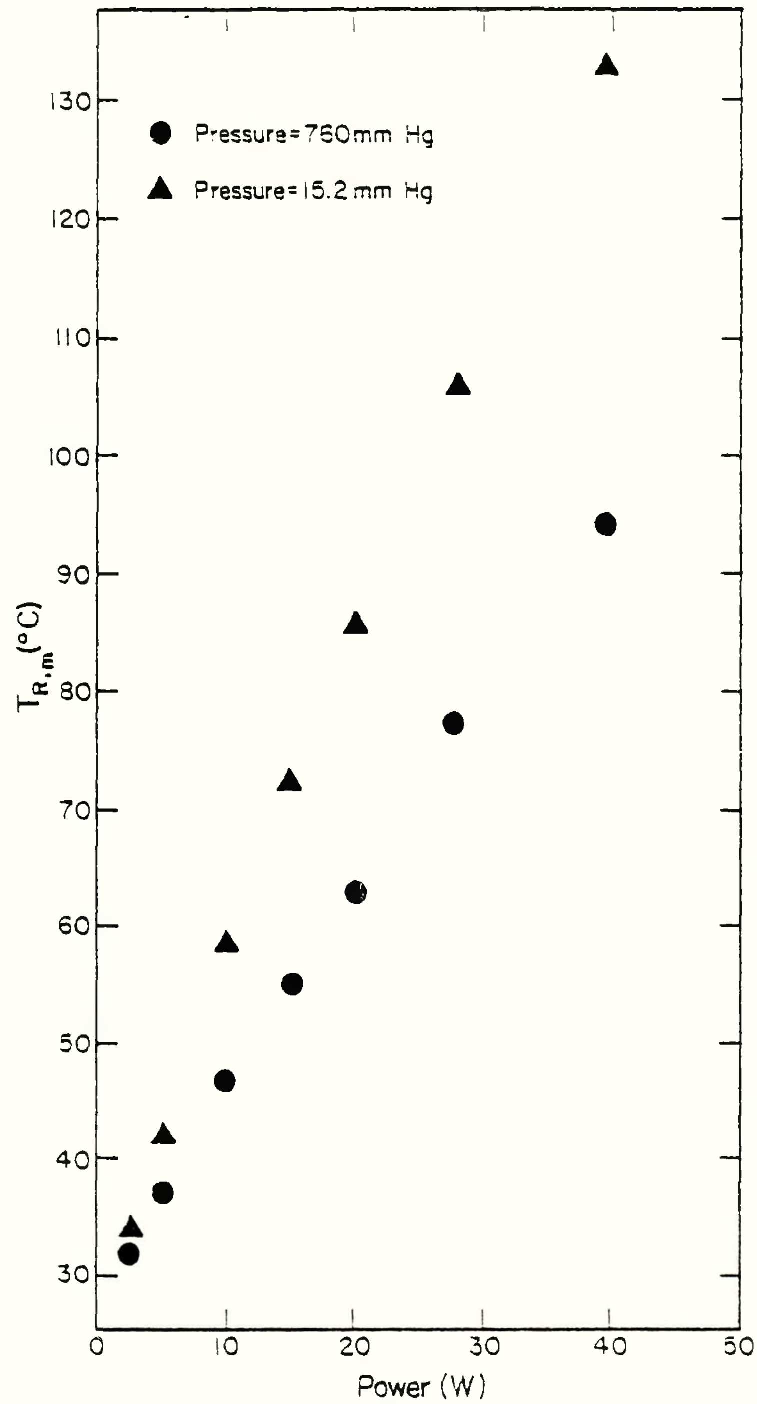


FIGURE 5. MEAN ROD SURFACE TEMPERATURE AS A FUNCTION OF INPUT POWER

NOMENCLATURE

A	Area, m^2
c_p	Specific heat at constant pressure, J/kg-C
C_r	Thermal conductance for radiation, Equation (2)
F_{i-o}	Radiation shape factor, inner to outer cylinder
g	Constant of gravitational acceleration, m/sec^2
Gr	Grashof Number, $(g\beta/\alpha\nu)\ell^3\Delta T$
h	Convective heat-transfer coefficient, W/m^2-C
H	Aspect ratio of cylinder, L/ℓ
k	Thermal conductivity, W/m-C
K	Radius ratio, r_o/r_i
ℓ	Length scale, r_o-r_i, meters
L	Height of annulus, meters
Nu	Nusselt Number, $h\ell/k$
P	Pressure, mm Hg
Pr	Prandtl Number, ν/α
q	Heat flux based on linear cylinder, W/m^2
r	Radius, meters
Ra	Rayleigh Number, Gr Pr = $(g\rho/\alpha\nu)\ \ell_3\ \Delta T$
T	Temperature, C
ΔT	Characteristic temperature difference, C
W	Power, W

Greek Symbols

α	Thermal diffusivity, $k/\rho c_p$, m^2/sec
β	Isobaric coefficient of thermal expansion, C^{-1}
ε	Emissivity
ν	Kinematic viscosity, m^2/sec
ρ	Density, kg/m^3
σ	Stephan-Boltzmann constant, 5.669×10^{-8}, W/m^2-K^4

Subscripts

c	Cylinder
i	Inner
m	Mean value
mc	Mean value on cylinder
mr	Mean value on rod
o	Outer
r	Radiation
R	Rod

REFERENCE

Thomas, R. W., and de Vahl Davis, G. 1970. "Natural Convection in Annular and Rectangular Cavities. A Numerical Study", *Proceedings, Fourth International Heat Transfer Conference,* held in Paris, France, Vol. 4, Paper NC 2.4, Elsevier, Amsterdam.

WBS 1.1.2

Project: Salt Model Pillar Studies

Principal Investigator: Oak Ridge National Laboratory (T. F. Lomenick)

ONWI Project Manager: G. Raines

Objective

The objective of this work is to provide data for the proper design of excavated cavities in rock salt which are candidates for the storage/disposal of radioactive wastes.

Progress Reported Previously

This is the first technical report under this project.

Activities During the Reporting Period

The long-term creep data from five model salt pillar tests have been analyzed to obtain preliminary estimates for the parameters in the power-law formulation:

$$\text{Pillar shortening} = C\, t^{a}\, \theta^{b}$$

where t is in hours, θ in K, and the constant C is a function of stress. Since all tests, except for the Lyons salt, are being run at 4000 psi, it is not possible to determine the stress dependency from the data under consideration. The temperature exponent may be estimated only for the Asse, Germany, salt that is being tested at room temperature (Sample 89) and at 100 C (Sample 90). The most reasonable estimate of the temperature exponent is about 8.5, which appears to be good from about 6,000 to 56,000 hours where the time exponent is about 0.3.

For the Lyons, Kansas salt (Sample 1) and the Salina Basin salt (Samples 3 and 4), it is possible only to determine the time exponent. Results for the time exponent for all five experiments are summarized in Table 1. Note that four of the five samples being tested have apparently gone through an initial stage where the time exponent is relatively low and then a rather distinct second stage where the exponent on time increases to the 0.3 to 0.4 range. The Lyons, Kansas salt is the exception where the time exponent has apparently decreased after about 5,000 hours, but then remains nearly constant to 100,000 hours. The unheated Asse salt has apparently gone through three creep stages where the time exponent is consistent with that of 56,000 hours. For the heated Asse salt, the second stage time exponent is consistent with that of the unheated Asse salt. The Salina Basin salt data are reasonably consistent with one another. These findings should be considered very preliminary and subject to change.

TABLE 1. SUMMARY OF PRELIMINARY DATA REDUCTION FOR LONG-TERM MODEL PILLAR CREEP TESTS

Salt	First Time Range, hr	Time Exponent	Second Time Range, hr	Time Exponent
Lyons, KS Sample 1	10 ≤ to <5000	0.370	5000 ≤ to <100,000	0.239
Salina Basin Sample 3	100 ≤ to <5000	0.158	5000 ≤ to <75,000	0.396
Salina Basin Sample 4	1000 ≤ to <3200	0.124	3200 ≤ to <75,000	0.438
Asse, Germany Sample 89	1 ≤ to <6000	0.105	6000 ≤ to <56,000	0.314
Asse, Germany Sample 90 at 100 C	1 ≤ to <100	0.090	100 ≤ to <100,000	0.30

Pillar shortening = Kt where t is in hours.

WBS 1.1.2

Project: Horizontal Emplacement Simulations

Principal Investigator: Scientific Applications, Incorporated (D. E. Maxwell)

ONWI Project Manager: G. Raines

Objective

The objective of this program is to provide a technology base for the study of the horizontal emplacement concept sufficient to warrant programmatic decisions to further consider its viability or to reject the concept entirely.

Progress Reported Previously

This is the first progress report under this project.

Activities During the Reporting Period

The objective of this task is to determine the extent and significance of the sag of horizontally emplaced canisters. The canister sleeve sink due to the unbalanced buoyant force and the creep of the hot salt were shown to be insignificant. Though only the SAI-Lyons salt model (Wahi, Maxwell, and Hofmann, 1978) was required, the methodology was applied to a wide spectrum of models employing extreme assumptions to enhance the creep. A preliminary report has been forwarded for review to ONWI.

The objective of this task is to perform two-dimensional evaluations of the thermomechanical response of canisters emplaced horizontally in salt. The two-dimensional computation has been designed and the computation is under way. Figure 1 shows the STEALTH 2D (Hofmann, 1976) grid corresponding to the upper right-hand quadrant. The room quadrant lies in the lower left corner and is four zones wide (3 meters) and two zones high (1.5 meters). The source region corresponds to the eight zones along the bottom, starting at 14 meters and extending to the right. The heat from these zones diffuses through the grid encountering (a) the adiabatic room walls, (b) the adiabatic left, right, and lower boundaries, and (c) the time-dependent temperature boundary condition applied to the upper boundary. The upper boundary temperature condition corresponds to an infinite column of salt above. Standard roller boundaries are applied at the bottom, left, and right. The overburden pressure corresponding to a room midheight of 2000 feet is applied at the top boundary. Employing a common technique, gravity is omitted in the grid, and hence the room midheight actually corresponds to the 2000 feet. The perturbation from reality by this method is negligible in this case and removes any question about the application of a horizontal symmetry plane through the room midheight. This reduces the number of zones required and allows the three-dimensional grid to have the same xy plane grid, which is obviously advantageous for comparisons.

The objective of this task is to perform a three-dimensional evaluation of the thermomechanical response of canisters emplaced horizontally in salt. The three-dimensional computation is designed and ready. Letting z be the direction parallel to the corridors, the 60 kw/acre case of the two-dimensional grid corresponds to a pitch (z spacing of the canister sleeves) of 4.5375 meters. The z width of the three-dimensional grid is half of the pitch due to symmetry which results in 2.26875 meters. The 0.75 zone widths around the room in the xy plane of the two-dimensional grid applied to the z direction results in three zones (four zone boundaries) in this direction. This can be handled by STEALTH 3D without modifying the xy plane grid, which is an obvious advantage. Though the z width may seem small, it does describe the infinite corridor with the same spatial resolution as that in the xy plane.

The objective of this task is to perform a two-dimensional evaluation of the thermo-mechanical response of canisters emplaced horizontally in granite under the assumed condition of no active slip or tensile cracking. The initial and boundary conditions were established for horizontal emplacement in granite. Overall mesh dimensions of 30 meters (height) and 36.5 meters (width) were chosen to represent a unit cell at a depth of 600 meters. The material property data were presented to and approved by ONWI. The initial conditions, the boundary conditions, and the mesh dimensions are shown in Figure 2. The nominal material property data are summarized in Table 1.

To model the joint slip in a passive fashion, five additional parameters were introduced into the calculation using the Cracking and Void Strain (CAVS) model. These parameters represented the principal orientation, orientation of the worst potential slip, and the associated joint slip safety factors that are a measure of the proximity to slip.

TABLE 1. NOMINAL MATERIAL PROPERTY DATA FOR GRANITE

Bulk Density	2650 kg/m^3
Thermal Conductivity	2.5 W/m-K
Specific Heat	810 J/kg-K
Coefficient of Expansion	8 x 10^{-6}/K
Young's Modulus	35 x 10^9 Pa (5 x 10^6 psi)
Poisson's Ratio	0.2
Bulk Modulus	19.2 x 10^9 Pa (2.8 x 10^6 psi)
Shear Modulus	14.4 x 10^9 Pa (2.1 x 10^6 psi)
Hydrostatic Pressure	5.9 x 10^6 Pa (840 psi)
(Pore pressure reaches hydrostatic by 12 meters)	

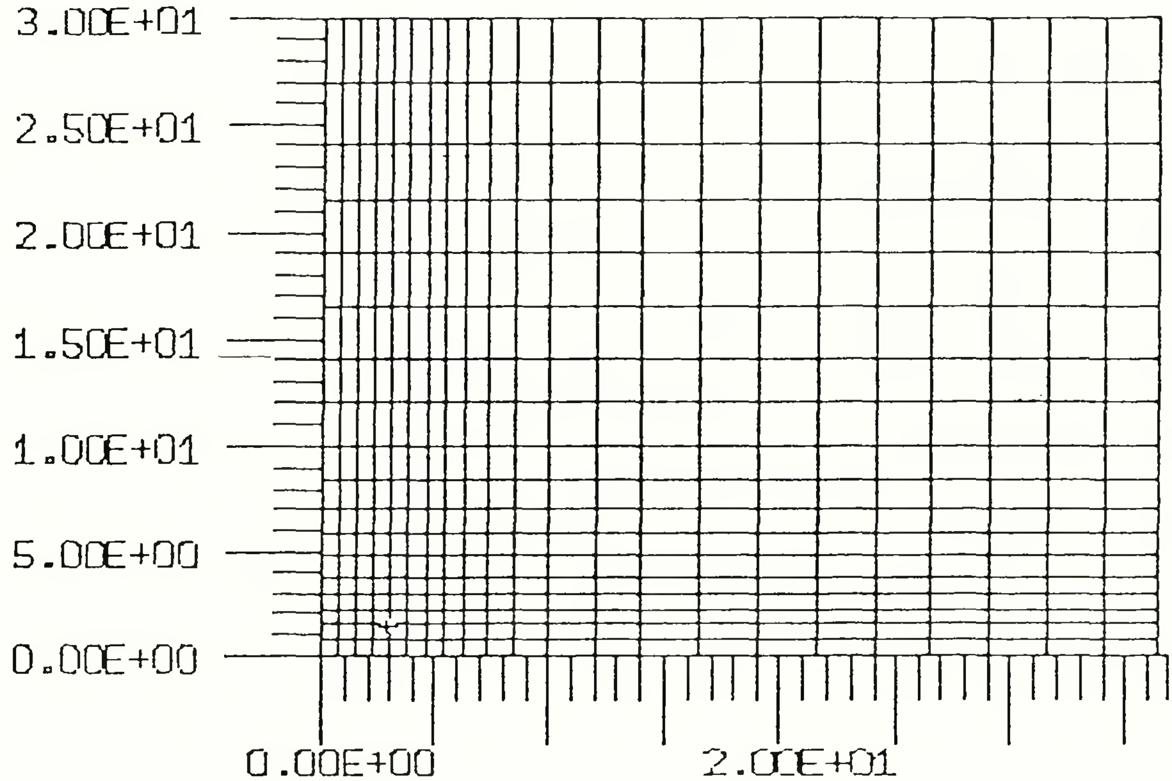


FIGURE 1. STEALTH 2D MESH

Because of the extensive number of updates necessary in this task, a special version of STEALTH 2D was created such that a minimal number of FORTRAN changes would be needed in each production run. This special version has built-in capabilities for time-step scaling (Maxwell, Hofmann, and Wahi, 1978), heat-source description, passive joint-slip modeling, and a time-dependent thermal boundary condition using the concept of sources and sinks.

The simulation has already been carried out to a time of 10 years out of the 25 years specified. The thermomechanical response appears to be extremely stable for the conditions encountered (i.e., when active slip or tensile cracking are not allowed) in the first 10 years. The worst slip orientation at a given location shows little variation with time. On the other hand, large spatial variations are noted as shown in Figure 3.

Temperature histories at three different locations are plotted as a function of time in Figure 4. The deformation of the tunnel walls in the first 10 years is very small. This may or may not be the case in the next task when tensile cracking, crack opening, and joint slip are permitted.

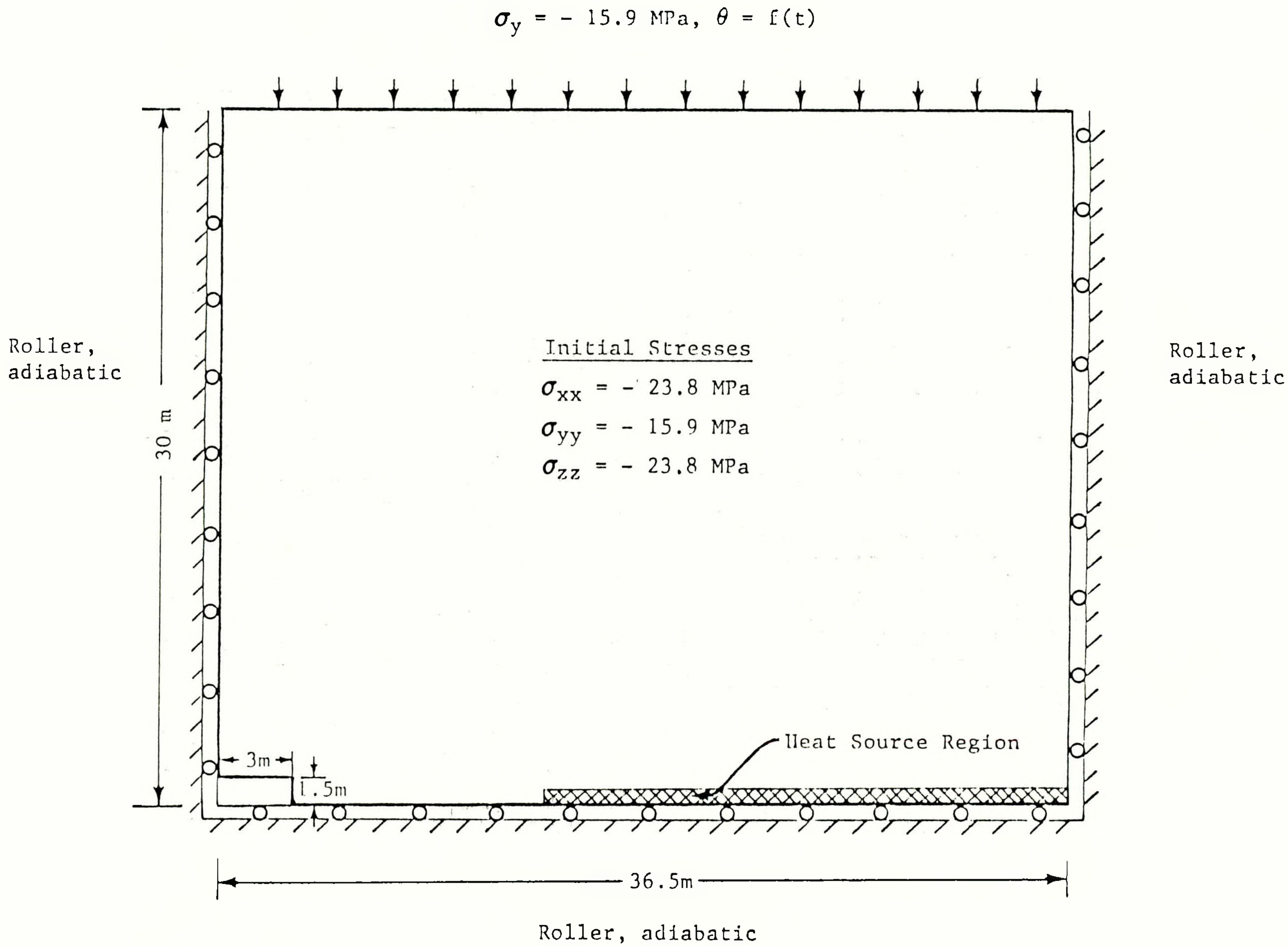


FIGURE 2. INITIAL AND BOUNDARY CONDITIONS

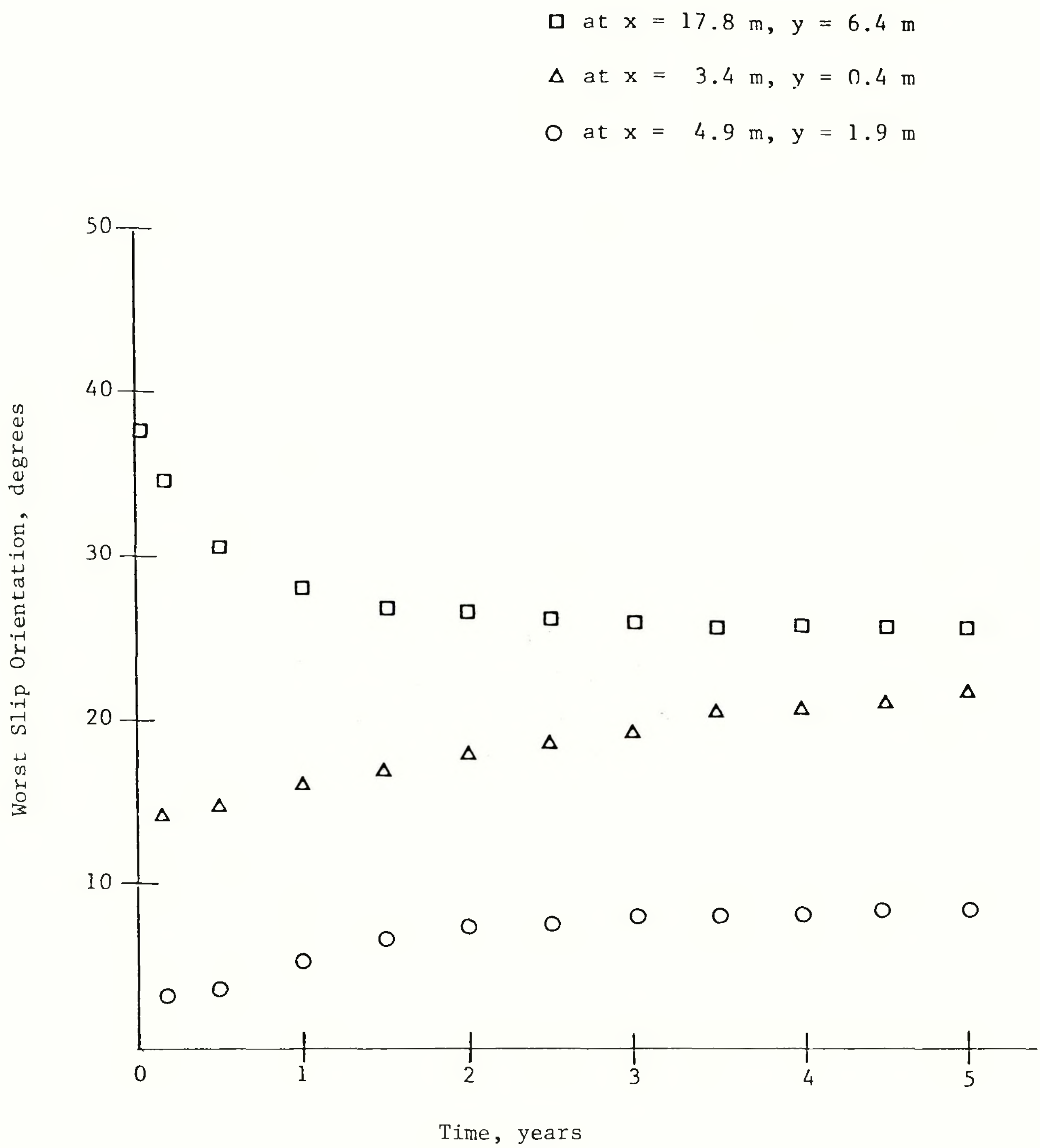


FIGURE 3. TIME HISTORIES OF WORST SLIP ORIENTATIONS AT SELECTED LOCATIONS

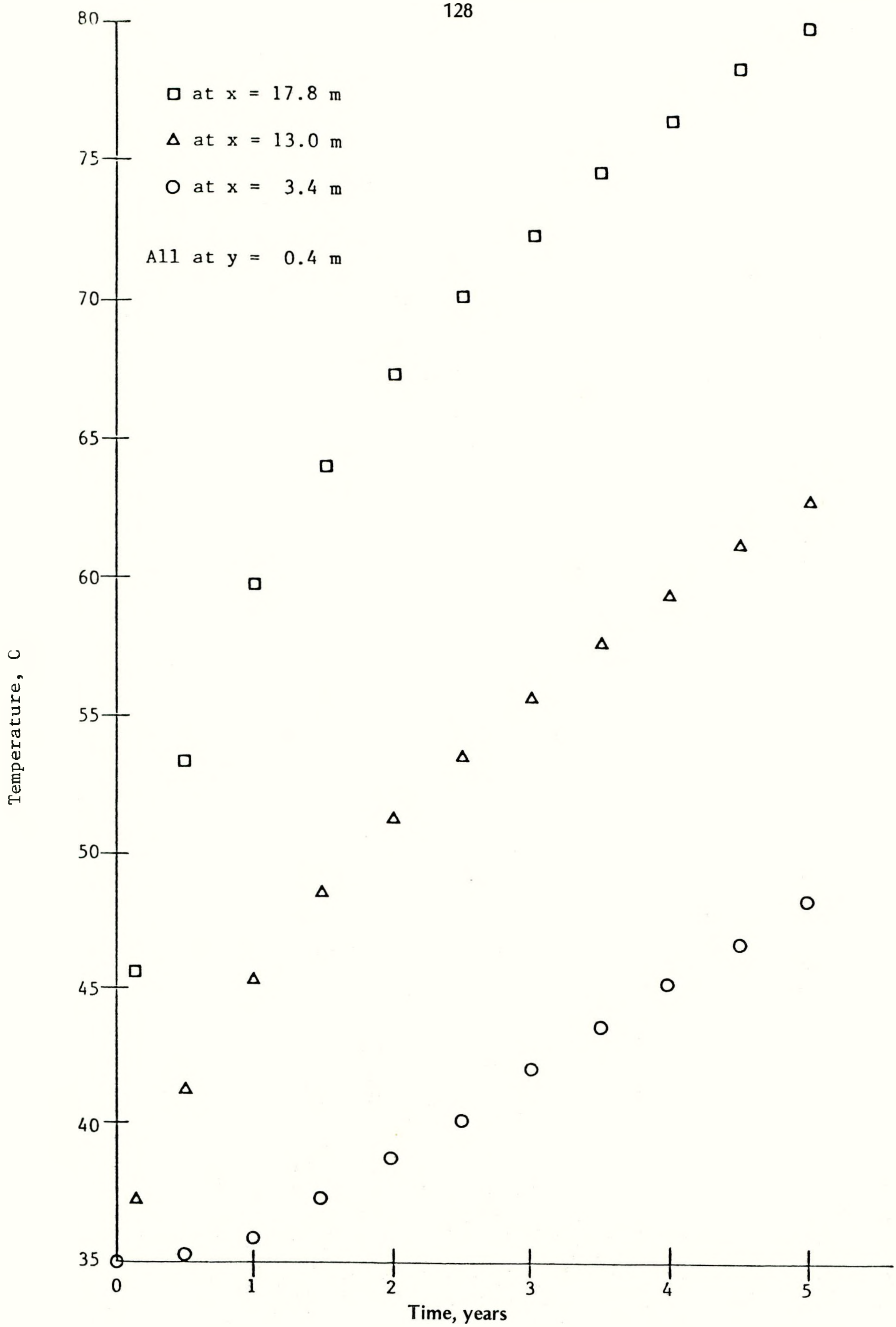


FIGURE 4. TEMPERATURE/TIME HISTORY AT SELECTED LOCATIONS

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WBS 1.1.3

Project: Fission Product Release

Principal Investigator: Los Alamos Scientific Laboratory (E. A. Bryant and A. E. Norris)

ONWI Project Manager: D. P. Moak

Objective

This program has been undertaken to measure both the rates of fission product release from UO_2 materials and the rates of dissolution of UO_2 matrices under controlled conditions. The major emphasis in this work is the determination of the function of oxidizing and reducing conditions in maintaining the integrity of the UO_2 matrix, with consequent retention of reactor fission products. The temperatures in these controlled conditions will be chosen to obtain data pertinent to long-term storage of UO_2 spent fuel elements. The results of the measurements obtained in this experimental program will be correlated with the observed retentions of fission products in UO_2 ores at the Oklo natural fission reactor site.

Progress Reported Previously

This project was derived from studies of the Oklo natural fission reactor system. In that work, many fission products and actinide elements were found to have been retained during the periods of their radioactive decay following their formation in the natural reactor system some two billion years ago. Reasonable explanations for this remarkable retention involve both the extreme insolubility of uraninite (UO_2) in the Oklo environment and the fission products' slow rate of diffusion out of the host mineral. This fission product release project was established to investigate these hypotheses and their implications for the geologic storage of spent UO_2 fuel elements.

Since this project's inception, work has resulted in a literature survey of the diffusion, chemical, and morphological data available concerning reactor products in UO_2 fuel elements; design of the procedures and the equipment necessary for the experimental efforts; construction of a hot cell slave box for use in the empirical measurements of fission product release from nuclear power reactor spent fuel; procurement of the spent fuel for use in this work; and assembly of an apparatus for measuring the rate of dissolution of uraninite materials under controlled conditions.

The experimental results showed initially that the rate of dissolution of powdered UO_2 in deionized water was about ten times faster in the presence of oxygen than in the presence of hydrogen gas. Another experiment was performed in which UO_2 was heated at 550 C for 3 hours in a hydrogen atmosphere to eliminate any oxygen on the surface of the UO_2 grains. This material dissolved in deionized water in the presence of hydrogen nearly 100 times more rapidly than material that was not heated before dissolution. Additional results from a continuation of this experiment are reported this quarter.

Wafers of spent reactor fuel have been leached to compare the fission product releases under oxidizing and reducing conditions. Lanthanide and actinide elements were observed to be leached about ten times faster under oxidizing conditions at 25 C than under reducing conditions. The differences between oxidizing and reducing conditions were much less apparent in the leach rates of reactor fuel measured at 70 C than at 25 C. The rates at which ^{90}Sr was leached also were ten times faster under oxidizing conditions than under reducing conditions, but for ^{137}Cs the rates under the two conditions were comparable. A second pair of spent fuel wafers was leached at 25 C under the same conditions as the first pair. Duplicate results were obtained. The spent fuel leaching data show that equilibrium or pseudoequilibrium conditions are attained about 20 days after introduction of fresh leachant.

Activities During the Reporting Period

Empirical Measurements of Fission Product Release from Spent Fuel

An electron microprobe examination of an H. B. Robinson reactor spent fuel element was completed this quarter. The purpose of this examination was to determine whether fission product and actinide element concentrations in the wafer could be correlated with the UO_2 grain structure or other physical properties of the spent fuel that might help our understanding of the observed leaching characteristics under oxidizing or reducing conditions. Figure 1 is a photomosaic of the surface of the polished, unetched wafer that was used for the microprobe examination. The outer rim visible in the photomosaic is the Zircaloy-4 cladding surrounding the UO_2 fuel. The results of radial point-count scans for strontium, antimony, cesium, uranium, and plutonium are shown in Figures 2 and 3 for the paths indicated in Figure 1. The plutonium data show an increase in concentration in the outer 500 μm of the wafer. The small absolute values of the plutonium concentrations require the assignment of a large uncertainty in the ratio of Pu/(U + Pu), but the same increase in plutonium concentration toward the edge of spent fuel from the same reactor was observed by Y. B. Katayama, Bradley, and Harvey, 1980. However, our cesium data showed variable distributions that displayed no trends along the radii. Thus, these data do not support the interpretation of the data given by Katayama, in which an increase in cesium concentration was noted at the outer edge of the fuel material. Our strontium and antimony data show no radial trends. The Katayama work cited above did not give data for these elements, but did include data for elements that we did not measure. The relatively uniform distribution for elements other than plutonium led us to conclude from these electron microprobe investigations that we could not observe differences in distributions that would correlate with physical features in the fuel element material.

Another aspect of the spent fuel leaching study is that of correlating the UO_2 dissolution under oxidizing conditions and under reducing conditions with the quantities of fission products and actinides that are leached at the same times. Those reactor products capable of existing in solid solution of UO_2 were hypothesized to exhibit leaching rates congruent with the UO_2 dissolution. Testing this hypothesis requires measurement of the uranium concentrations in the leachant solutions collected in this work. The method chosen originally to assay the uranium concentrations, that of irradiating aliquots of the solutions in a neutron flux and counting delayed neutron emission, proved much more difficult to use than expected. The reason was an inexplicable inconstancy of the $^{235}U/^{238}U$ and the $^{239}Pu/^{240}Pu$ ratios in the solutions. Therefore, other methods are being investigated to measure the uranium in the more than 100 solutions requiring analysis. One result of this investigation is the comparison of the uranium analyses shown in Table 1. The mass spectrometric assays are the most accurate of the three listed, but the delayed neutron counting techniques with corrections for uranium

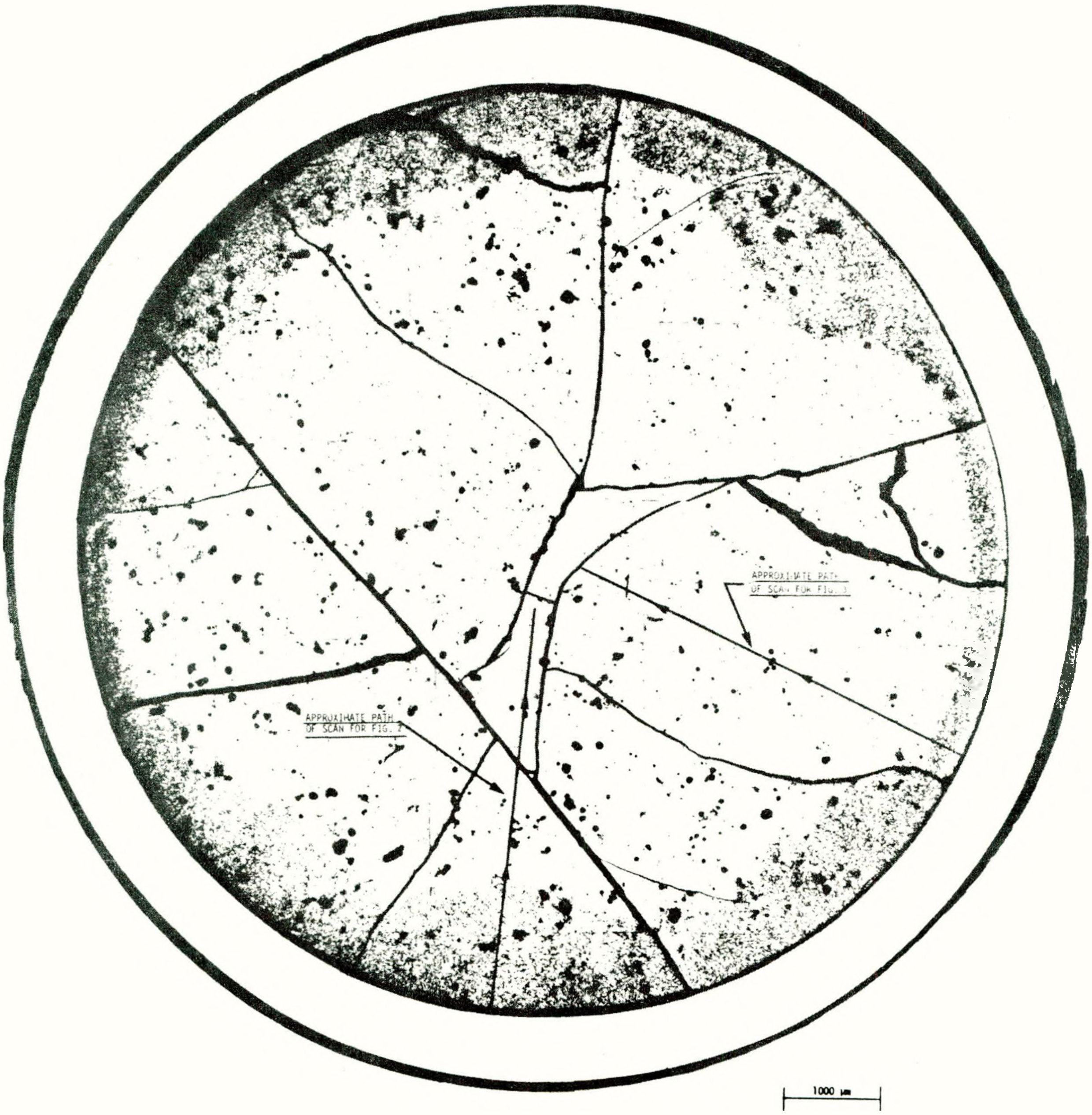
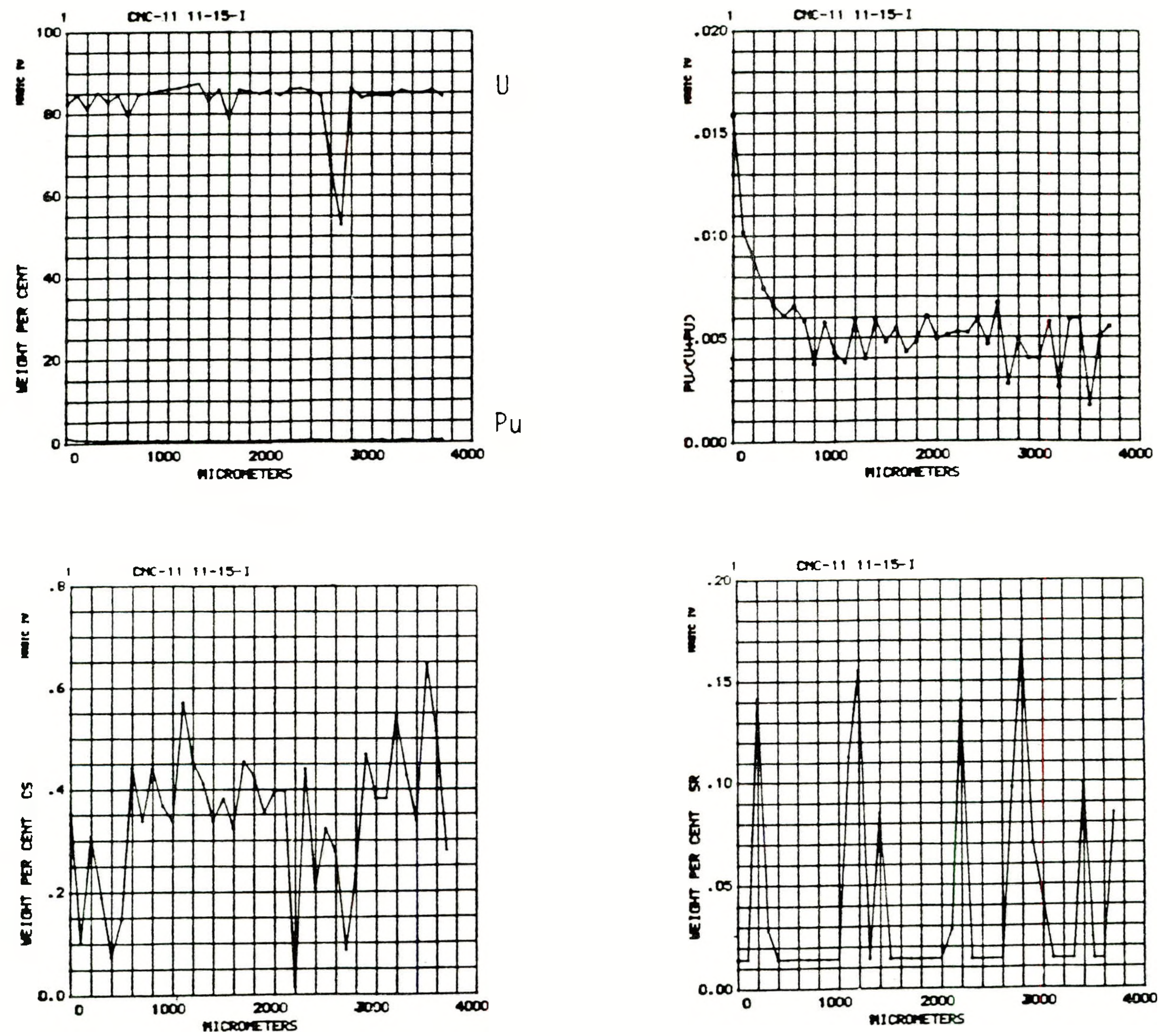


FIGURE 1. PHOTOMOSAIC OF THE SURFACE OF CNC-11, H. B. ROBINSON WAFER NUMBER 32-D

The approximate locations of scan paths are indicated. Polished, unetched.



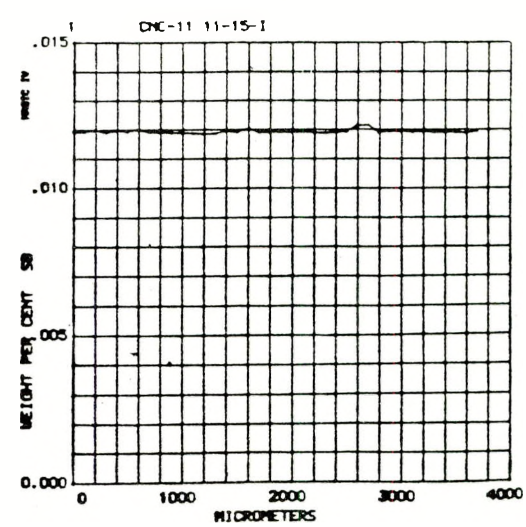
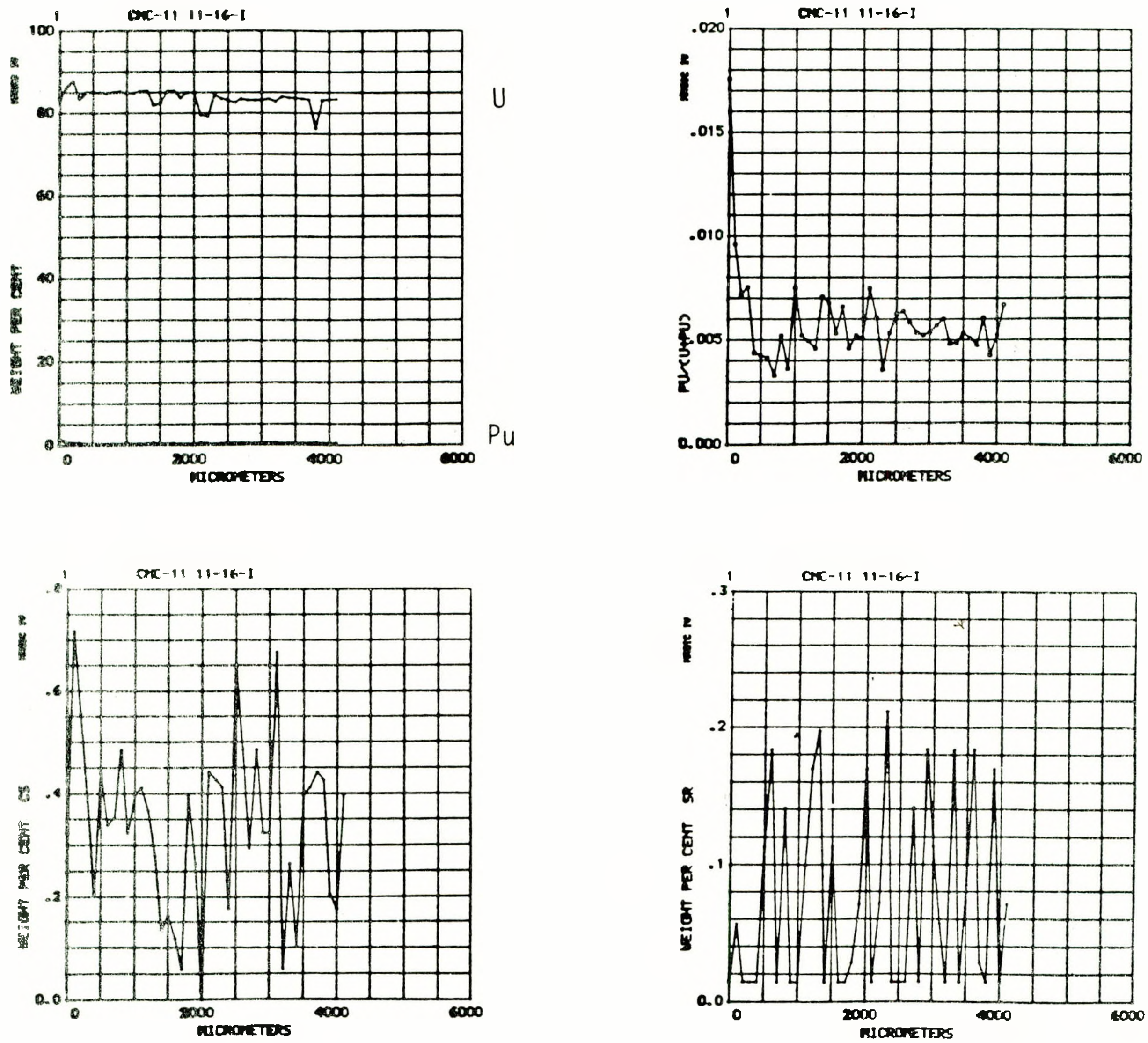


FIGURE 2. DISTRIBUTIONS OF U, Pu, Cs, Sr, AND Sb ALONG A PATH INDICATED APPROXIMATELY BY THE LOWER SOLID LINE IN FIGURE 1

On the upper right is a plot of the ratios wt % Pu/(wt % U + wt % Pu) corresponding to the data points in the upper left plot. The zero on the micrometer scale corresponds approximately to the fuel O.D.



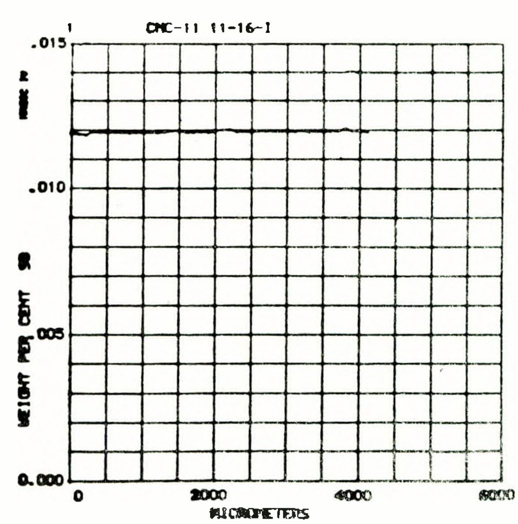


FIGURE 3. DISTRIBUTIONS OF U, Pu, Cs, Sr, AND Sb ALONG A PATH INDICATED APPROXIMATELY BY THE SOLID LINE AT THE RIGHT IN FIGURE 1

On the upper right is a plot of the ratios wt % Pu/(wt % U + wt % Pu) corresponding to the data points in the upper left plot. The zero on the micrometer scale corresponds approximately to the fuel O.D.

TABLE 1. COMPARISON OF URANIUM ANALYSIS RESULTS (ppm U)

Spent Fuel Sample	Mass Spectrometric Assay	Delayed Neutron Counting	Colorimetric Assay
3211-14	0.14	0.16	1.23
3221-14	3.24	3.34	1.96
3251-01		1.51	1.8
3251-02		0.11	0.05
3251-12	0.30	0.30	0.1
3261-12	0.23	0.30	0.6
3252-07	0.06	0.07	0.92
3262-02		1.15	1.10
3262-07	4.42	4.45	4.54

and plutonium isotopic compositions appear to give very similar results. The colorimetric technique used 1,3-diphenyl-1,3-propanedione in ethanol as the complexing agent. This method of analysis appears to be accurate only for uranium concentrations greater than 1 ppm.

UO_2 Dissolution Studies

Studies are being conducted to measure the dissolution of pure uraninite under oxidizing and reducing conditions. This will help our understanding of processes that result in the dissolution of UO_2 in spent fuel under leaching conditions. Last quarter we reported the results of an experiment in which UO_2 powder was heated in a hydrogen atmosphere to remove any oxygen absorbed onto its surface. The UO_2 was cooled and transferred in an anoxic environment to deionized water for measurement of its solubility under reducing conditions. The uranium concentrations measured in the leachant were unexpectedly high until a palladium-black catalyst was added to the system. The uranium concentration then decreased dramatically.

The experiment just described was continued this quarter. Results are shown in Figure 4. The increase in uranium concentration at day 118 corresponds to the time when the gas bottle supplying hydrogen to the experiment was changed. Apparently oxygen was admitted inadvertently.

The pH of the leachant was 3.3 at the time that the palladium-black catalyst was added. The pH rose to 4.5 by the 138th day. An ascarite filter was placed in the hydrogen supply line to remove any CO_2 that might be present. Subsequently, the Ph was measured at 5.9. This

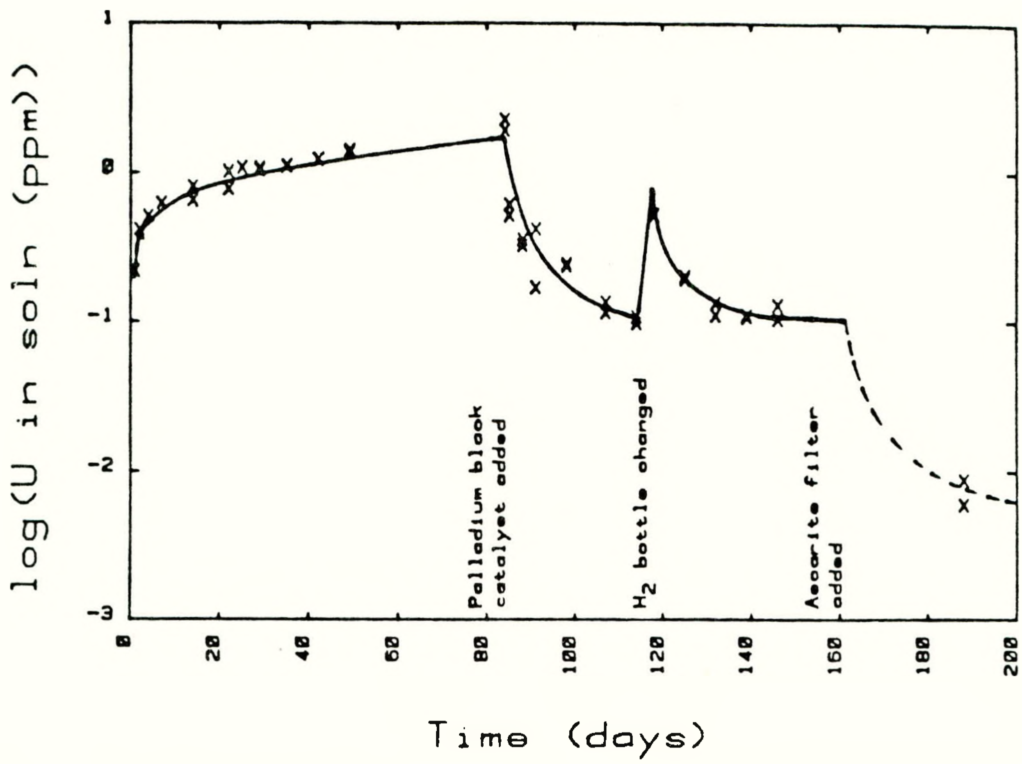


FIGURE 4. MEASURED URANIUM CONCENTRATIONS RESULTING FROM UO_2 POWDER IN H_2O UNDER REDUCING CONDITIONS

The final segment of the line is dashed to indicate uncertainty about the shape of the curve until additional data are collected.

increase may be due to the transfer of a small amount of NaOH from the ascarite filter to the solution. The uranium concentration fell to 8 ppb.

Data in a paper by Langmuir (1978) have been used to construct several UO_2 equilibrium solubility diagrams to aid in interpreting the current experiment. Figure 5 shows the solubilities of crystalline and amorphous UO_2 in pure water as a function of pH for selected oxygen fugacities. The oxygen fugacity of $10^{-83.1}$ (indicated in Figure 5 only by its exponent) is that calculated for H_2O in equilibrium with H_2 at a pressure of 1 atmosphere. The decrease in uranium concentration that was observed when the pH increased to 5.9 is consistent with an interpretation that the solid phase is crystalline UO_2, rather than amorphous, and that the oxygen fugacity in solution may be $\sim10^{-50}$. This interpretation can be confirmed by determining the equilibrium solubility of uranium in this experiment.

Figure 6 was constructed to show the effect of pH and CO_2 fugacity on UO_2 solubility at an oxygen fugacity of 10^{-50}. The atmospheric fugacity of CO_2 is about $10^{-3.5}$. This figure indicates, then, that carbonate complexing of uranium is unlikely to have had any effect on the experiment thus far.

Studies of Reducing Conditions

The uranium concentrations that result from leaching UO_2 in spent fuel and UO_2 powders, both under reducing conditions, have been much higher than expected from known

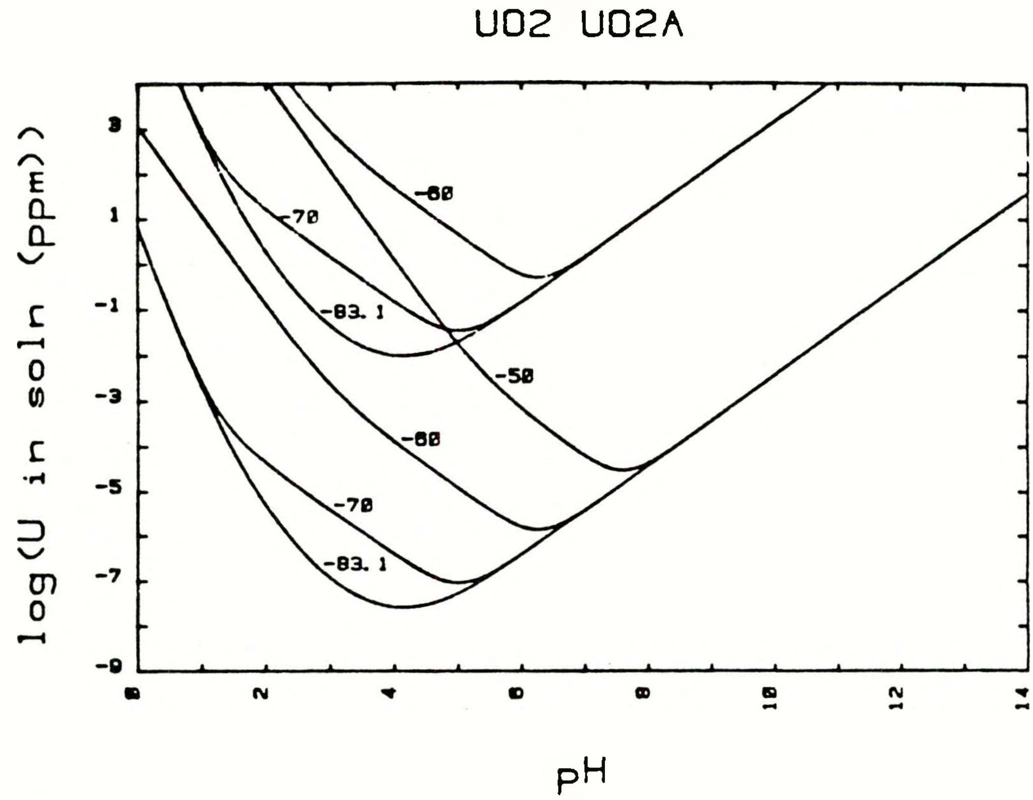


FIGURE 5. CALCULATED UO_2 SOLUBILITIES IN PURE H_2O AS A FUNCTION OF pH FOR SELECTED OXYGEN FUGACITIES, WHICH ARE INDICATED ONLY BY THEIR EXPONENTS

The upper set of curves represents the values calculated for amorphous UO_2, while the lower set contains the values for crystalline UO_2.

and estimated thermodynamic data. The reducing conditions in the experiments have been produced by bubbling hydrogen gas or a mixture of 6 percent H_2 and 94 percent Ar through the leachant, generally in the presence of a platinum gauze catalyst. The Eh values measured with a platinum electrode indicate reducing conditions (about -150 mV), but the high uranium concentrations in solution have led us to suspect that the hydrogen reduces any oxygen or any UO_2^{2+} present in the leachants so slowly that the uranium concentrations are not representative of true aqueous reducing conditions. Therefore, experiments are being conducted to find reducing agents better than hydrogen gas that will be part of a stable system with an extremely low oxygen concentration in solutions having pH values in the range of 7 to 9.

The status of all the experiments performed to date is discussed here. Four reducing agents have been investigated. Two of the four, Cr^{2+} and Eu^{2+}, react rapidly with oxygen. These reducing agents are sufficiently strong to reduce UO_2^{2+} to U(IV). However, the investigations of these two were terminated when they were found to be unstable at pH 7 to 9. The instability resulted in their being almost impossible to handle in this pH range, although they can be used easily in lower pH solutions.

The remaining two reducing agents investigated are ferrous ion in Fe^{2+} (o-phenanthroline)$_3$ and iron metal, Fe^0. The Fe^{2+} (o-phenanthroline)$_3$ experiments was described in the previous quarterly report. Measurements were made with a 5 x 10^{-5} M solution of the reductant in deionized and degassed H_2O at pH 7 and at a temperature of 25 C. The uranium in solution

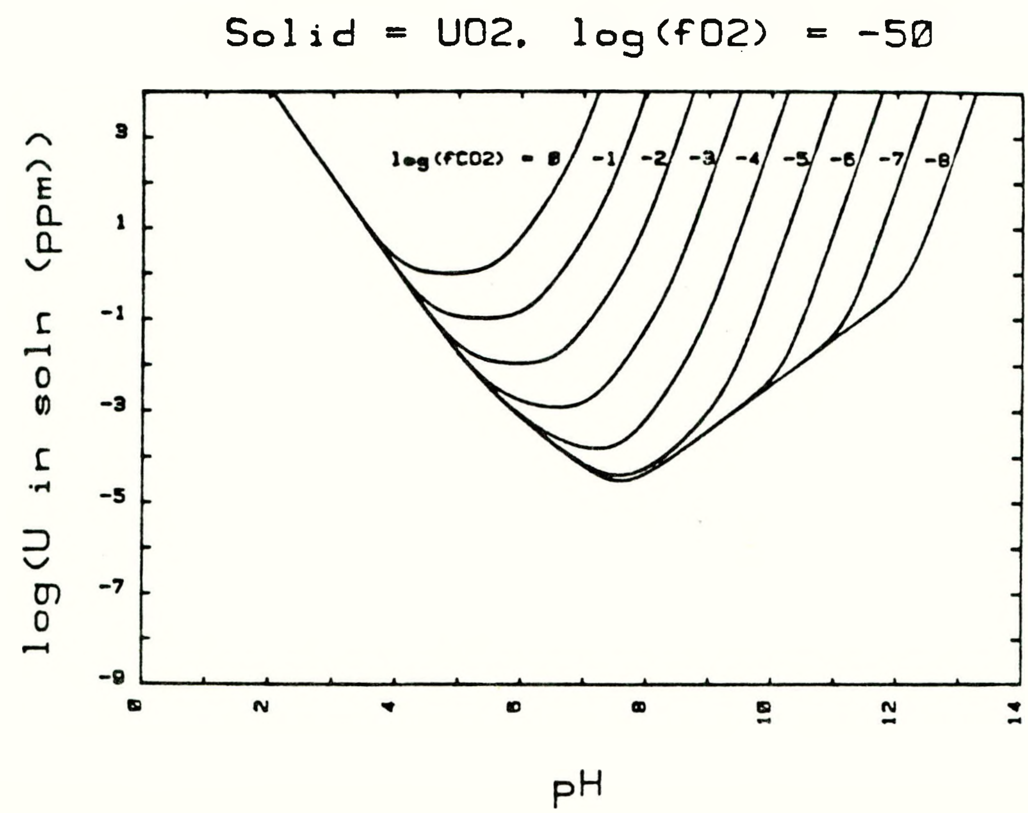


FIGURE 6. CALCULATED UO_2 SOLUBILITIES IN PURE H_2O AS A FUNCTION OF pH FOR SELECTED CO_2 FUGACITIES AT AN OXYGEN FUGACITY OF 10^{-50}

shortly after the sintered UO_2 pellet was placed in the leachant was measured to be 1.5 ppb. Two weeks later, the uranium concentration was 3.0 ppb. From that time on, the uranium concentrations were measured to be $(17 \pm 2) \times 10^{-2}$ ppb for contact times that varied from 2 to 4 weeks. The system appears to be either at equilibrium or changing extremely slowly. These low uranium concentrations are three orders of magnitude smaller than those observed in the hydrogen-produced reducing conditions in the spent fuel leaching experiments. Longer contact times will be performed with the Fe^{2+} (o-phenanthroline)$_3$ system to determine whether the uranium concentration is changing with time.

The fourth reducing agent being investigated is an iron foil. Iron is sufficiently strong to reduce any UO_2^{2+} that may be present in solution. Iron also is capable of reducing oxygen in solution. The iron foil experiment is being performed in the following manner. An iron foil and a small amount of ortho-phenanthroline were placed in water that was degassed with an Ar-H_2 gas mixture. The purpose of the ortho-phenanthroline is to complex and keep in solution any ferrous ion formed from the oxidation of the iron foil. The pH of the solution was observed to rise to values in the range of 8.9 to 9.3. This change in pH is a sensitive indication that the iron is reducing residual oxygen in the solution, according to the reaction

$$Fe + \tfrac{1}{2}O_2 + H_2O \rightarrow Fe^{2+} + 2OH^-.$$

The oxygen content of the solution was measured with an EIL membrane-covered probe after the pH stabilized. The probe indicated <50 ppb, which is its lower limit of detectability.

The UO_2 dissolution studies in this system began with the addition of sintered UO_2 to the pH 9.3 water. The results are given in the following tabulation.

Contact Time	15 m	15 m	2 d	2 d	3 d	15 m	7 d
U, ppb	6.2	3.6	3.5	3.9	0.35	0	0.02

The uranium concentrations measured after the five contact times can be seen in Table 2 to be one to two orders of magnitude higher than the last value listed, which is the lower limit of detection for the uranium analysis procedure. This phenomenon of high initial concentrations is characteristic of other UO_2 solubility or leaching experiments too. The explanation of this observation may involve an initial cleansing of the UO_2 surface of loose and small particles or of an oxidized layer.

We conclude that iron is an effective agent to produce reducing conditions for our experimental programs.

Conclusions

The most difficult part of this work is obtaining solutions with extremely low oxygen concentrations for measuring the dissolution of UO_2 and the release of fission products under reducing conditions. The experiments with iron and with ferrous ions as reducing agents have demonstrated that, after an initial period of leaching, very low concentrations of uranium are measured in the leachants. When iron is used, the result is a uranium concentration at the limits of detectability. These results constitute significant progress in this work.

The concurrent experiment to measure the solubility of UO_2 powder under reducing conditions obtained through the use of hydrogen gas and a palladium-black catalyst has been continued this quarter. The uranium concentrations decreased one order of magnitude when the pH of the solution increased from 4.5 to 5.9. Thermodynamic calculations are helping to give insight into this experiment. These calculations rule out the possibility of interference from uranium carbonate complex formation.

In the spent fuel element part of this work, electron microprobe scans were completed. The distribution of plutonium was that expected from work done at PNL. Some progress has been made in developing a reliable uranium measuring technique for the large number of leachant solutions on hand, but additional assay work remains to be done.

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WBS 1.1.3

Project: Thermodynamic Properties of Chemical Species in Nuclear Waste

Principal Investigator: Lawrence Berkeley Laboratory (N. Edelstein, S. Brown, R. Silva)

ONWI Project Manager: J. F. Kircher

Objective

The program is investigating the thermodynamic properties of anticipated actinide and fission product ions and the compounds they may form in geologic environments so that their chemical behavior and potential migration in a nuclear waste setting can be assessed with improved capability.

Activities During the Reporting Period

Experimental Survey of the Electrochemical Properties of the Actinides

During this quarter, considerable effort was devoted toward improving computer facilities, both by implementing a more stable operating system, and by equipping one computer with extended memory. This increased memory now allows an expanded capacity to perform fits or multifeature graphics, both of which should see considerable use in the present studies.

Programs were written to utilize the 16 bit digital-to-analog computer and a computer-controlled drop timer in differential pulse, normal pulse, and square-wave polarography, as well as differential pulse and square-wave voltammetry. These techniques are expected to be especially useful in studies of irreversible systems. A study of the UO_2^{2+}-OH^--$X^=$ system (where X is CO_3^{2-} or SO_4^{2-}) using differential pulse polarography and square-wave polarography was begun. The aim is to measure the mixed stability constant(s), which has been suggested to control uranium solubility in near-neutral waters. To attempt this, it is planned to vary both pH and pX and use a three-dimensional fit of the $E_{1/2}^{IRR}$ surfaces obtained from the study.

The Nd^{+3} -OH^- system has also been examined in more detail, using both forward and back titrations and measuring the [OH^-]. Plots of $\bar{n}$ versus [OH^-] indicate that the day-to-day reproducibility is not as good as observed in similar study of the Cu^{+2} -OH^- system. A thorough examination of about 40 titrations indicates that Models 1, 3, and 4 give similar fit parameters, as shown in Table 1. The simplest model, $NdOH^{++}$(1,1), would seem best from present data. The ambiguity seen between the models probably arises, in part, from the very small $\bar{n}$ values obtained for the Nd^{+3}-OH^- system (due to solubility constraints), and from a possible small CO_2 contamination problem, as extreme steps to exclude CO_2 from the experiment were not taken. Stability constants obtained for the Nd^{+3}-OH^- system are included in Table 1. Future work will emphasize careful exclusion of CO_2, and back titrations of the Nd^{+3}-CO_3^{2-} system will be attempted to determine the Nd^{+3}-CO_3^{2-} stability constants.

TABLE 1. COMPARISON OF NEODYMIUM HYDROLYSIS MODELS

	Model	-log β	Standard Deviation	Goodness of Fit
(1)	1,1	-9.21	0.0196	45.87
(2)	2,2	-13.85	0.061	74.26
(3)	1,1	-9.21	—	
	2,2	-15.36	0.1592	47.59
(4)	1,1	-9.21	—	
	1,2	-17.58	0.315	46.64
(5)	1,1	-9.21	—	110.58
	2,2	-15.36	—	
	3,5	-30.99	0.312	
(6)	1,1	-9.21	—	190.23
	1,3	-20.399	0.304	
	2,2	-13.85	—	
(7)	1,2	-16.84	1.19	74.85
	2,2	-13.85	—	

Construction and Testing of Laser
Spectroscopy Equipment

This quarter has seen the construction of the laboratory facility intended for laser spectroscopy. Most of the components required have now been received, with exception of the 8W Ar^+ laser and the modulator driver. Construction of the computer interface and assembly of other required components is now essentially complete. The optical table, dye lasers, and photodiode units are all assembled and are waiting for the pump laser to be aligned.

Experiments on laser-induced photoacoustic spectroscopy were attemped using a dye laser pumped by a 400 kW N_2 laser. A 0.1 M solution of Nd^{+3} was examined using R6G dye over the range 580 to 600 nm. No obvious signal was observed, probably because of a poor cell design, which involved use of a pressure fit to hold windows on a piezoelectric tube. The cell is being redesigned, and the experiment will be repeated using the Ar^+ laser to pump a dye laser using R6G. This arrangement will allow significantly higher input powers (~1 W) and should generate much larger signals.

Solubilities of Americium Hydroxide and
Americium Carbonate and the Identification
of Americium Species in Solution

Solubility of Americium in Solution. Measurements of the concentration of americium in aqueous 0.1 N $NaClO_4$ solutions in the pH range 5 to 10 have been completed. The procedures and results are summarized below.

To exclude CO_2 from the system, the sample preparations and subsequent measurements were carried out in an inert atmosphere box under an argon atmosphere. In addition, the box atmosphere was circulated through a canister containing soda lime to decrease the CO_2 content as low as possible. Unfortunately, there is no way to measure the exact CO_2 content. However, the O_2 content of the box atmosphere was measured periodically using a Teledyne model 310 oxygen analyzer. By purging the box with argon, the oxygen content of the box atmosphere was maintained at less than 2000 ppm O_2 or ~1 percent of room air. Since nothing was done to the box atmosphere to remove O_2 except purging with argon, an estimate of the upper limit to the CO_2 content could be made by assuming the CO_2/O_2 ratio in the box atmosphere was the same as the room air. This estimate was $<3 \times 10^{-6}$ atmospheres CO_2. Circulation of the box atmosphere through the canister should have reduced the CO_2 content substantially below this limit.

Before the americium solutions were prepared it was necessary to ensure sample purity. The purification of the Am^{3+} was accomplished by ion-exchange chromatography. The $^{243}Am^{3+}$ was loaded on a Dowex 50x8 cation-exchange resin column from 0.1 M HCl. The column was first washed with 3 column volumes of 0.1 M HCl and then 3 column volumes of 3 M HCl. The Am^{3+} was then eluted with 6 M HCl. The eluate was taken to near dryness and a stock solution of 1 ml of 5.996×10^{-3} M ^{243}Am was prepared with 0.1 M HCl. Alpha pulse height analysis of samples taken from the stock solution showed that the isotopic composition was 99.8 percent ^{243}Am, 0.15 percent ^{241}Am, and $<10^{-4}$ percent ^{244}Cm by weight.

Care was taken in the preparation of solutions so as not to introduce contaminants. All solutions were prepared with distilled-deionized water from which CO_2 had been removed by boiling for about 1 hour, followed by flushing with argon. Ultrapure HCl, NaOH, and $NaClO_4$ were used to prepare the americium solutions and to adjust pH.

It was found in the previous studies that sorption of americium by the container walls and/or on dust or other particles suspended in solution in the near-neutral or alkaline range was not significant for initial americium concentrations of 10^{-6} M or greater using 0.1 N $NaClO_4$ as supporting electrolyte. Therefore, duplicate samples (labelled Am I and Am II) of 100 ml volumes, $1.023 \pm 0.031 \times 10^{-5}$ M in ^{243}Am and 0.1 N in $NaClO_4$, were prepared. The pH of these solutions was initially adjusted to 5 with dilute NaOH. The pH was then increased in steps of ~1 pH unit to pH 10. The pH measurements were made using an Orion Model 399A pH meter with a Beckman Model 39505 combination glass electrode. At each new pH value, the solutions were allowed to sit for several days to reach equilibrium. The pH was checked nearly daily and readjustments were made as necessary. Initially it was planned to allow the solutions to sit at each pH for about 4 days. However, in the range 6 to 9, the pH tended to drift slowly, usually to lower values, with time. Therefore, waiting times were extended to longer periods to allow the pH to more or less stabilize. However, even after the longer periods, some drift was observed at pH 7, 8, and 9.

At the end of the waiting periods, samples of the two solutions were taken and centrifuged at 15,000 rpm for 5 minutes. One ml of the centrifuged solutions was taken directly for analysis for ^{243}Am content. Two ml of the centrifuged solutions was passed through 0.4-micron Gelman disposable filters. In an attempt to minimize the effect of possible sorption of americium by the filters, the first milliliter of solution through the filters was discarded and the second was taken for analysis for ^{243}Am. Since any precipitated americium could be in a finely divided form, at pH 8, 9, and 10 portions of the centrifuged solutions were also passed through 0.015-micron Nucleopore filters to determine whether there might be an effect due to filter pore size. All aliquots of the centrifuged and filtered solutions were acidified to 0.1 M in HCl before removal from the inert box for analyses.

The ^{243}Am content of the aliquots was determined by gross alpha counting using a Packard 460 liquid scintillation counter. Since the ^{239}Np daughter of ^{243}Am could contribute to the counting rate and was not necessarily in equilibrium with americium, the ^{243}Am was separated from the ^{239}Np by cation-exchange chromatography before counting. One ml of the aliquots (0.1 M in HCl) was passed through a 3-mm-diameter, 6-cm-long Dowex 50x8 cation-exchange resin column and the americium was absorbed on the top of the column. The column was then washed with 1 ml of 1 M HCl to elute the neptunium; then the americium was eluted with 1 ml of 6 M HCl. This procedure consistently gave greater than 95 percent recovery of the ^{243}Am free of ^{239}Np. Aliquots of the eluted americium solutions were made up to 1 ml with 0.1 M HCl, and 10 ml of Packard Insta-Gel scintillating cocktail was added. The ^{243}AM content of the solutions was then determined by liquid scintillation counting.

The concentrations of ^{243}Am, expressed as moles per liter, in the various samples as a function of pH are given in Table 2. From a consideration of errors associated with counting and sampling, the precision of the reported values for the americium concentrations is ~3 percent. The errors in the pH values were estimated from the inherent reproducibility of the pH meter and probe (~0.05 of a pH unit) and the observed drift in the pH during the waiting periods.

There was essentially no observed loss in americium from solution for both Am I and Am II at pH values of ~5, 6, and 7. Both the centrifuged and 0.4-micron filtered samples gave nearly the same results. At pH ~8, americium began to be lost from solution and the centrifuged and filtered samples began to give slightly different results. At pH values of 9 and 10, the centrifuged samples contained considerably more americium in solution than the filtered samples. These higher values, compared with those for the filtered solutions, could have resulted from finely divided $Am(OH)_3$ or americium sorbed on very small contaminant particles that were not centrifuged down at 15,000 rpm. They could also have resulted from sampling problems since it is possible that some of the centrifuged material could have been stirred up when the 1-ml samples were taken from the 1.5-ml centrifuge cones. However, the values obtained for the centrifuged samples do represent an upper limit to the solubility of americium under these conditions. At pH 9, the 0.4- and 0.015-micron filtered samples gave similar results, but at pH 10, the 0.4-micron samples contained approximately a factor of three less americium than the 0.015-micron samples for both Am I and Am II. This leads one to suspect that the filtration process may have removed americium from solution. The 0.4-micron Gelman filters are more massive and probably present a larger possible sorption area to the solutions than the 0.015-micron Nucleopore filters. Since the source of the difference between the 0.4 and 0.015 micron filtered samples is not known, values of americium concentration in solution for both filter sizes and for both Am I and Am II were averaged for the pH values of 8, 9, and 10 and least-square errors were calculated. For pH values of 5, 6, and 7, the results for the 0.4-micron samples for both Am I and Am II were averaged. The results of these calculations are displayed in Figure 1 as the points on Curve C.

Allard and Beall (1978) have reported estimates for the hydrolysis constants for Am^{3+} in aqueous solution as well as for the solubility product of $AM(OH)_3$. His estimates are given in Table 3. Using a computer program which includes corrections for ionic strength by the Davies equation, the solubility limit for americium in a 0.1 N $NaClO_4$ solution has been calculated as a function of pH from Allard's estimates. The results of the calculation are shown in Figure 1, Curve A.

TABLE 2. CONCENTRATION OF AMERICIUM[a] IN SOLUTION AS A FUNCTION OF pH

		Concentration, moles/liter					
		Am I (M)			Am II (M)		
pH	Time, days	1[b]	2[b]	3[b]	1[b]	2[b]	3[b]
4.95 ± 0.05	4	0.954×10^{-5}	0.964×10^{-5}		0.9451×10^{-5}	0.913×10^{-5}	
5.90 ± 0.15	5	1.020×10^{-5}	1.048×10^{-5}		1.059×10^{-5}	1.042×10^{-5}	
6.85 ± 0.20	7	0.873×10^{-5}	0.912×10^{-5}		0.921×10^{-5}	0.936×10^{-5}	
7.90 ± 0.15	23	3.757×10^{-6}	3.393×10^{-6}	2.131×10^{-6}	5.715×10^{-6}	5.322×10^{-6}	3.975×10^{-6}
8.95 ± 0.10	21	1.699×10^{-7}	1.140×10^{-8}	2.362×10^{-8}	7.700×10^{-8}	1.288×10^{-8}	1.297×10^{-8}
10.00 ± 0.05	12	1.595×10^{-7}	1.750×10^{-9}	5.040×10^{-9}	7.716×10^{-8}	1.698×10^{-9}	4.394×10^{-9}

(a) Initial Am concentration = $1.023 \pm 0.031 \times 10^{-5}$ M.

(b) 1 — centrifugation; 2 — centrifugation plus 0.40-micron filtration; 3 — centrifugation plus 0.015-micron filtration.

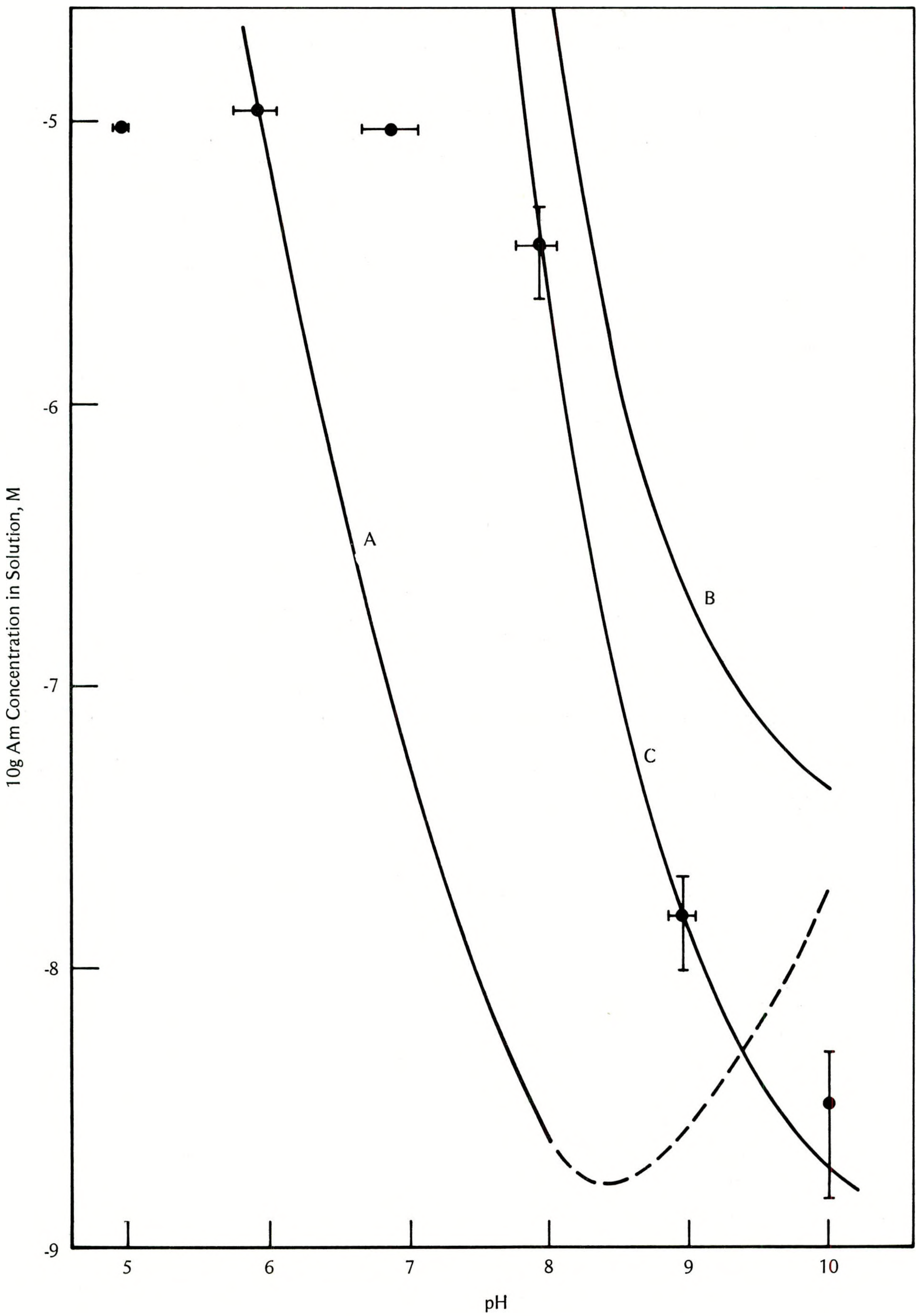

FIGURE 1. Am CONCENTRATION VERSUS pH

TABLE 3. ESTIMATES OF HYDROLYSIS AND SOLUBILITY CONSTANTS OF Am^{3+}

Reaction	log k (Allard)	log k (Baes & Mesmer)
Hydrolysis		
$Am^{3+} + H_2O \rightleftharpoons Am(OH)^{2+} + H^+$	-5.8	-8.0
$Am^{3+}\ 2H_2O \rightleftharpoons Am(OH)_2^+ + 2H^+$	-13.0	-16.9
$Am^{3+} + 3H_2O \rightleftharpoons Am(OH)_3^0 + 3H^+$	-21.0	-26.5
$Am^{3+} + 4H_2O \rightleftharpoons Am(OH)_4^- + 4H^+$	-30.0	-37.1
$2Am^{3+} + 2H_2O \rightleftharpoons Am_2(OH)_2^{4+} + 2H^+$	-11.0	-13.8
Precipitation		
$AM^{3+} + 3H_2O \rightleftharpoons Am(OH)_3 + 3H^+$	-12.0	-18.7

Baes and Mesmer (1976) have also estimated the solubility product for $Am(OH)_3$ from a comparison with a lanthanide ion of nearly the same ionic radius, i.e., Nd^{3+}, and their estimate is given in Table 3. It seems reasonable to go a step further and to use the measured or estimated values for the hydrolysis constants for neodymium as estimates for americium. These values, taken from Baes and Mesmer, are also shown in Table 3. The solubility limits for $Am(OH)_3$ in 0.1 N $NaClO_4$ were calculated as a function of pH using these estimates and these are shown in Figure 1, Curve B. Clearly the experimental data favor the solubility limit line calculated from the Baes and Mesmer estimates (Curve B) over the line calculated using Allard's estimates (Curve A). In fact, if the solubility of $Am(OH)_3$ estimated by Baes and Mesmer is decreased about a factor of 10, i.e., changing log K = -18.7 to log K = -17.5, the calculated Curve C in Figure 1 results.

To check the reversibility of the reaction, the solutions are being returned from pH 10 to pH 5 in steps of 1 pH unit.

REFERENCES

Allard, B., and G. W. Beall. 1978. "Predictions of Actinide Species in Groundwater", presented at Workshop on Environmental Chemistry of the Actinide Elements, Warrington, Virginia, October 9-12.

Baes, C. F., Jr., and R. E. Mesmer. 1976. *The Hydrolysis of Cations,* John Wiley & Sons, New York.

WBS 1.1.3

Project: Desiccant Materials Screening

Principal Investigator: Lehigh University (D. R. Simpson)

ONWI Project Manager: D. P. Moak

Objective

One setting considered for the disposal of radioisotopes is within salt beds. Although these salt beds appear to be essentially dry, a small quantity of brine may migrate toward the storage area as a result of heat generated by the radioactive decay. This brine results from minute droplets trapped during the crystal growth, and it migrates toward a heat source by solution and precipitation of the host salt crystal. Backfilling around the disposed waste with a desiccant material would establish the anhydrous environment.

This research is aimed at appraising various materials for their suitability as desiccant backfill. The appraisal began with literature searches and continues with experimentation to provide further data on the behavior of the substances in saline brines.

Activities During the Reporting Period

No progress report was submitted for the period.

WBS 1.1.3

Project: Development of Backfill Material

Principal Investigator: Battelle Pacific Northwest Laboratory (E. J. Wheelwright)

ONWI Project Manager: D. P. Moak

Objectives

The objectives for this project are described separately for the individual tasks below.

Introduction

Concepts currently under investigation for the disposal of spent nuclear fuel or separated high-level nuclear waste involve deep emplacement of the waste in continental geologic formations. In such disposal concepts, primary canisters or primary canisters contained within one or more overpacks are placed in an oversized hole bored into the geologic medium; the space between the surface of the canister or overpack and the geologic medium is then backfilled with a suitable material or combination of materials. Emplacement of properly engineered backfill materials can significantly reduce the possibility of radionuclide migration into the geologic medium by increasing the redundancy of barriers. A properly placed multi-component backfill could provide a high-integrity seal against ground-water penetration and could ensure selective sorption of specific radionuclides such as ^{129}I and ^{99}Tc in the event that ground-water penetration and leaching of the waste does eventually take place. Backfill components can improve the chemical stability of the canister or overpack by controlling the Eh and pH of the immediate environment.

Activities During the Reporting Period

PRELIMINARY DEMONSTRATION OF A MULTIFUNCTIONAL BACKFILL MATERIAL

Objectives

The objectives of this activity are to provide an early laboratory-scale demonstration of a multifunctional backfill material and, in doing so, to gain experience for use in designing the subsequent screening experiments employed in the laboratory evaluation of selected backfill materials.

Initial laboratory experiments include evaluation of pure bentonite clay plus clay mixed with other selected exchange materials. The compaction properties, the permeability of the compacted forms in a dynamic-flow system, and the migration properties of selected ions of interest (e.g., ^{129}I, ^{137}Cs, ^{90}Sr, and ^{99}Tc) will be determined.

Procedures

Pure bentonite pellets 1 inch in diameter have been pressed to densities of 2 g/cm^3 at ~2 tons/in.^{2}. The pressed pellets are mechanically stable and do not crack or crumble with reasonable handling. Additional pellets are being evaluated as a function of pressing conditions, water content, and clay-exchange material ratio.

In initial experiments, a heavy-wall stainless steel cylinder with a fritted plate in the bottom was used to investigate the effects of pumping water through pressed bentonite clay. It quickly became evident that the clay must be constrained by a fritted plate on top of the bed. The equipment is being redesigned to include this feature and hopefully, to provide a measure of the pressure exerted by the bentonite against the confining cylinder and end plates as water is forced through the pressed clay bed at high pressures.

Techniques have been developed to determine batch distribution (Kd's) for a number of candidate backfill exchange materials as a part of the screening process to select a manageable number of materials (6 to 12) for a more comprehensive evaluation.

DEFINITION AND PRIORITIZING OF BACKFILL REQUIREMENTS

Objectives

The objectives of this activity are to define the "reasonable purposes" of a backfill (what functions it should fill) and then convert the "reasonable purposes" to a prioritized and quantified list of backfill performance attributes. Backfill material could be used simply to fill in the space between the waste canister and the host geologic media. A much more meaningful purpose would be to provide a redundant barrier(s) to the migration of radioactive species from the waste to the biosphere. Any emplaced backfill material will be subjected to five influences:

(1) Mechanical pressure and stress

(2) A high radiation field

(3) Above-ambient temperature

(4) Hydraulic flow of ground water

(5) Materials dissolved in the ground water.

The backfill material must continue to fulfill its function(s) while subjected to these five influences for time periods ranging up to 10^6 years.

Procedures

Two backfill functions being examined that do provide redundant barriers are (1) minimizing the penetration of ground water to the encapsulated waste and (2) controlling the chemical environment surrounding the encapsulated waste.

If ground water cannot reach the canister or if the rate of migration is so slow that the amount of water that can come into contact with the waste canister even in 10^6 years is small, canister corrosion will be significantly reduced and the principal mechanism for transporting radioactive species to the biosphere eliminated. Results of initial experiments described in the Procedures section imply the possibility that compacted bentonite clay can provide such a barrier.

Chemical control of the environment surrounding the encapsulated waste can be accomplished by placing carefully selected materials in the backfill that will buffer the pH to a desired range and reduce the oxygen fugacity to near zero. Such careful control will minimize corrosion of the canister system and greatly reduce the migration rate of most cationic radioactive species. Additional chemical control is achieved by using backfill material such as bentonite clay with high cation-ion-exchange capacity or by adding specialized absorbing material for selected nuclides such as ^{129}I.

A preliminary list of backfill attributes (see Table 1) has been compiled.

SCREENING OF POTENTIAL BACKFILL MATERIALS

Objective

Potential backfill materials and combinations of materials will be screened to select a small number for exhaustive laboratory testing. Those that show the greatest promise of meeting the performance attributes defined in the activity described in the previous section will be chosen. As noted, major emphasis has been placed upon expanding clays, but other materials have not been excluded from consideration.

Procedures

Activities to date include an extensive literature search and documentation of materials properties to provide a basis for the ultimate selection.

LABORATORY EVALUATION OF SELECTED BACKFILL MATERIAL

Objective

The objective in this task is to experimentally measure the performance characteristics of the selected backfill materials and to evaluate the experimental results in terms of the defined attributes.

TABLE 1. UNORDERED LIST OF POSSIBLE BACKFILL MATERIALS ATTRIBUTES

	Relative Importance											
	High			Medium			Low					
Attribute	1	2	3	1	2	3	1	2	3	Experimentally Measurable Property	References	General Comments
1. Water Exclusion										-Porosity (θ) -Permeability (ϵ) -Diffusivity (D) -Low hydraulic conductivity -Capillary pressure		-Hydrophobic surfaces -Very small pores
2. Radionuclide Retention										-Distribution coefficient (K_d) -Dispersion coefficient (K_f) -Radionuclides - Specific Loading Capacity		-Channeling (seams, cracks) -Thickness (boundary effects)
3. Mechanical Stability										-Modulus of elasticity • in shear (G) • in tension } (E) • in compression } (E)		
										-Bulk modulus of elasticity (K) -Modulus of resilience (U_p) -Modulus of rupture (S_R) - in bending - in torsion		
										-Atterberg limits		-Atterberg limits are the plasticity index, liquid limit, plastic limit
										-Activity		-Activity = Ratio of Atterberg plastic limit to fraction of clay in the substance
4. Thermal Stability										-Retention of chemical and physical properties during and after thermal stress -Coefficient of thermal expansion (β)		-Cracking -Diagenesis

TABLE 1. (Continued)

	Relative Importance											
	High			Medium			Low					
Attribute	1	2	3	1	2	3	1	2	3	Experimentally Measurable Property	References	General Comments
5. Radiation Stability										-Retention of chemical and physical properties during and after irradiation		-Diagenesis
6. Satisfactory Heat-Transfer Capability										-Thermal conductivity (k) -Emissivity (ϵ) -Overall heat-transfer coefficient (U)		
7. Mitigation of Long-Term Intrusion												-Possible colored material -Do not utilize materials that are currently, or projected to be, valuable or in short supply
8. Availability										-Resource assessment -Supply capabilities -Resource utilization/conservation		
9. Cost/Cost-Benefit												-Resource available in adequate quantity
10. Homogeneity/Reproducibility												-Can the selected backfill be adequately reproduced with the same attributes?
11. Resistance to Biological Degradation										-Retention of physical and chemical properties during and after exposure to biological attack		
12. Self-Sealing Ability/Ductility										See Item 3		
13. Ease of Emplacement/Formability										See Item 3		

TABLE 1. (Continued)

Attribute	Relative Importance									Experimentally Measurable Property	References	General Comments
	High			Medium			Low					
	1	2	3	1	2	3	1	2	3			
14. Compactibility										See Item 3		
15. Faulting Characteristics										See Item 3		
16. Shear Resistance										See Item 3		
17. Long-Lived Physical and Chemical Properties										-Retention of physical and chemical properties with time periods up to and beyond 1000 years		
18. Radiation Attenuator										Shielding properties		
19. Unconfined Compressive Strength										See Item 3		
20. Hydrophobic										See Item 1		
21. Swelling Capability										See Item 1		
22. Large and Permanent Molecular and Cationic (Anionic) Sorption Capacity										See Item 2		
23. High Consolidation Rate												-Rate of compression

TABLE 1. (Continued)

Attribute	Relative Importance: High 1	High 2	High 3	Medium 1	Medium 2	Medium 3	Low 1	Low 2	Low 3	Experimentally Measurable Property	References	General Comments
24. Low Sensitivity										-Strength in undisturbed state divided by strength in remolded state		
25. Compatibility a. With Geology b. With Package c. With Media Solutions d. With Other Backfill Components Prior to and Following Any "Reaction" (i.e., Sorption)										-Change in physical and chemical properties following exposure to or reaction with (a), (b), (c), or (d)		
26. "Permanent" Retention of Radionuclides										See Items 2 and 17		
27. Enhances Package Retrievability												
28. Barrier to Corrosion Products/High Ion-Exchange Capacity										-Sorption capacity for possible corrosion products, H^+, OH^-, radionuclides, etc.		

TABLE 1. *(Continued)*

Attribute	Relative Importance									Experimentally Measurable Property	References	General Comments
	High			Medium			Low					
	1	2	3	1	2	3	1	2	3			
29. Available in Adequate Purity										–Low organic impurities		
30. Corrosion Resistance												
31. High Oxidation Resistance												
32. General Items										a. Diagenesis		
										b. Thixotropy		
										c. Precipitation in reaction		
										d. Transport phenomena		
										e. Filtration capability		
										f. Radionuclide convection		
										g. Particle shape (ψ), (η)		
										h. Particle size (Do)		
										i. Void ratio		
										j. Swelling versus sorption/ cross effects		
										k. Density (ρ)		
										l. Cushion effect		
										m. Fluids content at time of emplacement		
										n. Are any properties directional; isotropy and anisotropy		
										o. What is the effect of density on mechanical stability?		
33. High Redox Potential												

TABLE 1. (Continued)

Attribute	Relative Importance: High 1	High 2	High 3	Medium 1	Medium 2	Medium 3	Low 1	Low 2	Low 3	Experimentally Measurable Property	References	General Comments
34. Enhances pH and Eh of environment										See Items 29 and 34		
35. Gettering properties for O_2, etc., are high										See Items 2, 29, and 34		

Procedures

Work has been started to define the number and kind of experimental tests that will be done and the specific procedures that will be used.

WBS 1.1.4

Project: ONWI Support Program; Program Coordination and Special Problems

Principal Investigator: Oak Ridge National Laboratory (A. L. Lotts)

ONWI Project Manager: G. E. Raines

Heat Transfer Studies

Objective

Two thermal analyses studies are in place: (1) direct comparison of thermal analyses computer codes and (2) limits of applicability of computer codes, models, and data used in repository design. The objective of the first study is a direct comparison of the calculated results for the two- and three-dimensional representations of a hypothetical repository using the finite difference codes HEATING5, THAC-SIP-3D, TRUMP and SINDA and the finite element codes ADINAT and TRANCO (renamed SPECTROM 41). The objective of the second study is to investigate some areas involving limits of applicability of codes, models, and data used in waste repository designs and to demonstrate by a sample problem the efficacy of the techniques used along with recommendations for future work.

Progress Reported Previously

The final draft of a report entitled *A Statistical Sensitivity Analysis of a Simple Nuclear Waste Repository Model in Salt* was completed.

A similar analysis was made for a granite repository. For this study 51 input parameters were considered. These parameters describe the physical properties of the materials in the repository, the geometric modeling, and the initial temperature distribution.

Using engineering judgment, 22 input parameters were assumed to be important, i.e., to have high sensitivity values. The engineering judgment was based on the sensitivity analysis performed for the salt repository. For all the assumed important input parameters, the exact sensitivity values were calculated. The calculations were done by rerunning the HEATING5 code for each change in the input parameters and comparing it to the base case. The sensitivities obtained are time dependent for the first 50 years of the repository life.

The next stage in the analysis was to determine whether there are other important parameters besides those assumed. To do that, a validation test was applied. With this test all the assumed unimportant input parameters were randomly changed by ± 1 percent. The probability that more important parameters exist besides those that were calculated is less than 0.5 percent.

Activities During the Reporting Period

The report mentioned above was published in June.

A sensitivity analysis was conducted for a granite repository. The nonlinearity effects were considered by calculating the second order derivatives of the important temperatures in the repository with respect to the important input parameters. The nonlinearity effects were small.

A crude estimate of the uncertainties of the input parameters was used to calculate the uncertainties of the important temperatures in the repository (uncertainties of the responses). The response uncertainties were obtained by combining the uncertainties of the input parameters and the obtained sensitivity coefficients.

The standard deviations of the responses (the important temperatures in the repository) were between 4.1 to 4.9 percent at the beginning of life t=0, and between 9 to 10.4 percent after 50 years.

All these results are summarized in a draft report entitled *Sensitivity and Uncertainty Analysis of a Simple Near Field Granite Nuclear Waste Repository*.

Expected Repository Environments

Objective

The objective of this task is to identify the expected environments for nuclear waste and spent fuel repositories in bedded and in domal salt. The environments or effects include temperature distributions and histories, brine flows, brine chemistry, and pressure.

Progress Reported Previously

The ERE-Salt document was revised as additional calculations were performed.

The decay characteristics for Defense High Level Waste (DHLW) have been defined for calculational purposes. DHLW is difficult to characterize because of the composition variability.

Activities During the Reporting Period

The effort in this period was devoted primarily to preparing the report on the expected repository environments for final publication. A draft of a report on recommended repository conditions for salt was prepared.

WBS 1.1.4

Project: The Chemistry and Physics of Nuclear Waste-Rock Interactions

Principal Investigator: Pennsylvania State University (W. B. White, J. V. Biggers)

ONWI Project Manager: D. P. Moak

Objective

The objective is to identify and characterize chemical reactions and physical property changes between representative simulated nuclear waste forms and sedimentary rocks, primarily shale and salt.

Activities During the Reporting Period

NUCLEAR WASTE-ARGILLACEOUS ROCK INTERACTIONS

Long-Duration Experiments

Work is continuing on the analysis of the long-duration runs with shales plus waste. One impression obtained during the Scanning Electron Microscope (SEM) examination is that there is a regular ordering to the distribution of some of the elements between phases—as would be expected for chemical equilibrium. In particular, strontium appears to be partitioned into sulfates in preference to molybdates and in molybdates in preference to carbonates. So far strontium has not been recognized in silicates in a regular pattern. Barium is found in molybdates in preference to feldspars and in feldspars in preference to carbonates. The position of sulfates in this series is not certain; it seems that the preference of strontium for the sulfate is strong enough to account for most of the sulfate. Cesium is found in pollucite in preference to micas and is apparently absent in feldspars; several compounds of cesium, uranium, and molybdenum have been recognized, but their position in this scheme is not known. It is suspected that the presence of oxidized uranium is the controlling factor. All of these generalizations depend upon the presence of sufficient "anions", sulfate for example, to allow the identification of the expected phase (strontium sulfate). They also depend upon the interaction of the separate series. This hypothesis will have to be checked more carefully against the data which have already been collected and against the data yet to be collected. If it still seems reasonable, then a set of experiments using simple pairs of phases (calcium sulfate and strontium carbonate for example) would be reacted to determine rather quickly whether the predicted reaction (producing calcium carbonate and strontium sulfate) occurs.

The distribution of alkaline earths between competing phases is quite nicely demonstrated by sample S7D 306 13/50 (1:1:1 Conasauga Shale : PNL 76-68 glass : deionized water reacted at 300 C and 300 bars for 6 months). In this sample, large euhedral crystals of $BaSO_4$ containing minor amounts of strontium coexist (nearby) with large euhedral crystals of $CaMoO_4$, also with minor amounts of strontium. Elsewhere in this sample are clusters (akin to "barite roses") of euhedral grains of a compound of strontium, with lesser calcium and a low atomic number cationic group (most likely $CO_3^{=}$ or $BO_3^{=}$; NO_3^{-}, and OH^{-} are other possibilities). Calcium is also present as a minor component of one or more silicate phases (minor strontium is difficult to detect in a silicate; barium would be readily detected).

Tellurium has been found (among the solid phases) only as a compound with noble metals, presumably as the telluride. The occurrence in sample S7D 306 10/50 was a (Au, Pd)Te compound; previous occurrences had been of PtTe, with (at least) the platinum present in the run as an impurity in the gold.

The occurrence of albite ($NaAlSi_3O_6$) at higher temperatures and analcime-pollucite solid solutions $(Na, Cs)AlSi_2O_6 \cdot xH_2O$ at lower temperatures persists in the longer (6 month) runs, as was reported for the 1-month experiments.

For some of the 6-month experiments with glass (PNL 76-68) and shale, angular cavities are present in the coherent body of the charge. These may be places where the glass (or some other phase, but the shape, abundance, and occurrence apparently restricted to runs with glass suggest glass) has been removed completely, or nearly so; in some cases, a drusy lining is present.

Role of Brine Chemistry

The bicarbonate/sulfate "connate water" described in a previous report is now being used as a fluid in the waste-rock interaction runs. This should enable one to contrast the effects of carbonate complexing with the effects of chloride complexing.

Role of Oxygen Buffers

Little experimental work was done during this quarter on the question of oxygen fugacity and oxygen buffer capacity of shales. Attempts were made to devise either an experiment or a calculation that will allow the estimation of oxygen-consuming capacity of the rock since it is this parameter, rather than the oxygen fugacity itself, that is most critical to the immobilization of radionuclides in their lower valence states.

Waste-Rock Interactions in the Presence of Canister Metals

A major effort of this quarter was the initiation of studies on the quaternary interactions of a waste form, a specific shale, a specific canister metal, and a specific fluid.

The gold-capsule technique that has been used for all other waste-rock interaction experiments is not satisfactory for this series because of the possibility of electrolytic corrosion between the gold (anode) and the strip of canister metal (cathode). This problem has been resolved by the use of Teflon as an encapsulating material. Successful sealing of reactant materials into Teflon tubing was achieved only after an extensive set of trial-and-error experiments using various types of Teflons and various procedures for sealing.

Welding of Teflon using a torch (hydrogen-oxygen), a hot air gun, and a soldering iron has been tried, but without success. Because the Teflon is translucent to transparent (as contrasted, for example, with gold), it is possible to see the charge after it has been sealed in the capsule. In the 2 weeks since the capsules were prepared (the entire suite of capsules had not been completed and loaded), significant reaction had taken place (as indicated by color changes) at room temperature. The most spectacular example was the set with Brallier Shale (the only light colored shale in the set) and NBT-6a brine (shown to be very corrosive at higher temperatures with just the waste forms). There are signs of reaction with all four metals used: extensive discoloration in the case of copper or mild steel and only discoloration adjacent to the metal with the stainless steel or Zircaloy.

The metal plus shale plus waste experiments are still in preparation. The full set of experiments can be described as all of the possible terms of the product:

$$A_iB_jC_kD_lE_m$$

where

A_i i = 1,2,3	are the shales 01, 10, and 11
B_j j = 1,2,3,4	are the waste forms SPC-2+U, SURFP, 76-78, and blank
C_k k = 1,2,3,4	are the metals mild steel (1008), stainless steel (304L), Zircaloy, (2) and copper
D_l l = 1,2,3,4	are the fluids H_2O bicarbonate, brine NBT 6a, bittern brine, and NaCl + H_2O
E_m m = 1,2	are the temperatures 150 C and 250 C.

There are 384 combinations, and all of these except for B_2 (SURFP) have been prepared. The capsules are to be loaded into Teflon jars—each jar containing all capsules with the same values for A_i, D_l, and E_m. The jar will then be packed with more of the same shale and filled with the same brine to minimize the gradients in water and oxygen activity across the walls of the capsules.

Characterization of Interaction Products

Cesium Interactions with Shales. Cesium iodide is a highly soluble compound which is present in spent fuel elements. One hundred milliliters of distilled water dissolves 85.5 g of CsI at 25 C. This cesium phase did not react with clays or shales as readily as the Cs_2MoO_4 or CsOH at either 200 or 300 C, as indicated by the percentage of added cesium remaining in solution (Table 1). At 200 C, no pollucite could be detected with shales by X-ray diffraction analysis, but at 300 C, pollucite was detected only with chlorite of the clays and four of six shales (Table 2). In the case of montmorillonite, cesium from CsI was mainly fixed in the interlayers, as indicated by a decrease in the interlayer spacing, i.e., from 15.5 A to ~12 A. Cesium from CsI seems to have readily reacted with feldspars to produce pollucite (Table 2) but not with illite, as indicated by the percentage of cesium remaining in solution in the cases of illite and green mica (Table 1). Thus, this cesium phase is slow in reacting with clays or shales compared with Cs_2MoO_4 or CsOH.

Uranyl Silicate Phases. Two difficulties encountered in this study of uranyl silicate phase equilibria have been the presence of residual nitrate in the samples after the hydrothermal

TABLE 1. ANALYSES OF CESIUM REMAINING IN SOLUTION FROM VARIOUS MIXTURES OF CLAYS OR SHALES WITH CsI SOURCE WHICH WERE HYDROTHERMALLY TREATED AT 200 AND 300 C/300 BARS FOR 2 MONTHS AND 1 MONTH, RESPECTIVELY

Sample and Particle Size	Weight of Clay or Shale[(a)] +Cs Phase, mg	Weight of CS Added[(b)], mg	Cs in Solution, percent 200 C	Cs in Solution, percent 300 C
Kaolinite, pulverized	125.2	12.9	–	92.9
Montmorillonite, pulverized	133.6	17.2	–	49.4
Green mica, <105 μm	124.5	12.5	–	81.5
Illite, <105 μm	134.8	17.8	–	75.4
Chlorite, <105 μm	117.6	9.0	–	81.8
Salona shale, <75 μm	125.5	13.0	–	30.8
Antrim shale, <75 μm	132.4	16.6	–	69.4
Brallier shale, <75 μm	130.7	15.7	–	84.3
Conasauga shale, <75 μm	129.7	15.2	85.0	63.7
Catskill shale, reduced, <75 μm	142.1	21.5	99.9	66.6
Catskill shale, oxidized, <75 μm	136.5	18.7	–	48.9

(a) Weight of clay or shale is 100 mg in all cases.
(b) Molar ratio of silicon in clay or shale to cesium added is 8 in all cases.

runs and the reduction of uranium in the samples due to hydrogen diffusion through the gold capsules. In order to proceed with the project it was first necessary to resolve these problems.

The problem with the residual nitrate was resolved through the use of a slightly modified sample-preparation procedure. In this procedure, the sample is thoroughly ground to a very fine powder before denitration. Apparently, if the sample is not thoroughly ground before denitration, nitrate adsorbed within the interior of the sample will not be able to diffuse through the sample to the surface and escape. Thus, a small amount of residual nitrate remains which later appears in the analysis of the samples after the hydrothermal runs. By thorough grinding before denitration, the surface area of the sample is increased enough so that all of the nitrate will readily escape.

A sample having the composition $K_2O \cdot 13UO_3 \cdot 6SiO_2$ was reacted hydrothermally at a temperature of 300 C and a pressure of 300 bars for 8 days. Analysis of the sample after the run indicated the absence of nitrate in the sample.

TABLE 2. X-RAY DIFFRACTION ANALYSIS OF VARIOUS MIXTURES[a] OF CsI WITH CLAYS OR SHALES HYDROTHERMALLY TREATED AT 200 AND 300 C/300 BARS FOR 2 MONTHS AND 1 MONTH, RESPECTIVELY

Sample and Particle Size	Pollucite Formation by XRD	Clay or Shale Behavior by XRD	Other Phases by XRD
Shales + CsI mixtures at 200 C			
Conasauga shale	ND[b]	No obvious change	ND
Catskill shale, reduced	ND	No obvious change	ND
Clays or shales + CsI mixtures at 300 C			
Kaolinite, pulverized	ND	No obvious change	ND
Montmorillonite, pulverized	ND	15.5 A collapsed to ∿12 A	ND
Green mica, <105 μm	ND	No obvious change	ND
Illite, <105 μm	ND	Better crystallized	ND
Chlorite, <105 μm	Slight	No obvious change	ND
Salona shale, <75 μm	Very strong	F[c] disappears, I+[c] decreases	ND
Antrim shale, <75 μm	Strong	F and I decrease	
Brallier shale, <75 μm	ND	I better crystallized	ND
Conasauga shale, <75 μm	ND	I better crystallized	ND
Catskill shale, reduced, <75 μm	Strong	F disappears, I decreases	ND
Catskill shale, oxidized, <75 μm	Very strong	F disappears, I decreases	ND

(a) Molar ratio of silicon in clay or shale to cesium added is 8 in all cases.
(b) ND = None detected.
(c) F = feldspars; I = illite; K = kaolinite.

The problem with the reduction of the uranium in the sample by hydrogen diffusion through the gold capsules was resolved by using H_2O_2 as the fluid medium. The presence of the H_2O_2 maintains a sufficiently oxidizing environment within the capsule so as to prevent reduction from occurring.

A set of samples having the composition $K_2O \cdot 13UO_3 \cdot 6SiO_2$ was reacted hydrothermally at 300 C and 300 bars for 8 days. For one control set of samples, deionized water was used as a fluid medium; for the other set, H_2O_2 was used as the fluid medium. After the run was completed, both sets were examined for reduction. The set with H_2O_2 showed no observable reduction of the uranium. However, the set with water showed extensive reduction.

The next phase of this project will involve the preparation of 30 new sample compositions. The purpose of these compositions will be (1) to define more precisely the locations of the boundaries between the compatibility triangles, (2) to attempt to define the location of the unknown phase reported in the prior quarterly report, and (3) to verify that the presence of the residual nitrate in the previous runs did not have an appreciable effect on the phase reduction.

BRINE MIGRATION IN SALT

Microstructural Characterization of Hot-Pressed Salt: Grain Size and Subgrain Size Analyses

As described in previous reports, a series of nominally pure recrystallized commercial loose salts with a grain-size variation representing that of natural salt have been consolidated by hot pressing for use as test samples in the investigation of brine migration in salt.

The grain size of hot-pressed samples was analyzed by linear intercept techniques and the results were reported in a previous Quarterly Report.

Subgrain Formation in Sodium Chloride. Many investigators have documented the formation of an extensive subgrain structure in crystals with the rock-salt structure as a result of high-temperature deformation, that is, at temperatures exceeding the 0.5 C melting temperature.

In a paper describing etching techniques for sodium chloride, Mendelson (1962) found that after annealing for 3 hours at 600 C the highly strained area around a crack had polygonized, showing a subgrain structure. Later Mendelson (1962) found that polygonization occurred in the later stages of primary creep in synthetic-salt single crystals.

Carter and Heard (1970) performed an extensive study of the deformation behavior of reagent-grade salt single crystals from room temperature to 500 C at stresses up to 150 bars. They found that salt deforms on one primary slip system $\{110\}\langle 1\bar{1}0\rangle$, and two secondary systems, $\{100\}\langle 110\rangle$ and $\{111\}\langle 1\bar{1}0\rangle$, with slip on the primary system occurring at room temperature and 50 bars and with the secondary systems becoming activated at higher temperatures and pressures.

In general, higher temperatures and lower strain rates tended to favor dislocation interaction effects, which resulted in polygonization of the single crystal into a network of slightly misaligned cells bounded by subgrain boundaries. For the primary slip system, the transition to polygonization behavior occurred at rather low temperatures (near room temperature) at geological strain rates (see Figure 1; Carter and Heard, 1970).

Dislocations were found to rearrange into polygon walls by climb of edge dislocations and cross-slip of screw dislocations. At the highest temperatures and the lowest strain rates, the dislocation density within the polygon walls was near the as-grown density ($\sim 10^4$/cm) and the disorientation across the boundary was estimated by Berg-Barret X-ray topographs and

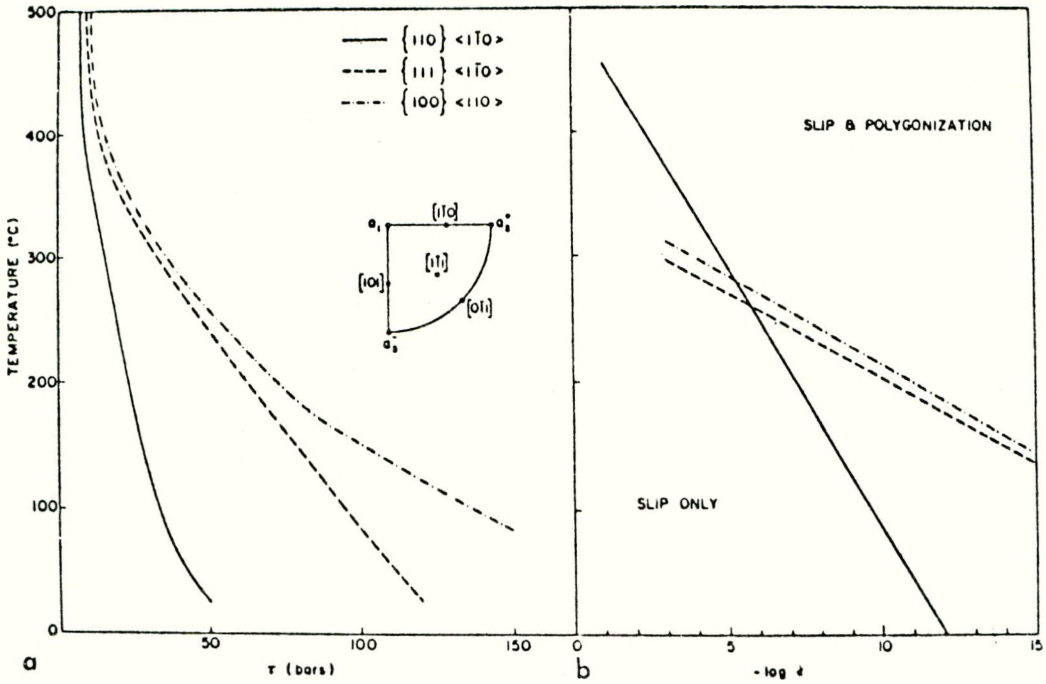

FIGURE 1. HALITE SINGLE CRYSTALS

rocking curves to be 0.1 to 0.5 degrees, with dislocation spacings from 2300 to 500 A. The average subgrain diameter produced was 0.5 to 0.15 mm.

Later work by Heard (1972) documented the same effect in reagent-grade polycrystalline salt. Again, pit and X-ray topograph studies indicated that steady-state creep was accompanied by polygonization, and recrystallization was not observed.

More recently, work by Bernal et al (1974) on hot forging of materials with the rock-salt structure has shown that above the brittle-ductile transition temperature (where five independent slip systems operate) subgrain boundaries may be introduced into single crystals by a process of polygonization and recrystallization. In general, the subgrain diameter decreases (subgrain boundary network becomes more extensive) as the working temperature is decreased and the strain rate (or pressing stress) is increased. Their study produced subgrains in KCl in the 0.005 to 0.010-mm range.

In the rock-salt structure, dislocations intersecting at 90 degrees (conjugate slip) to form a network is not favored since there is no lowering of the dislocation strain energy; however, the oblique slip (60 degree) reaction

$$\frac{a}{2}[110] + \frac{a}{2}[\bar{1}0\bar{1}] \rightarrow \frac{a}{2}[01\bar{1}]$$

is favored energetically and forms a theoretical subgrain network very similar to those seen after hot forging. These subgrain structures were first studied in detail by Amelinckz (1957).

Bernal et al (1974) recognize recrystallization as a competing recovery process occurring during polygonization which serves to reduce the strain energy built up in the crystal structure by the subgrain network. Extensive long-term deformation can lead to subgrain boundaries that become so misoriented that they are in fact grain boundaries. Bernal et al (1972) showed that large deformations can result in high degrees of orientation or crystal texture, and also that extremely fine subgrain structures developed under extensive deformation can be destroyed by spontaneous recrystallization at room temperature. This phenomenon was observed to occur from nucleation at points on the surface of the sample and in the interior, after hot forging was completed, and obviously was a factor during the forging, as the subgrain size was found to vary in banded zones throughout the sample.

At present, no documentation of the subgrain structures observed in natural salts has been found, even though polygonization is likely to occur during the deformation processes in salt beds and especially in salt domes. It may be that the recrystallization process removes this fine structure under equilibrium conditions. High degrees of crystal orientation have been documented, especially in domal salt (Carter, 1976).

Subgrains in Hot-Pressed Salt. After etching polished samples with etchants I and II, a fine subgrain structure was revealed in all samples. The subgrain structure was not evident in all grains in all samples (only 70 percent of the grains in Salt C showed subgrains), probably because of masking of the structure on specific crystallographic planes. All samples contained sufficient areas of subgrain structure for analysis.

The subgrain size was found to vary greatly with pressing temperature and to a lesser extent with grain size. It is likely that the subgrain size is also a function of pressure and strain rate during pressing, but these data are unavailable since all samples were pressed at the same pressure and densification data were not taken.

The pressure dependence of subgrain size was evident in the variation in this parameter in different portions of the sample. In general, the subgrain size was different near the periphery of the sample where die-wall friction causes variation in the stress field. The magnitude and the sign of the size difference varied with grain size of the material being pressed. At the point where the small brine cup is pressed into the sample, the average subgrain size was similar to that in the interior, but subgrain shape was more elongate and shape factors were significantly different from one measured. Subgrain data are compared with previous microstructural data in Table 3. $\bar{L}_3$, the mean intercept chord length, and S_v, the grain boundary surface area per unit volume, are both determined from the lineal intercept analysis of the microstructure. Data $\parallel \alpha$ and $\perp \alpha$ are for lineal analysis parallel and perpendicular to the applied stress, respectively. The shape factors (minimum to maximum chord length ratio) are determined from these values, and an average shape factor is shown for both grain size and subgrain size data. Since all values for a single sample are determined from the same basic data, the average standard deviation is shown as a percentage. In the case of the subgrain analysis, the quality of the data may best be described by the number of points on the sample where the analysis was performed.

Portions of all samples have been annealed at 500 C for 24 hours to determine the effect of annealing on the subgrain size, but data are available only for Salt E (Purex fine). In this case annealing resulted in a 25 percent reduction in subgrain diameter.

Chemistry of Hot-Pressed Samples. The commercial salts used for hot-pressed samples are nominally pure recrystallized salt. They are, in general, free from insoluble contaminants, but their purity with respect to soluble ions is in doubt. Samples were submitted for bulk spectrochemical analysis, with the results shown in Table 4.

TABLE 3. MICROSTRUCTURAL PARAMETERS FOR HOT-PRESSED SALTS

Starting Parameters

Salt	Morton-Norwich Commercial Design	Prepressed Grain Size, mm	Hot Pressing Parameters Temp, C	Pressure, psi	Time, min
A	K.D. Solar Extra Coarse	9.65	400	2500	5
B	K.D. Solar Coarse (-4 + 6m)	4.05	400	2500	5
C	K.D. Solar Coarse (-10 + 14m)	1.70	450	2500	15
D	Purex Evaporite	0.46	450	2500	5
E	Purex Fine Evaporite	0.27	450	2500	5

Hot Pressed Grain Size Data

Salt	$\bar{L}_3$, mm	$\bar{D} = \pi/2 \cdot \bar{L}_3$, mm	Shape Factor, $\parallel\sigma:\perp\sigma$	Boundary Surface, mm^2/mm^3 $\parallel\sigma$	$\perp\sigma$	Avg	Stnd Dev., %
A	6.33	9.94	0.723	0.378	0.273	0.326	5.9
B	3.62	5.68	0.639	0.711	0.454	0.583	3.8
C	1.22	1.92	0.781	1.86	1.46	1.66	2.5
D	0.28	0.44	0.719	8.77	6.33	7.55	5.8
E	0.15	0.24	0.706	16.28	12.14	14.21	5.2
Avg			0.714				7.1

Subgrain Data

Salt	$\bar{L}_3$, mm	$\bar{D} = \pi/2 \cdot \bar{L}_3$, mm	Shape Factor, $\parallel\sigma:\perp\sigma$	Boundary Surface, mm^2/mm^3	Stnd Dev., %	Number of Points on Sample
A	0.0127	0.0199	0.925	158.9	11.2	3
B	0.0090	0.0141	1.240	225.6	12.4	1
C	0.0183	0.0287	1.049	110.6	12.1	4
D	0.0176	0.0276	1.068	114.6	7.9	3
E	0.0159	0.0250	1.062	126.7	8.3	4
E(ANN.)[a]	0.0119	0.0187	1.005	174.8	21.4	2

(a) Sample E(ANN.) is Purex fine evaporite after annealing at 500 C for 24 hours in air.

TABLE 4. SPECTROCHEMICAL ANALYSIS OF COMMERCIAL SALTS

Salt	Commercial Designation	Elements Detected by Emission Spectroscopy, ppm				
		Ca	K	Mg	Sr	Fe
A	K.D. Extra Coarse Solar	430	150	100	35	<2
B & C	K.D. Coarse Solar	320	130	20	25	2
D	Purex Evaporite	480	80	20	16	<2
E	Purex Fine Evaporite	8300	230	50	50	<2
E sol	Purex Fine Soluble Material	3400	130	22	36	ND

Also, the percentage of insoluble material in each of these salts was determined by filtration of solutions. Insoluble contaminants were at a negligible level in all but the Purex fine (Salt E). This was found to contain 1.33 wt percent of a fine white powder, probably an anticaking agent. Since most anticaking agents are volatile, it was decided to determine the insoluble content of a hot-pressed sample of this salt. After hot pressing the sample still contained 1.01 wt percent of insoluble fine white powder. The soluble fraction of Salt E was as also submitted for spectrochemical analysis (see Table 4). The insoluble remains from both the bag salt and the hot-pressed sample were X-rayed but have not been identified.

Characterization of Avery Island Natural Salt Cores

Microstructural Characterization. A number of cores have been obtained from the Avery Island test site for use in brine migration testing. Characterization of these samples is still under way, but some preliminary data are now available. The first task, since a request for cored samples was filled but with essentially no accompanying data, was to determine the variability from core to core. Single lengths of core will be insufficient for the proposed testing schedule. The best gauge for this was to check the grain size in the plane perpendicular to the core length (sacrificing only a small amount of core) and to check the bulk chemistry. Grain size was determined using the lineal intercept method and data on each core received are listed in Table 5.

The average value of $\bar{L}_3$ falls within the standard deviation range of all cores analyzed, and all cores except core 8-1b are within 4 percent of the average value. On the basis of grain size, all cores are equivalent except possibly core 8-1b. The grain-size range of the natural cores appears to fall in between that of hot-pressed Salts B and C.

Samples of 8-1b and one of the other cores have been selected for more complete analysis, including grain size texture and subgrain size analysis. This work is not yet completed.

Chemistry of Natural Salt Cores. The Avery Island salt was chosen as the first natural salt for testing purposes because of its outward purity and uniform grain size as compared with salts at

TABLE 5. GRAIN-SIZE ANALYSIS OF NATURAL SALT

Core Label	$\bar{L}_3$, mm	$D = \pi/2 \cdot \bar{L}_3$, mm	Boundary Surface, mm^2/mm^3	Number of Grains
Barrel 6-5b-30'2"	2.74±0.13	4.30	0.731±0.35	367
Barrel 7-5b-70'0"	2.65±0.20	4.16	0.758±0.58	297
Barrel 7-2b-	2.72±0.35	4.27	0.745±0.94	381
Barrel 7-3b	2.69±0.16	4.23	0.745±0.43	367
Barrel 8-1b-35'2"	2.95±0.26	4.63	0.681±0.56	354
Barrel 8-2b-36'6"	2.77±0.21	4.35	0.726±0.56	380
Average Values	2.75±0.23	4.32	0.731±.061	Total 2156

other test sites (i.e., the WIPP site). Upon completion of the preliminary grain-size analysis, samples of core 8-1b and core 6-5b were submitted for bulk spectrochemical analysis. Also a portion of core 7-2b was dissolved and the dried solution submitted for spectrochemical analysis. The results are shown in Table 6.

Most notably, 8-1b and 6-5b differ in their potassium (KCl) and magnesium [$CaMg(CO_3)_2$-dolomite] content. If the bulk chemistry could be assumed to be the same between 6-5b and 7-2b, then it can be seen that a good portion of the calcium present is found to be soluble material associated with the NaCl, perhaps as calcium defects rather than as calcium in $CaSO_4$. The insoluble portion of 7-2b (0.36 wt %) was analyzed by X-ray diffraction and found to be anhydrite ($CaSO_4$) with perhaps 10 percent dolomite (determined by computer peak subtraction).

Comparison of Natural and Synthetic Samples. As suspected, these preliminary results indicate that the Avery Island cores are relatively clean and have minor element chemistries comparable to those of the synthetic samples. The major differences are:

(1) Avery Island samples contain a small amount of relatively fine-grained insoluble phases, primarily anhydrite with minor amounts of dolomite.

(2) Avery Island samples contain calcium in the 2000 to 3000 ppm range, primarily as soluble ions and probably as calcium defects in the NaCl.

(3) Avery Island samples contain an as-yet undetermined amount of contained brine.

(4) Although analysis has not been completed, it is likely that the natural salt samples do not contain a well-developed subgrain microstructure, if any at all.

(5) Although not yet ascertained, it is probable that the natural samples will show some grain orientation, perhaps similar to that in the synthetic samples.

TABLE 6. CHEMISTRY OF NATURAL SALTS

Sample	Portion	Elements Detected by Emission Spectroscopy, ppm					
		Ca	K	Mg	Sr	Al	Fe
Barrel 8-1b	Bulk	2800	70	23	19	4	ND
Barrel 6-5b	Bulk	2300	<10	4	17	2	ND
Barrel 7-2b	Solubles	1800	<10	3	12	2	ND

Brine Migration

Brine migration runs in the new cell on both synthetic and natural samples indicate slower migration rates than indicated by previous tests. This may be due to the fact that earlier tests were conducted on samples that had not been pressed to full density and which contained pressing flaws in the form of cracks. These defects, which would not necessarily be found in natural salt or the present suite of more flaw-free samples, could easily be the source of enhanced migration through polycrystalline samples. However, some of the tests, especially the two long-term runs shown in Table 7, indicate that part or all of the brine was lost to evaporation. Better seals may be required in the cell to prevent evaporation.

One of the long-term runs (Salt D in Table 7) was polished and etched and the microstructure was examined for migration artifacts. Areas of different contrast were seen emanating from the brine cup area which disappeared near the center of the sample. None of the rounded, elongate, pore-type artifacts seen in the lower density samples reported previously were noted. Upon examination under high magnification, it was noted that these rather broad areas tended to follow grain boundaries and that the grain boundaries within the areas showed fine separations along their length. These features were lost toward the center of the sample.

TABLE 7. BRINE MIGRATION TEST RUNS

Sample	Gradient, C/cm	Pressure, psi	Brine Added, ml	Brine Entered	Brine Exited	Time, hours	Maximum Velocity, cm/hr
Core 8-2b	9.0	400	0.25	Yes	No	24	0.13
Core 7-2b	7.6	400	0.25	Yes	No	48	0.069
Core 7-3b	7.4	400	0.25	Yes	No	24	0.13
A	7.0	400	0.35	Some	No	39	0.084
C	7.0	400	0.85	Some	No	170.5	0.019
D	(6.1)var	400	0.70	Some	No	158	0.021

Up to now it has been the procedure to first heat the cell to thermal equilibrium and then introduce warm, saturated brine to the sample through a small port in the center of the migration cell. This port may be the source of brine evaporation during the migration run. The alternative is to place brine in, seal the cup, and then bring the system to thermal equilibrium. Since this procedure would take several hours, the precise time of initiation would be impossible to determine. However, if the migration time through the present samples is on the order of days instead of hours, this error may not be as serious as earlier envisioned. In the future the test procedure will be altered in this way.

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WBS 1.1.4

Project: Strain-Related Radiation Damage Measurements in Rock Salt for Waste Disposal Applications

Principal Investigator: Brookhaven National Laboratory (P. W. Levy and K. J. Swyler)

ONWI Project Manager: J. F. Kircher

Objective

The facets of radiation damage in both natural rock salt and synthetic NaCl crystals which will be important for selection of a radioactive waste repository site, site design and engineering, evaluation of interactions between waste and host rock, risk assessment, and other considerations are being investigated. Unique equipment at Brookhaven National Laboratory is being used to make optical and other measurements on samples before, during, and after irradiation with 0.5 to 2.5-MeV electrons. The ability to make measurements during irradiation is particularly important. Rock salt and other minerals surrounding emplaced waste will be continuously irradiated and it is essential to determine whether important radiation damage processes occur during irradiation which might not be detected in samples studied only after irradiation. The principal means of studying radiation damage used up to the present time is the determination of F-center, i.e., negative ion defect, concentrations, and the concentrations and size of sodium metal colloid particles. The formation of these and other defects during irradiation and annealing, and other effects occurring after irradiation, are being studied as a function of dose rate, total dose, sample temperature during irradiation, strain applied prior to, and during, irradiation, etc. Also, synthetic NaCl and natural rock salt samples from different geological locations, including some potential repository sites, are being studied. The goal of the research is to provide sufficient information, as analytical expressions, graphs, tables, etc., to determine the radiation damage developed in rock salt surrounding emplaced canisters as a function of radiation levels, time after emplacement, salt temperature, and other parameters. To extrapolate from the laboratory studies to the dose rates, exposure times, and other parameters applying to repositories, it will be necessary to make a reasonably complete determination of radiation-damage formation and annealing kinetics in rock salt. Also, it will be necessary to determine whether radiation damage in rock salt from different localities is similar or whether a detailed study must be made for each locality under consideration. Almost all current studies are being made on rock salt, but other minerals including granite and basalt will be phased into the program.

Activities During the Reporting Period

No progress report was submitted for the period.

WBS 1.1.4

Project: Salt-Brine-Waste-Canister Interactions

Principal Investigator: U.S. Geological Survey, Menlo Park, California (M. A. Clynne)

ONWI Project Manager: J. O. Duguid

Objectives

The objectives are to determine the likely interactions among salt, brine, canisters, and waste at a range of temperatures and pressures which may be considered in disposal of high-level radioactive waste or spent fuel, and to determine the properties of the resultant reaction products at temperatures up to 300 C and pressures up to 2600 psia.

Progress Reported Previously

Brines in contact with nuclear waste would tend to dissolve ^{90}Sr and ^{137}Cs as chlorides. Such a fluid would contain its own energy source and by migrating could change the thermal evolution of the repository from designed values. In order to define the problem, the solubility of Sr and Cs in complex brines must be known. The solubilities of $SrCl_2 \cdot 6H_2O$, $SrCl_2 \cdot 2H_2O$, and halite in the system $NaCl-SrCl_2-H_2O$ have been determined from 18 to 115 C with NaCl contents fixed at 0, 5, 10, 15, and 20 weight percent.

Activities During the Reporting Period

The solubility data in the system $NaCl-SrCl_2-H_2O$ described above, together with those of Assarsson (1953), were fitted with equations. The results are shown in Figures 1 and 2. Figure 1 shows the solubility relations in weight percent of $SrCl_2$ versus T(C), contoured in weight percent of NaCl content. Figure 2 shows the phase relations in weight percent of NaCl versus T(C), contoured in weight percent of $SrCl_2$ content. The presence of NaCl in the solution reduces the $SrCl_2$ content and the solution is readily saturated with halite as well as the solid $SrCl_2$ hydrates. In the system $KCl-SrCl_2-H_2O$, a similar reduction of $SrCl_2$ solubility occurs but the content of total dissolved solids is higher at comparable temperatures. $CaCl_2$ and $MgCl_2$ are more soluble than $SrCl_2$, and bitterns high in either of these components limit $SrCl_2$ solubility to a few weight percent. In solutions with significant SO^{2-}_4, Sr is soluble only to about 0.0005 weight percent. Therefore, addition of a soluble SO^{2-}_4 bearing phase, e.g.,Na_2SO_4 in a waste canister overpack, would limit Sr mobility in the event of canister breaching.

Densities of halite saturated WIPP-A and NBT-6 brines have been calculated from 0 to 100 C using the Potter-Haas model. A series of density measurements approaching halite saturation has been made for WIPP-A and NBT-6 brines at 50 and 30 C. The differences between the calculated and the measured densities were less than 0.15 percent for both brines. The density for $MgCl_2$ saturated solution measured at 50 C agreed well with that obtained from extrapolation of unsaturated data from the *International Critical Table* (National Research Council, 1928).

A Soret cell has been put together. The Soret coefficient obtained for 1 molal NaCl solution at 37.2 C is 1.27×10^{-3} (C^{-1}), which compares with the value of 2.48×10^{-3} reported by

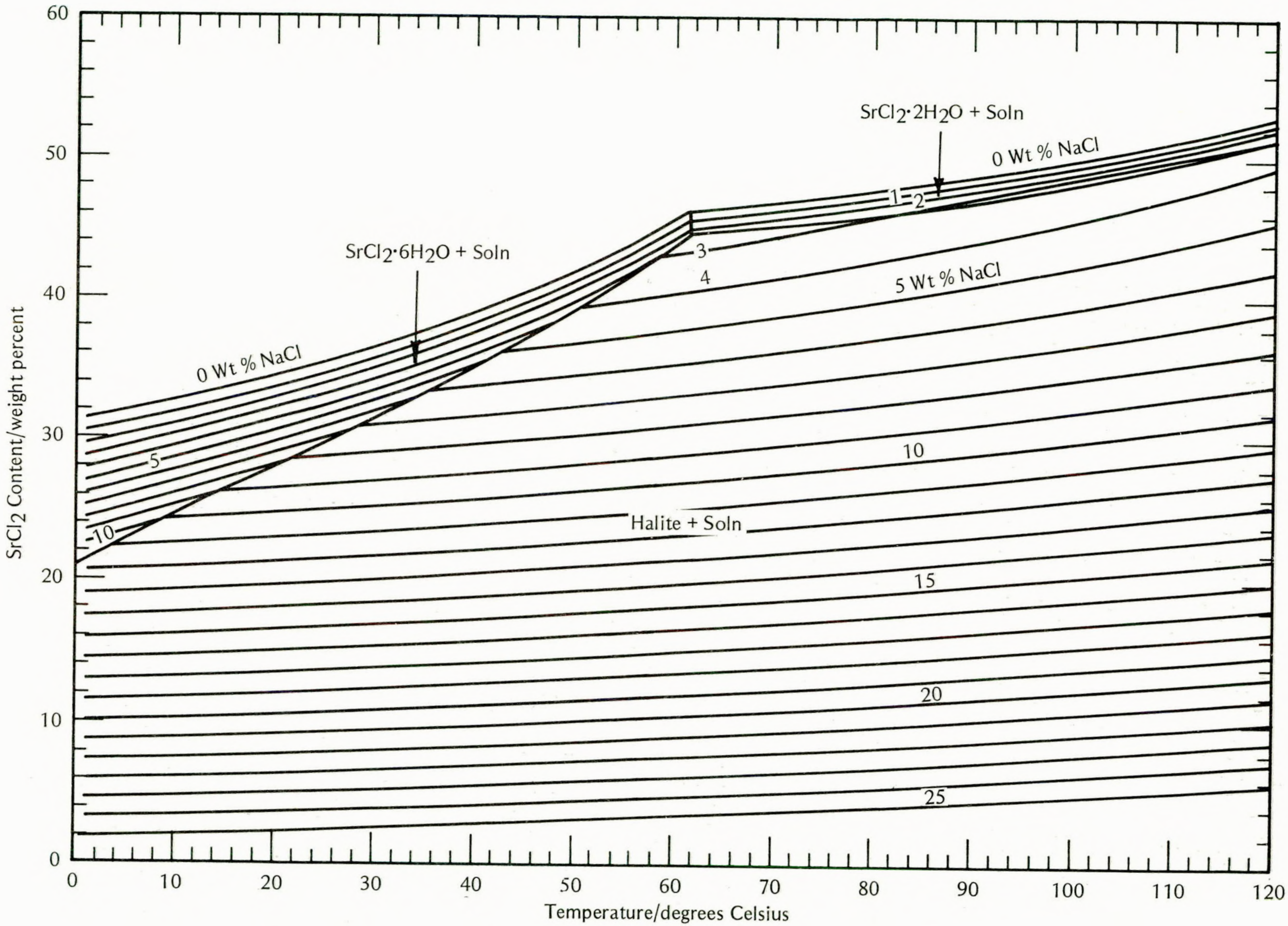

FIGURE 1. SOLUBILITY IN THE SYSTEM H_2O-NaCl-$SrCl_2$

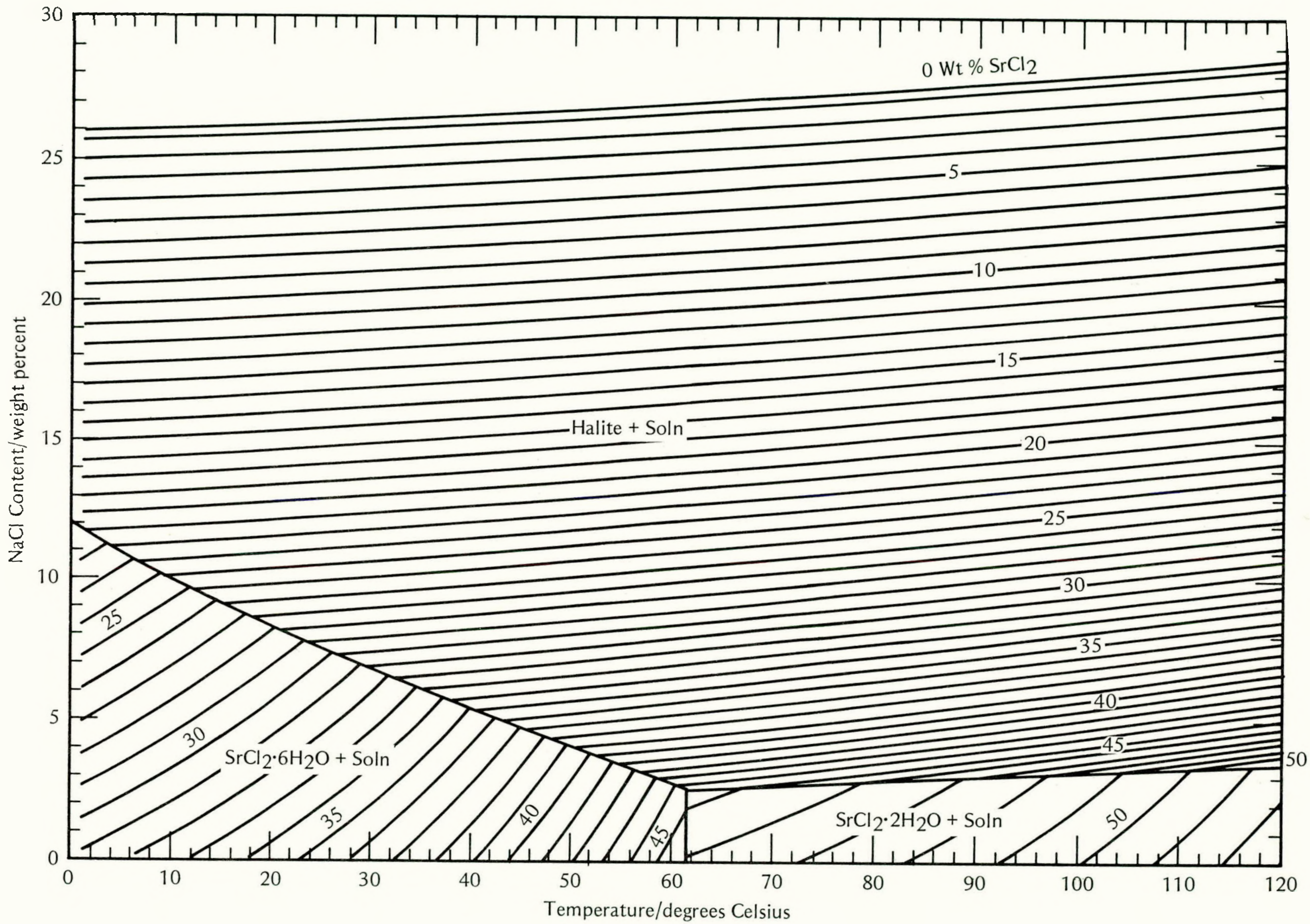

FIGURE 2. SOLUBILITY IN THE SYSTEM H_2O-NaCl-$SrCl_2$

Tanner (1927) for 1M NaCl at 37 C. The discrepancy is probably due to (a) the difference in analytical technique for solution concentrations, and (b) the possible convection flow in the cell.

Steam condensate samples from the brine migration experiment at Avery Island have been submitted for deuterium analysis. The results have not been received yet. The manuscript on Avery Island brine compositions and origin is being revised following USGS technical reviews.

Cu corrosion experiments are essentially complete for the 100 to 200 C range. Significant results are: (a) in the 3-month duration runs in WIPP-A at 100 C, atacamite (CuOHCl) precipitates on walls of the vessel in an H_2 permeable system; (b) upon cooling, Cu in solution precipitates as a Cu hydroxide; (c) if the system contains a second metal as a solid phase, Cu may be dissolved and electroplated onto the other metal, thereby greatly increasing the corrosion rate.

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WBS 1.1.4

Project: Thermal Gradient Brine Migration

Principal Investigator: University of California, Berkeley (D. R. Olander)

ONWI Project Manager: J. F. Kircher

Objective

The objective of this investigation is to develop a rigorous model of thermal gradient brine migration in natural rock salt.

Progress Reported Previously

From the experimental investigation, it was concluded that the crystal orientation does not appear to play a major influence in determining the magnitude of migration velocities of all-liquid inclusions in sodium chloride single crystals.

With regard to the theoretical modeling of the migration process of gas-liquid inclusions, some phenomena (surface tension effects, growth dispersion) usually unimportant may be playing an important role because of the small sizes of the inclusions. The complete mathematical description of the migration process does not lend itself to an analytical solution. Numerical schemes requiring considerable development are required.

Activities During the Reporting Period

THEORETICAL INVESTIGATION

Objective

The objective was to finalize an advanced model for describing the migration of gas-liquid inclusions in a salt matrix.

Results

An extensive compilation of the data and extrapolation techniques needed to provide the input parameters required to calculate the migration velocities of gas-liquid inclusions in NaCl or KCl single crystals has been prepared.

The preliminary model has been modified to take thermal diffusion (Soret effect) into account.

The migration velocities, calculated using the results of the data compilation and taking the Soret coefficient into account, are shown in Figures 1 and 2, together with data obtained by Anthony and Cline (1972), Wilcox (1969), and Olander, Machiels, Balooch, Muchowski, and Yagnik (1980).

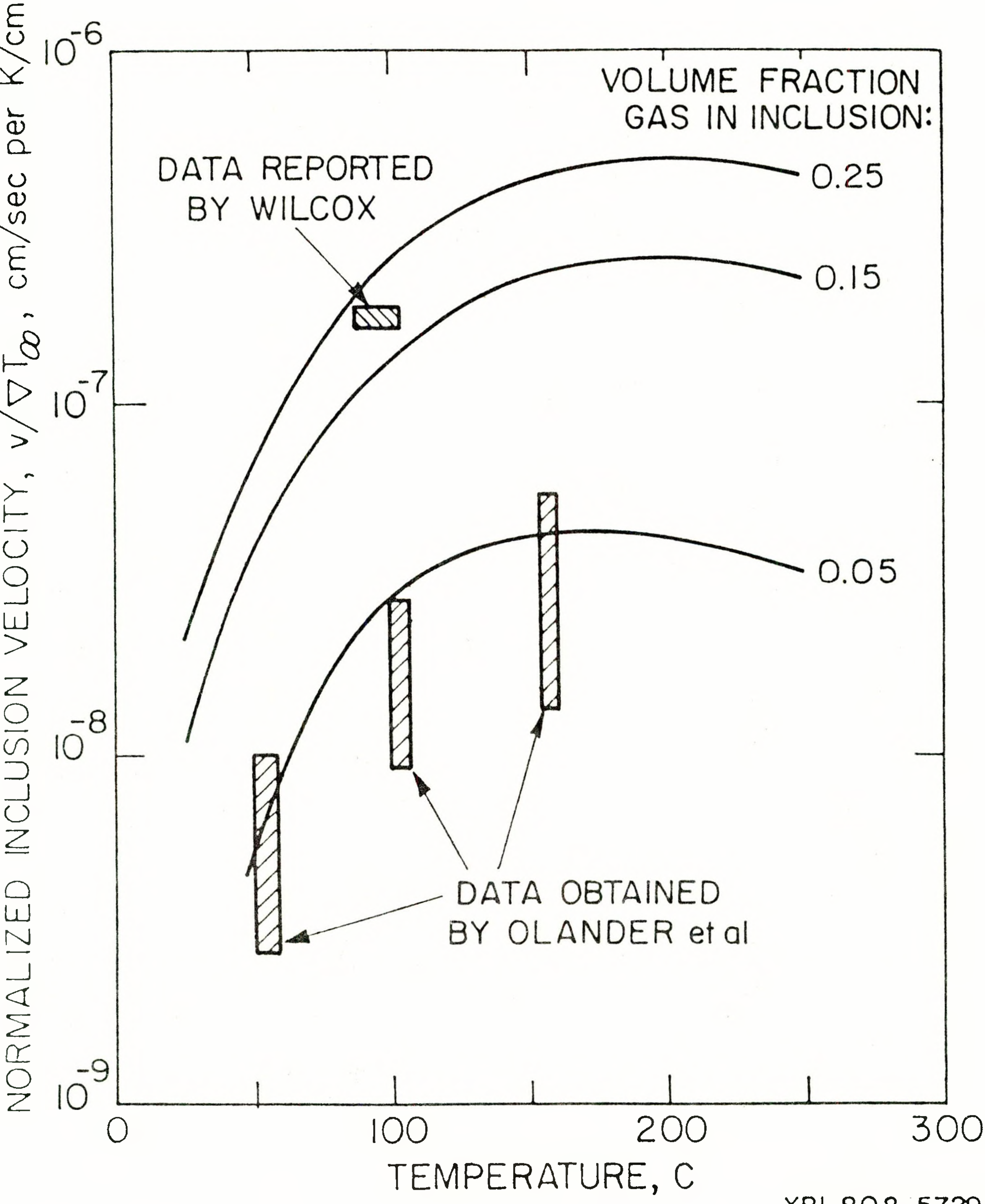


FIGURE 1. MIGRATION VELOCITIES OF TWO-PHASE INCLUSIONS IN A NaCl SINGLE-CRYSTAL FROM 25 TO 250 C

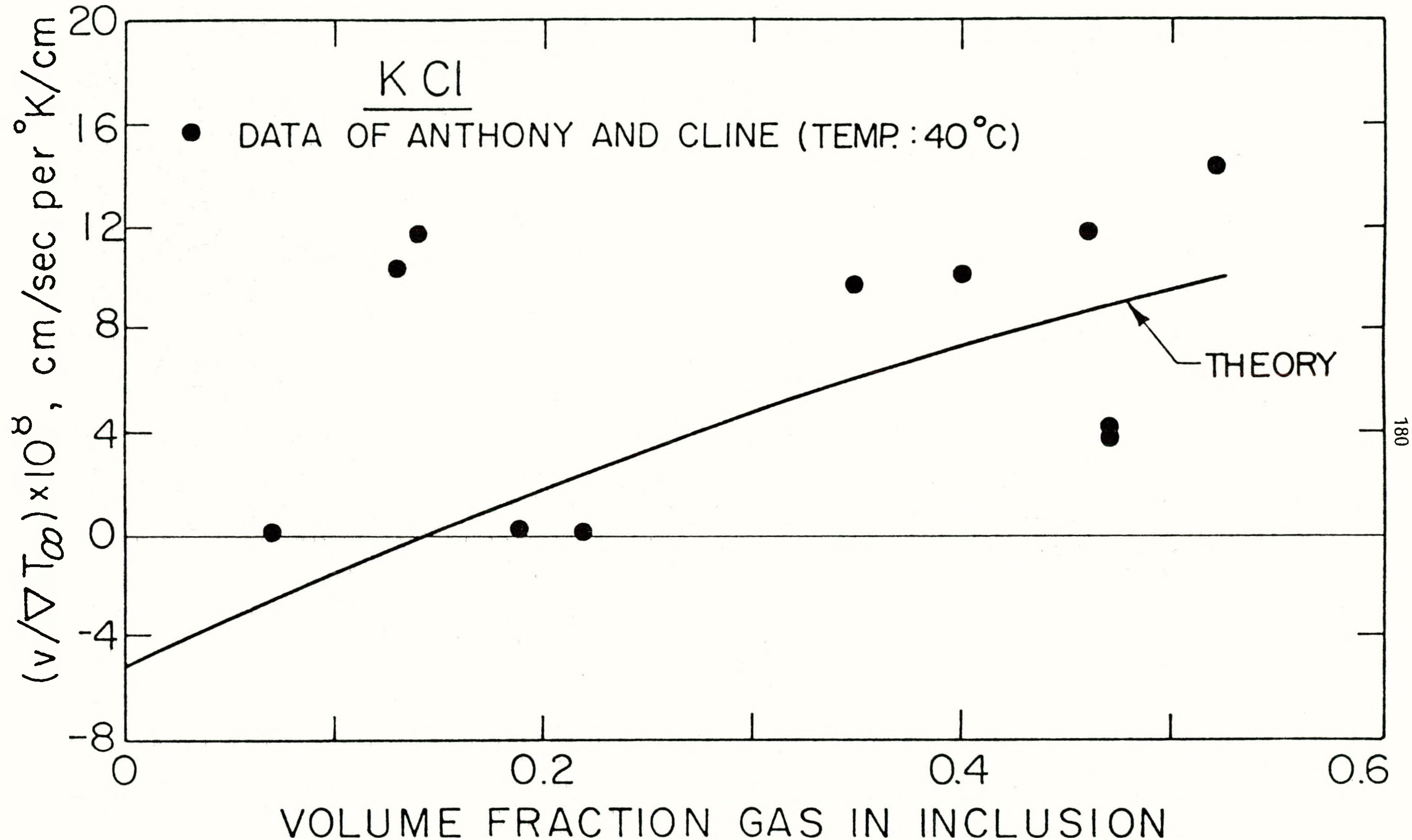


FIGURE 2. MIGRATION VELOCITIES OF TWO-PHASE INCLUSIONS IN A KCl SINGLE-CRYSTAL AT 40 C

XBL 808-5730

Discussion

For sodium chloride brines (Figure 1), the theory predicts a change in direction of inclusion migration at a gas volume fraction between 0.03 and 0.06, depending on the temperature. The experimental velocities obtained by Olander et al (for gas volume fractions between 0.06 and 0.22) are lower than the computed values, while Wilcox's data (gas volume fractions unreported) are within the range of calculated values.

For potassium chloride brines (Figure 2), the theory predicts a change in direction of inclusion migration at a gas volume fraction of 0.15. The experimental and theoretical values of the migration velocities are in good agreement.

Conclusions

The existing model predicts changes in direction of inclusion migration and velocities in the direction of decreasing temperatures in good agreement with the available experimental data.

The present theory predicts a linear dependence of migration velocities upon the temperature gradient but none on inclusion size. The incorporation of thermocapillarity processes should yield more exact dependences on temperature gradient and inclusion size but should not affect the absolute values of the migration velocities by more than an order of magnitude.

The theory is based on a diffusion-limited transport model. For all-liquid inclusions, it has been shown by Anthony and Cline (1972) that interface kinetics is generally rate controlling. Therefore, the theory is expected to generally overestimate the migration velocities.

EXPERIMENTAL INVESTIGATION

Objectives

The new experimental setup was to be made operational. Quantification of dislocation density effects was to be completed.

Results

Experimental Setup. The new experimental setup has been completed and is performing very well.

Effects of Dislocations. The effect of dislocations on the migration velocity of all-liquid inclusions is illustrated in Figures 3 and 4.

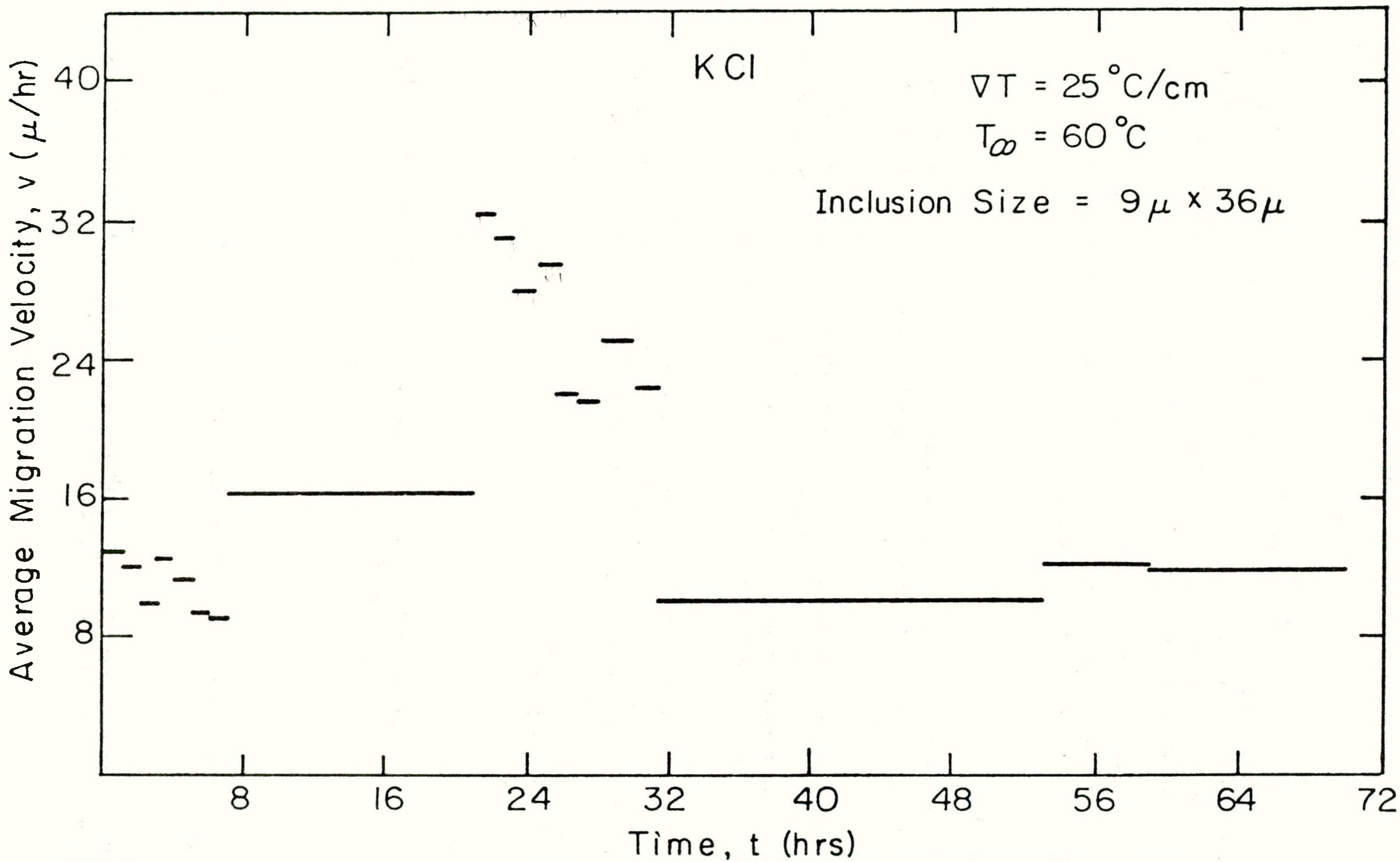


FIGURE 3. MIGRATION VELOCITY OF AN ALL-LIQUID INCLUSION IN A KCl SINGLE-CRYSTAL AS A FUNCTION OF TIME

XBL808-5646

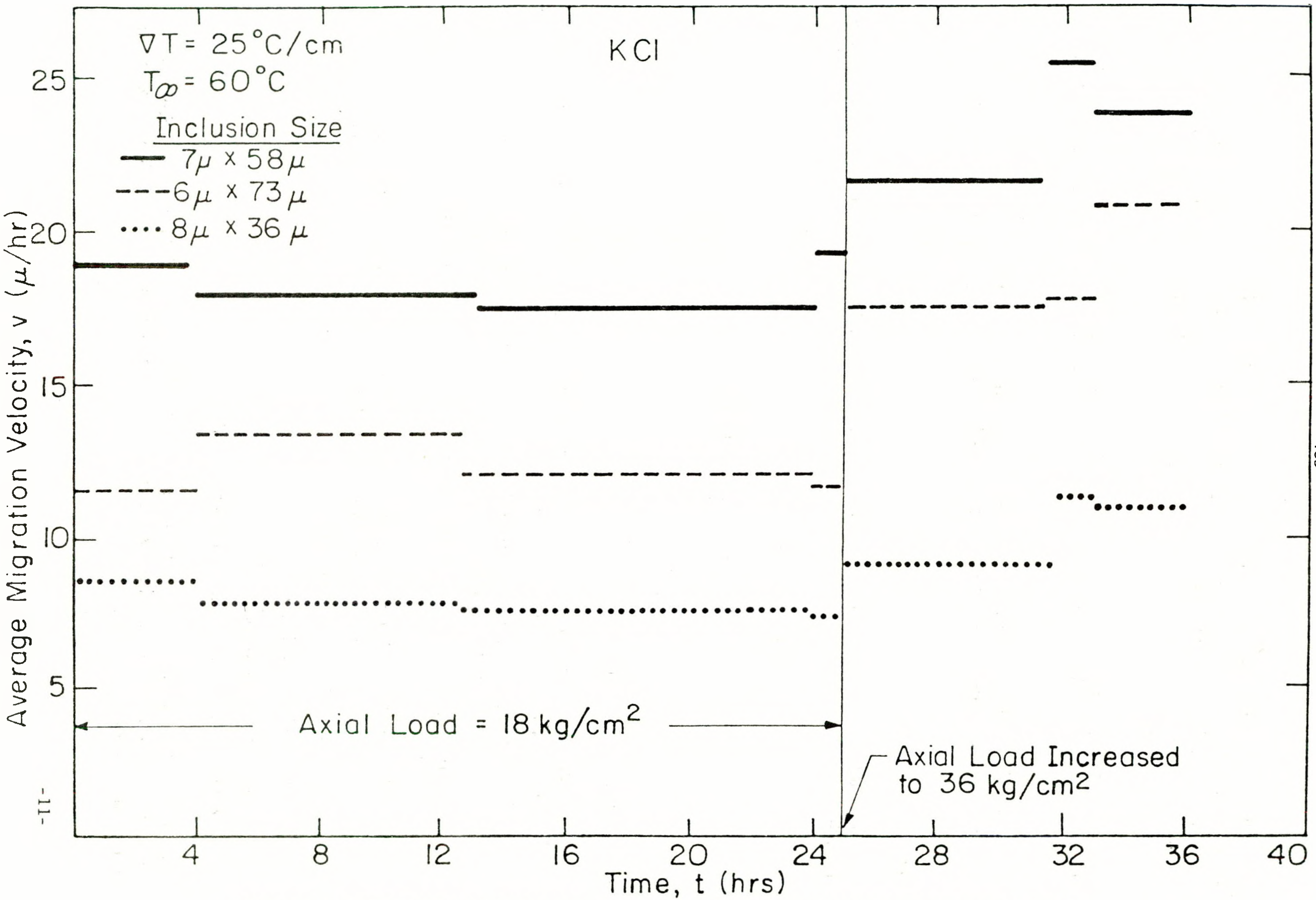


FIGURE 4. EFFECT OF A STEP CHANGE OF THE UNIXIAL LOAD ON MIGRATION VELOCITIES OF ALL-LIQUID INCLUSIONS IN A KCl SINGLE CRYSTAL

XBL808-5645

Figure 3 shows the velocity variations for a given inclusion in a KCl crystal as a function of time. Velocities were obtained by dividing the migration distance by the time of observation. The latter is indicated by the length of the bar representing the magnitude of the observed velocity. It can be seen that the velocity has changed by a factor of four (minimum: ~8 μ/hr, maximum: ~32 μ/hr).

Figure 4 shows the effect of increasing the crystal axial load by a factor of two after 25 hours of observation. The load increase results in a sudden increase in the migration velocities.

Quantification of Dislocation Densities. Etch-pitting techniques have been used successfully to visualize dislocations terminating on a surface. The results are shown in Figures 5 and 6.

Discussion

At steady state, the migration velocities can be modeled according to the following formalism:

$$J = k_{dis} f \left(C^h_{sat} - C^h\right) \quad (1)$$

$$= \frac{D_l}{L}\left(C^h - C^c\right) - \sigma D_l C_l \nabla T_l \quad (2)$$

$$= k_{dep} f^1 \left(C^c - C^c_{sat}\right) , \quad (3)$$

where J is the flux of salt

k_{dis} and k_{dep} are rate constants describing the dissolution and deposition processes occurring at the hot and cold faces, respectively

C^h_{sat} and C^c_{sat} are the saturation concentration corresponding to the temperatures existing at the inclusion faces

C^h and C^c are the salt concentration in the brine in contact with the hot and cold faces, respectively

$f\left(C^h_{sat} - C^h\right)$ and $f^1\left(C^c - C^c_{sat}\right)$ are two functions describing the dependence of the dissolution and deposition processes upon the local concentration conditions

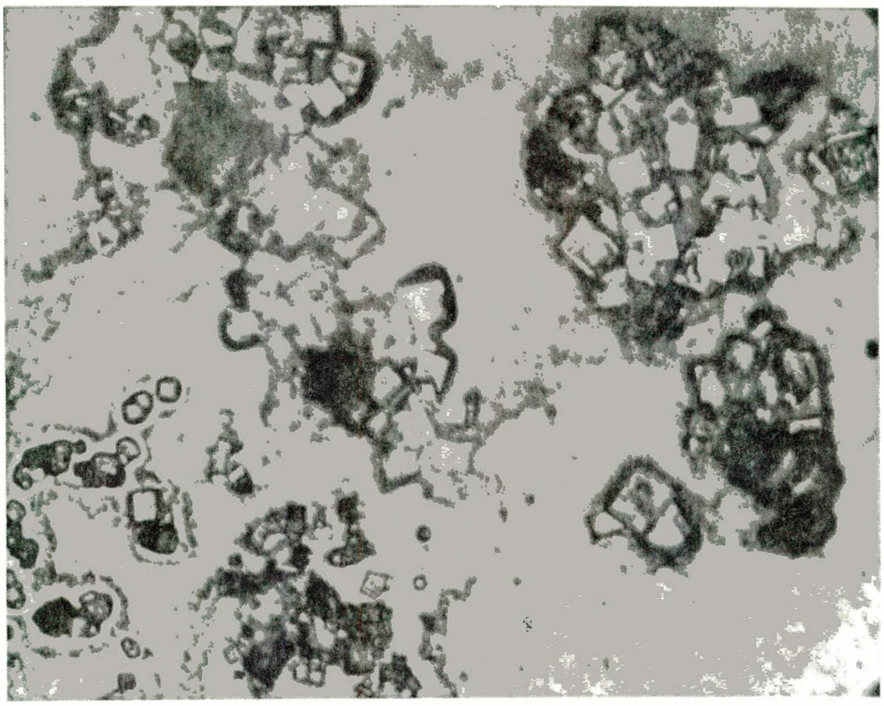
D_l is the salt diffusion coefficient in water

L is the inclusion thickness

σ is the Soret coefficient

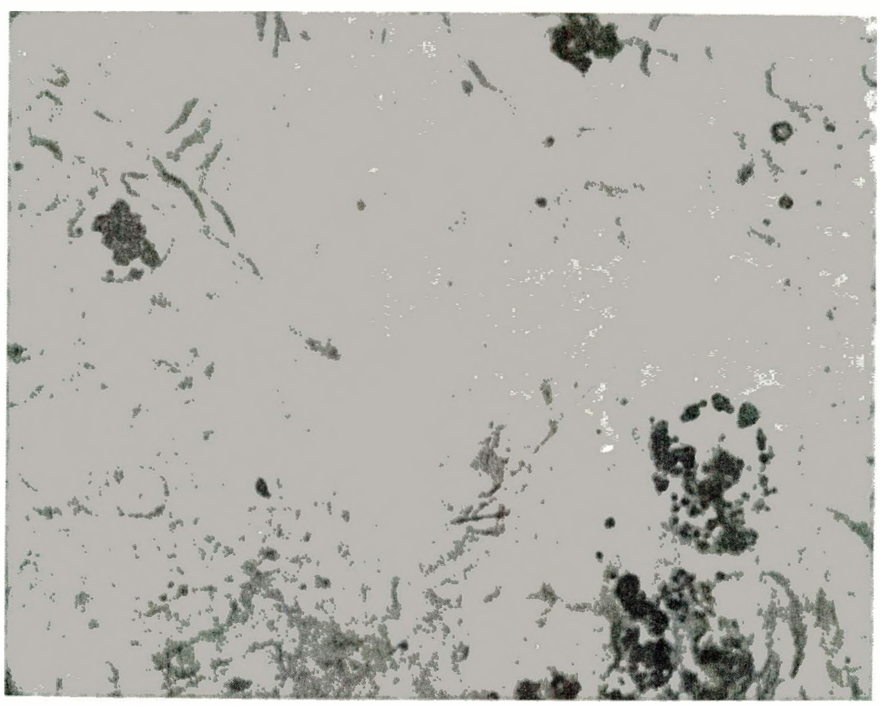
∇T_l is the temperature gradient in the liquid.

Equation (1) represents the dissolution of salt at the hot end of the inclusion. Equation (2) represents the transport of salt through the brine. Equation (3) represents the deposition of salt at the cold end of the inclusion.



MAGNIFICATION: 200 X

FIGURE 5. VISUALIZATION OF DISLOCATION THROUGH ETCH-PIT TECHNIQUES



MAGNIFICATION: 50 X

FIGURE 6. NONUNIFORM DISTRIBUTION OF DISLOCATIONS (DISLOCATION CLUSTERS)

It is well established that the migration process is rate controlled by phenomena occurring at the interfaces. k_{dep} is expected to be large while k_{dis} is expected to be small; therefore, the dissolution step, i.e., $k_{dis}f\left(C^h_{sat} - C^h\right)$, is expected to be rate determining.

$k_{dis}f\left(C^h_{sat} - C^h\right)$ is a function of temperature, number of dislocations ending at the dissolving face, location of dislocations, and strength of dislocations. Therefore, as an inclusion migrates in a salt crystal, the number, location, and strength of dislocations continuously change, leading to variations of the magnitude of the migration velocity as illustrated in Figure 3.

When the uniaxial load is increased, the resulting increase in stress activates a number of dislocation sources. The dislocations so created flow through the crystal. As a result, a number of dislocations can be intercepted by the dissolving face, leading to a faster dissolution rate (Figure 4).

Conclusion

The effect of dislocation density on migration velocity is qualitatively clear. It is also possible to obtain an order-of-magnitude determination of dislocation densities through etch-pitting techniques. However, as illustrated by Figure 6, dislocation densities are not uniform. Attempts to quantify this parameter are continuing.

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Wilcox, W. R. 1969. "Anomalous Gas-Liquid Inclusion Movement", *Indust. Eng. Chem.,* 61:76–77.

WBS 1.1.4

Project: Radiation Chemistry of Salt Mine Brines and Hydrates

Principal Investigator: Oak Ridge National Laboratory (G. H. Jenks)

ONWI Project Manager: J. F. Kircher

Objective

The objective of this program is to experimentally establish the value for $G(H_2)$ and G (accompanying oxidants) in salt mine brines and hydrates ($MgCl_2$ hydrates) under gamma irradiation at temperatures up to about 450 K, for some solutions for which the vapor pressure does not exceed about 0.3 MPa at the test temperature. The G-value is a measure of product yield during radiolysis. It is defined as molecules of product per 100 eV of energy absorbed by the system. The radiolytic products from brine irradiation may have deleterious effects on package components via hydrogen embrittlement or enhanced corrosion.

Progress Reported Previously

Experimental methods, equipment, and procedures were developed. A large number (27) of experimental measurements of $G(H_2)$ in NaCl-saturated $MgCl_2$ solutions were completed.

In addition, arrangements were made to investigate and develop methods of analysis for Cl_2, H_2O_2, and ClO_3^- in the irradiated brine.

Activities During the Reporting Period

Experimental measurements were continued on $G(H_2)$ in NaCl-saturated $MgCl_2$ solutions. The experimental conditions which were investigated and the results of gas analyses in the irradiated ampoules are shown in Table 1. Analogous information for previous experiments (up to No. 36) is included in Table 1.

Brief comments on the $G(H_2)$ experiments and/or calculations conducted this quarter are the following.

Gamma Dose Rate During Irradiation

A revised value of 8.35 E+17 eV/g/min for the gamma ray dose rate in pure water at the irradiation site was used in calculating the values for $G(H_2)$ reported in Table 1. This dose rate value was based on a value of 2.50 for $G(Ce^{+3})$ in the dosimeter solution.

Effects of Added HNO_3

HNO_3 was added to the test solutions for experiments 40 through 43, as shown in Table 1. There were no significant effects on $G(H_2)$.

TABLE 1. VALUES FOR $G(H_2)$ AND OTHER RESULTS OF GAS ANALYSES OF RADIATION CAPSULES

Experiment Number	Wt H_2O (g)	Rad. Time (Min)	Resulting Amount of Gases (μ mol) Total	H_2	O_2	N_2	$G(H_2)$	$\frac{2G(O_2)}{G(H_2)}$	Excess O_2 (μ mol)	Comment
Test Soln. 2.4 m $MgCl_2$ Temperature 73–85 C $1 + E_s/E_w$ 1.32										
6	0.72	110	208	0.87	2.57	9.72	0.60	<0	–0.48	He flush
14	0.79	210	200	1.45	3.64	13.04	0.48	0.18	–0.49	He flush
18	0.70	210	197	1.34	3.41	11.66	0.50	0.41	–0.40	He flush
21	0.64	210	215	1.27	0.34	0.52	0.51	0.32	–0.43	Freeze, evac.
22	0.75	210	205	1.54	0.49	1.07	0.53	0.26	–0.57	Backfill He
23	0.78	110	197	0.75	0.57	1.02	0.48	0.79	–0.08	Freeze, evac.
24	0.71	110	204	0.65	0.43	1.04	0.46	0.48	–0.17	Backfill He
27	0.83	110	189	0.81	0.59	1.36	0.49	0.56	–0.18	Freeze, evac.
28	0.86	110	180	0.81	0.43	1.15	0.47	0.31	–0.28	Backfill He, frozen
33	2.42	20	105	0.42	0.24	0.36	0.47	0.68	–0.07	Freeze, evac.
34	2.41	20	99	0.42	0.22	0.33	0.48	0.62	–0.08	Backfill He
40*	2.37	20	94	0.44	0.35	0.90	0.50	0.48	–0.12	Freeze, evac.
41*	2.41	20	119	0.41	0.39	0.87	0.46	0.79	–0.05	Backfill He
42**	2.41	20	84	0.39	0.24	0.35	0.44	0.73	–0.05	Freeze, evac.
43**	2.44	20	84	0.39	0.21	0.33	0.44	0.62	–0.08	Backfill He

*HNO_3 added to make solution 10^{-5} m in HNO_3.
**HNO_3 added to make solution 10^{-4} m in HNO_3.

TABLE 1. (Continued)

Experiment Number	Wt H_2O (g)	Rad. Time (Min)	Resulting Amount of Gases (μ mol)				$G(H_2)$	$\frac{2G(O_2)}{G(H_2)}$	Excess O_2 (μ mol)	Comment
			Total	H_2	O_2	N_2				
Test Soln. 5.8 m $MgCl_2$ Temperature 75–80 C $1 + E_s/E_w$ 1.49										
19	0.70	110	207	0.81	2.94	10.81	0.51	0.08	–0.44	He flush
20	0.71	110	215	0.75	2.09	7.76	0.48	0.01	–0.37	He flush
25	0.74	110	185	0.81	0.46	0.94	0.48	0.51	–0.20	Freeze, evac.
26	0.77	110	183	0.90	0.53	0.90	0.51	0.74	–0.12	Backfill He
Test Soln. 2.4 m $MgCl_2$ Temperature 112–140 C $1 + E_s/E_w$ 1.34										
7	0.71	110	207	0.89	3.11	11.96	0.62	<0	–0.55	He flush
8	0.68	110	216	0.91	2.51	9.89	0.66	<0	–0.61	He flush
29	0.84	55	183	0.42	0.27	0.35	0.49	0.84	–0.83	Freeze, evac.
30	0.80	55	167	0.41	0.15	0.30	0.50	0.37	–0.13	Backfill He
35	2.46	20	93	0.41	0.20	0.33	0.45	0.54	–0.12	Freeze, evac.
36	2.44	20	93	0.43	0.19	0.33	0.47	0.47	–0.12	Backfill He
Test Soln. 5.8 m $MgCl_2$ Temperature 106–143 C $1 + E_s/E_w$ 1.50										
31	0.81	55	167	0.45	0.22	0.27	0.49	0.65	–0.08	Freeze, evac.
32	0.84	55	169	0.44	0.19	0.32	0.46	0.67	–0.07	Backfill He

TABLE 1. (Continued)

Experiment Number	Wt H_2O (g)	Rad. Time (Min)	Resulting Amount of Gases (μ mol) Total	H_2	O_2	N_2	$G(H_2)$	$\frac{2G(O_2)}{G(H_2)}$	Excess O_2 (μ mol)	Comment
Test Soln. 2.4 m $MgCl_2$ Temperature 30–45 C $1 + E_s/E_w$ 1.31										
12	0.73	110	208	0.83	1.91	7.09	0.57	0.01	–0.41	He flush
13	0.73	110	215	0.73	2.51	9.35	0.50	0	–0.37	He flush
44	2.40	30	106	0.52	0.29	0.38	0.40	0.71	–0.08	Freeze, evac.
45	2.28	30	119	0.56	0.25	0.40	0.45	0.50	–0.14	Backfill He
52	1.93	30	140	0.41	0.22	0.39	0.39	0.58	–0.08	Freeze, evac.
53	1.98	30	129	0.43	0.19	0.33	0.40	0.49	–0.11	Backfill He
Test Soln. 5.8 m $MgCl_2$ Temperature 30–45 C $1 + E_s/E_w$ 1.49										
16	0.65	110	204	0.98	3.22	12.48	0.67	<0	–0.63	He flush
17	0.71	110	206	0.97	2.86	10.84	0.60	<0	–0.54	He flush
58	1.53	30	143	0.40	0.17	0.23	0.42	0.55	–0.09	Freeze, evac.
59	1.47	30	164	0.36	0.16	0.23	0.40	0.56	–0.08	Backfill He
62	1.41	30	122	0.32	8.67	24.69	0.36	12.79	1.87	Backfill He

TABLE 1. (Continued)

Experiment Number	Wt H_2O (g)	Rad. Time (Min)	Resulting Amount of Gases (μ mol) Total	H_2	O_2	N_2	$G(H_2)$	$\frac{2G(O_2)}{G(H_2)}$	Excess O_2 (μ mol)	Comment
Test Soln. 10.75 m $MgCl_2$ Temperature 160 C $1 + E_s/E_w$ 1.87										
37	1.26	30	116	0.45	0.05	0.20	0.46	–0.03	–0.23	Evac., Backfill He
Test Soln. 9.80 m $MgCl_2$ Temperature 160 C $1 + E_s/E_w$ 1.81										
38	1.37	50	121	0.92	0.15	0.67	0.54	–0.07	–0.49	Evac., Backfill He
Test Soln. 11.24 m $MgCl_2$ Temperature 170–180 C at end $1 + E_s/E_w$ 1.93										
56	1.06	30	161	0.76	0.02	0.08	0.89	–0.08	–0.41	Evac., Backfill He
Test Soln. 11.73 m $MgCl_2$ Temperature 169–182 C at end $1 + E_s/E_w$ 1.98										
57	1.05	30	163	0.59	<0.02	0.11	0.68	–0.10	–0.35	Evac., Backfill He

Values of $G(H_2)$ at 30 to 45 C

Additional experiments (Nos. 44, 45, 52, 53, 58, 59, and 62) indicated values for $G(H_2)$ which were slightly lower than those at 70 through 140 C which were determined previously.

Values of $G(H_2)$ at 160 and 180 C

Solutions highly concentrated in $MgCl_2$ were prepared from the 5.8 m $MgCl_2$ test solutions by placing the 5.8 m solution within an ampoule with NaCl crystals, and then heating the ampoule to the high temperature (160 or 180 C) while the space over the solution was purged with a slow stream of helium. The ampoule was weighed from time to time, and the loss in weight was assumed to represent loss of H_2O. After the loss in weight reached an acceptable value, the ampoule was prepared for irradiation in a usual manner, as indicated under "Comments" in Table 1. The concentrated solutions in Nos. 37 and 38 melted at temperatures between 120 and 130 C during heat-up. The solutions in Nos. 56 and 57 melted completely at about 170 C during heat-up.

The results of these experiments showed $G(H_2)$ values at 160 C which did not differ significantly from those in the 2.4 or 5.8 m $MgCl_2$ solutions at 70 to 140 C. However, the values for $G(H_2)$ in the more concentrated solutions at 180 C were significantly higher (35 and 80 percent higher) than the average of the 160 C values.

The investigation and development of methods for analysis for Cl_2, H_2O_2, and ClO_3^- in the irradiated brines were continued. The development of methods for H_2O_2 and Cl_2 analyses was completed and has provided detailed instructions for routine analyses for these species. The method for H_2O_2, which utilizes the oxidation of Fe^{+2} by H_2O_2, is applicable to the determination of 0.1 to 3 μg (0.003 to 0.09 μmol) with a precision of about $\pm$ 5 relative percent. The method for Cl_2 utilizes the reaction of Cl_2 with O-tolidine and is applicable to the determination of 0.1 to 6 μg (0.0015 to 0.085 μmol) with a precision of about $\pm$ 5 relative percent.

Thirteen irradiated ampoules (Nos. 14, 21, 22, 34, 40, 42, 19, 25, 7, 29, 30, 16, and 37) which had been stored after gas analyses were submitted for H_2O_2 determination. H_2O_2 was detected and measured in each ampoule solution except Nos. 29 and 30. The amounts in the other solutions ranged from 0.002 to 0.3 μmol, corresponding to 1 to 23 percent of the amounts indicated by the measured deficiencies of radiolytic O_2. Accordingly, these analytical results indicate the occurrence of other oxidants within the irradiated solutions.

WBS 1.1.6

Project: Waste/Rock Interactions Technology Program (WRIT)

Principal Investigator: Pacific Northwest Laboratories (PNL) (R. J. Serne)

ONWI Project Manager: J. F. Kircher

Objective

The objectives of the Waste/Rock Interactions Technology (WRIT) program are to:

- Identify and characterize mechanisms of waste form radionuclide release and subsequent geochemical interactions with engineered barriers and natural geologic media, e.g., leaching, solubility, and sorption

- Collect data and develop and evaluate the effectiveness of models (develop a perspective on applications/limitations of each model) that predict leaching, sorption, and release processes in the repository and surrounding media

- Obtain, through verification studies and documentation, the most acceptable test methodologies for sorption, leaching, solubility limitations, and waste package-geomedia interaction studies

- Support repository site characterization and licensing specifically through data generation and analysis and predictive model formulation.

To accomplish these objectives, the WRIT program will develop the necessary data and predictive capability on the release and subsequent geochemical interactions of radionuclides with engineered barriers and natural geologic media. The major activities of the planned research in the WRIT program are: (1) generation of defensible, reproducible data on leaching, sorption, and nuclide release processes through the use of scientifically acceptable methodologies, (2) synthesis of the data into readily retrievable data banks, (3) formal documentation of sorption, leaching, and release test methodologies, and (4) the development of credible models of leaching, sorption, and release processes based on underlying theory and experimental observation that can be used in consequence analysis.

Progress Reported Previously

Results of static leach tests at 25 and 75 C on doped 76-68 glass beads were reported. Results of Paige leach tests on spent fuel corrected for nuclide plateout onto the apparatus were reported. Results of single-pass continuous-flow leach tests of neptunium- and plutonium-doped 76-68 glass at both 25 and 75 C were reported.

Glass leach mechanism studies such as surface potential correlations with element release were described. It was hypothesized that the high surface potential which occurred each time the solution was changed can account for increased leach rates for the International Atomic Energy Agency (IAEA) and single-pass continuous-flow leach tests over static leach tests.

The initial six static waste package tests and results of solution and rock and glass surface analyses were reported. Under oxidizing conditions uranium was found to migrate from a glass to the surface of a granite pellet in contact with the glass. No uranium migration was observed under reducing conditions.

Leach tests on TRU waste emplaced in portland cement showed deionized water leached more plutonium than did WIPP brine B.

Electron spectroscopy for chemical analysis (ESCA) surface analysis of glass helped in the interpretation of increased leaching of glass in a radiation field versus a nonirradiated control glass. It was concluded that dissolution of neodymium and cerium is enhanced by the presence of gamma radiation. The mechanism for this enhanced lanthanide dissolution may involve radiolysis of water, leading to peroxide and other reactive species formation.

Results from spent fuel analysis by shielded microprobe show that in low-burnup fuel, element concentrations from edge to center are all near constant, except for plutonium which appears higher at the outer edge. In high-burnup fuel, the concentration of all the selected elements is higher at the edge than toward the center of the pellet. The large cesium gradient indicates that this element had migrated toward the pellet-cladding interface, and the material left on the cladding removed from the pellets may have contained significant amounts of cesium. Thus, leach rates reported from the unclad fragments may be lower than one would expect for an equal exposed surface area of spent fuel in a breached repository.

Laboratory work on development of relevant sorption testing methodology and on sorption mechanisms was reported. A key finding is that cesium sorption (Kd) onto basalt and limestone is quite sensitive to the tracer concentration between 10^{-11} and 10^{-6} M and may require that transport models use either a Kd that varies with tracer concentration or a minimum Kd value. Results from Rockwell Hanford Operations (RHO) and Argonne National Laboratory (ANL) indicate that a Freundlich isotherm fits some of the data on crushed rock. The Freundlich model is a simple expression relating the Kd to the radionuclide concentration in solution and should be easily incorporated into a mass transport model for repository safety assessment. Researchers observed that column sorption ratios (for materials with low Kd values) tend to be smaller than batch sorption ratios, which is possibly due, in part, to the shorter residence times. A study has shown that some retardation factors increase with decreasing flow rate through a column, and that, as the flow rate decreases, column and batch sorption measurements are in better agreement.

Studies of the effect of temperature on sorption of plutonium and americium onto argillite showed conflicting results. The formation of hard-to-centrifuge colloids is being investigated. Results for cesium and strontium sorption on clays show that sorption of multivalent radiocations is favored over sorption of univalent cations with increasing temperature.

Sorption experiments on several substrates have shown a very strong pH dependence for strontium. When the data are plotted as [Sr] versus pH, a relationship Log [Sr] = A – pH appears that indicates that mineral formation may control the strontium concentration rather than adsorption.

Sorption of neptunium under reduced oxygen levels shows that Kd(Np) apparently increases in an anoxic environment as compared with results of tests in the presence of air. However, the neptunium concentration in the influent solution varied by about five orders of magnitude in the two experiments (10^{-11} M in the anoxic experiment and 10^{-6} M in the ambient atmosphere experiment).

A batch Kd study of 15 sandstones with sorptions of ^{137}Cs, ^{141}Ce, ^{125}Sb, ^{75}Se, ^{85}Sr, and ^{237}Pu from brine was completed. Observed Kd values for strontium varied from –0.39 ml/g to 0.01 ml/g, which indicates that the sandstones do not adsorb strontium from brine. Values for cesium, antimony, and selenium were 0 to 8 ml/g, 0 to 14 ml/g, and 0 to 63 ml/g, respectively. The cesium and plutonium Kd values were 20 to 1800 ml/g and 60 to 9000 ml/g, respectively.

Plutonium (VI) sorption was shown to be controlled by an ion-exchange type of reaction and a redox reaction at pH 4. Similar studies at pH 7 with plutonium (VI) have shown that it is less exchangeable at the higher pH and that Kd values for iron (II) correlate well with the amount of plutonium removed from solution.

The weathering of basalt, granite, and argillite and its effects on cesium, strontium, neptunium, americium, and plutonium nuclide sorption were studied. Generally, weathering had little effect on Kd values for granite. Weathering of argillite in a nitrogen atmosphere seemed to reduce sorption of all nuclides except cesium. Kd values on weathered basalt (both in air and N_2) were higher than those observed on fresh basalt, especially for plutonium and americium. Only for argillite does it appear that weathering may adversely affect sorption for those nuclides studied.

Flow-through fracture experiments were begun. An intact core of Climax Stock granite was split along an existing fracture and recombined in a high-pressure flow apparatus. A spike (50 μl) of ^{233}U was dried in the center of the top of the core a few millimeters from the fracture, and granite ground water was pumped through the core until activity was observed. Slices of the core have shown activity to remain in the fracture. Several regions of high activity on the fracture surface are being analyzed to identify the minerals that strongly adsorb ^{233}U. It is hoped that results of analysis of fracture flow via these pressurized core runs will compare with sorption results predicted by batch and crushed rock column experiments, once the differences in surface areas are compensated. An added benefit of the fracture-flow tests is that granite permeabilities may be less than those previously measured. The tracer tests have shown that much of the water flowing through the core apparatus (similar to a permeability apparatus) passes between the rock core and the confining sleeve.

The solution chemistry of technetium and actinides neptunium, plutonium, and americium was studied. The solubility of crystalline NpO_2 was determined. The apparent solubility of plutonium and neptunium in doped glass beads is remarkably similar to PuO_2 and NpO_2, suggesting that, at low flow conditions, the leach rates of these two actinides may be predictable from knowledge of the solubility of the crystalline oxides.

Activities During the Reporting Period

WASTE PACKAGE INTERACTIONS—NUCLIDE RELEASE STUDIES

Waste Form—Solution Interactions

Radioisotope leachate analysis is essentially complete for five leach time periods in the static tests at 25 and 75 C, using actinide-doped 76–68 glass. Results will be reported at the end of the next quarter. Elemental analysis by inductively coupled plasma (ICP) is also nearly complete, and some important results are presented here. Table 1 compares silicon release under modified IAEA and static leaching conditions for nearly equivalent times and temperatures. For deionized water, roughly equivalent release occurs by these test methods, but for bicarbonate ground water, a twofold increase in release is found in the IAEA test. The boron, sodium, and molybdenum release fractions are nearly the same, whereas silicon and calcium are removed to a lesser degree. The fractional release curves are approximately represented by a $t^{1/2}$ functionality. A comparison of silicon release from the three leachates used in this study shows that more silicon is released in the bicarbonate than in the deionized water and that the least silicon release occurs in WIPP brine B. The deionized water and WIPP brine leachates appear to be equilibrating with the glass after 341 days, whereas the bicarbonate ground water continues to leach at this stage. Temperature has an inconsistent effect on release enhancement for glass constituents, as shown in Table 2.

Technetium-99 release from a static leach test using spent fuel with a burnup of 28,000 MWd/tU has been measured. The releases of ^{99}Tc in the five leach solutions after 8 days of static leach testing are shown in Table 3, along with the available release data for nine other elements. The ^{99}Tc-based release of the fuel is higher than the matrix (uranium)-based release, but lower than the cesium-based release. Elements in spent fuel do not leach congruently with respect to the uranium.

Results of the anoxic static leach test reported earlier lacked only some uranium analysis to complete the set of actinide leach data for the first 30 samples. Each datum includes the uranium recovered by scrubbing the polypropylene leach container with concentrated HF and O_3. In the 75 C brine solutions, much of the uranium (2 to 88 percent) was found on the container walls; the 23 C brine leachings retained the uranium in solution (except for the 2-day leaching). All of the 2-day leaching results showed relatively high wall adsorption. There appear to be two effects: an adsorption mechanism, accounting for about 0.03 μg uranium, and precipitation (over 3 grams of uranium in the case of the 75 C brine, 106-day leaching).

TABLE 1. RELEASE OF SILICON AT LONG TIMES FROM 76-68 GLASS UNDER STATIC AND IAEA CONDITIONS

	Release Fraction	
Leachate	Static 25 C, 341 Days	IAEA 21 C, 331 Days
Deionized water	6×10^{-4}	5.3×10^{-4}
Bicarbonate ground water	1.1×10^{-4}	2.5×10^{-3}

TABLE 2. LEACH ENHANCEMENT GOING FROM 25 C to 75 C

(Ratio of fraction released at 75 C to that at 25 C at 341 days)

	B	Ca	Na	Si
Brine	3	(a)	—	4.5
Bicarbonate	25	3	—	15
Deionized water	34	4	25.5	18

TABLE 3. LEACH SOLUTION CONCENTRATION (PPM) AFTER STATIC LEACH TESTING SPENT FUEL WITH A BURNUP OF 28,000 MWd/tU $NaHCO_3$ AT 25 C FOR 8 DAYS

	Deionized Water	0.03 M $NaHCO^3$	WIPP B Brine	0.03 M NaCl	0.015 M $CaCl_2$
^{137}Cs	8.8 E-02	1.3 E-1	7.1 E-2	9.8 E-2	5.7 E-2
Uranium	2.7	5.7	10	8.4	7.6
$^{239,240}Pu$	1.7 E-2	5.9 E-2	1.0 E-3	1.3 E-2	1.8 E-2
^{244}Cm	7.2 E-6	4.9 E-4	1.1 E-3	8.9 E-4	5.5 E-4
$^{90}Sr + ^{90}Y$	(a)	(a)	(a)	(a)	(a)
^{125}Sb	(a)	(a)	(a)	(a)	(a)
^{106}Ru	(a)	(a)	(a)	(a)	(a)
^{144}Ce	(a)	(a)	(a)	(a)	(a)
^{154}Eu	(a)	(a)	(a)	(a)	(a)
^{99}Tc	5.3 E-2	5.3 E-2	3.2 E-2	3.2 E-2	3.4 E-2

(a) Analytical data not available at time of publication.

The results of the completed (to date) uranium analysis for the anoxic static leach tests of PNL 76-68 simulated waste glass can be compared to the results for plutonium and neptunium reported earlier. The amount of leaching by bicarbonate solution at 75 C is more than a thousandfold greater for uranium than for plutonium. In 23 C water, the amount of uranium leached is comparable to that for plutonium and less than that for neptunium.

Waste Package Interactions

This quarter was devoted to characterization of the components from the first series of waste package tests conducted in 850-ml direct sampling autoclaves. Anion determinations will be incorporated in all future waste package tests.

Additional effort was also spent examining the glass surfaces from the minicanisters by Scanning Electron Microscopy (SEM). Problems of rock powder matrix material adhering to the glass surface and interfering with SEM analysis have led to the development of a modified package configuration with an exposed surface for use in future tests.

Some of the solution analysis data from the first series of direct solution sampling tests are reported for basalt and granite matrices in Figures 1 and 2. These tests were run for 30 days at 250 C/2000 psi. Solutions were sampled at the following intervals: (1) after reaching pressure and temperature, (2) after 1 week, (3) after 2 weeks, (4) after 3 weeks, and (5) after 4 weeks. In addition, samples were collected at 50 C intervals during cooldown, and the solution remaining in the autoclave after cooldown was also analyzed.

About 600 ml of solution was used in these first waste package tests and the components had the following masses (in grams):

Granite		Basalt	
Minicanister + glass	50.1	Minicanister + glass	49.4
Glass wafer	12.5	Glass wafer	12.9
Granite wafer	6.5	Basalt wafer	6.7
Granite powder	122.5	Basalt powder	136.8

Figure 1 shows the solution concentrations as a function of time for boron and molybdenum. The initial solution was dionized (DI) water, so this illustrates the buildup of some of the most mobile glass components in solution as the solution itself interacts with the rock matrix. Also shown in Figure 1 are solution concentrations of boron and molybdenum from some gold capsule autoclave tests with glass and water only at the same pressure and temperature but differing solution volume-to-surface area ratio, 20:1 cm (as opposed to 10:1 cm for the gold capsule tests). Figure 1 suggests that solutions in a basalt matrix have less effect in preventing boron and molybdenum leaching than granite solutions. This may be the result of a greater probability of forming molybdate alteration products in a granite environment than in a basaltic one, although such an interpretation is entirely speculative at this point.

Solution data for silicon, sodium, and cesium from both waste package and gold capsule experiments are presented in Figures 2 and 3. As reported previously, the high silicon content in solutions from basalt experiments may be the result of partial dissolution of the glass component of basalt rather than of the whole rock. A speculation on the differences in cesium

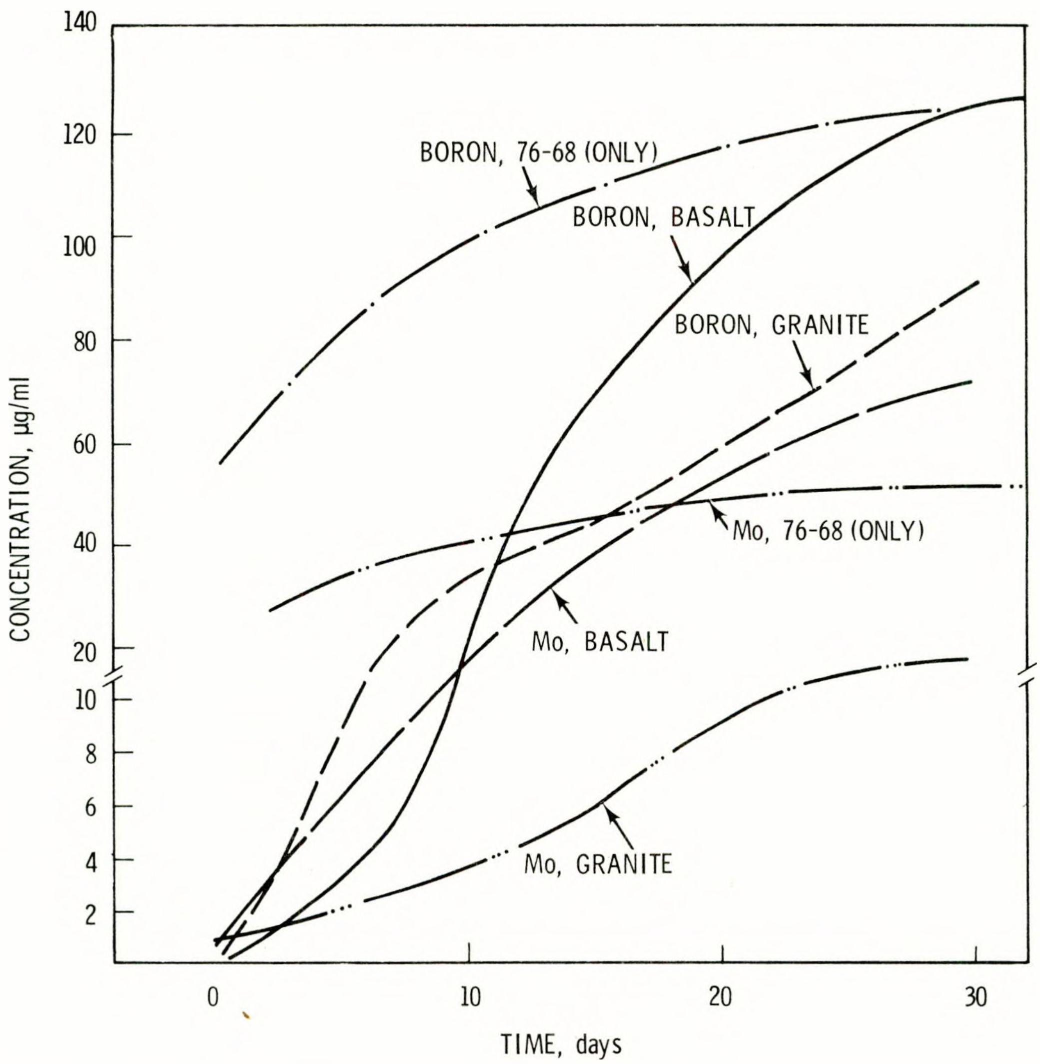

FIGURE 1. SOLUTION CONCENTRATIONS AS A FUNCTION OF TIME FOR BORON AND MOLYBDENUM FROM WASTE PACKAGE TESTS COMPARED WITH 76-68 GLASS WITHOUT ROCK MEDIA PRESENT

concentrations between basalt and granite may be that the granite has a higher cesium content than basalt in the original rock. The source of elements common to several components can be determined with spiked glasses or from experiments using fully loaded high-level waste (HLW) glass such as the one planned.

Table 4 shows concentrations of selected elements in solution from samples taken during autoclave cooling. The most mobile elements do not seem to change concentration significantly during cooling, although silicon is, as expected, considerably reduced. SEM study also showed a pervasive coating of silicon, probably as a gelatinous material, over all glass surfaces.

The test plan for the joint PNL-WIPP large-volume (5-gallon) waste package tests has been revised after receiving comments on the first draft. A large-volume (5-gallon) autoclave has been identified for use in the first cold (UO_2)-doped 76–68 glass test. A liner for this autoclave

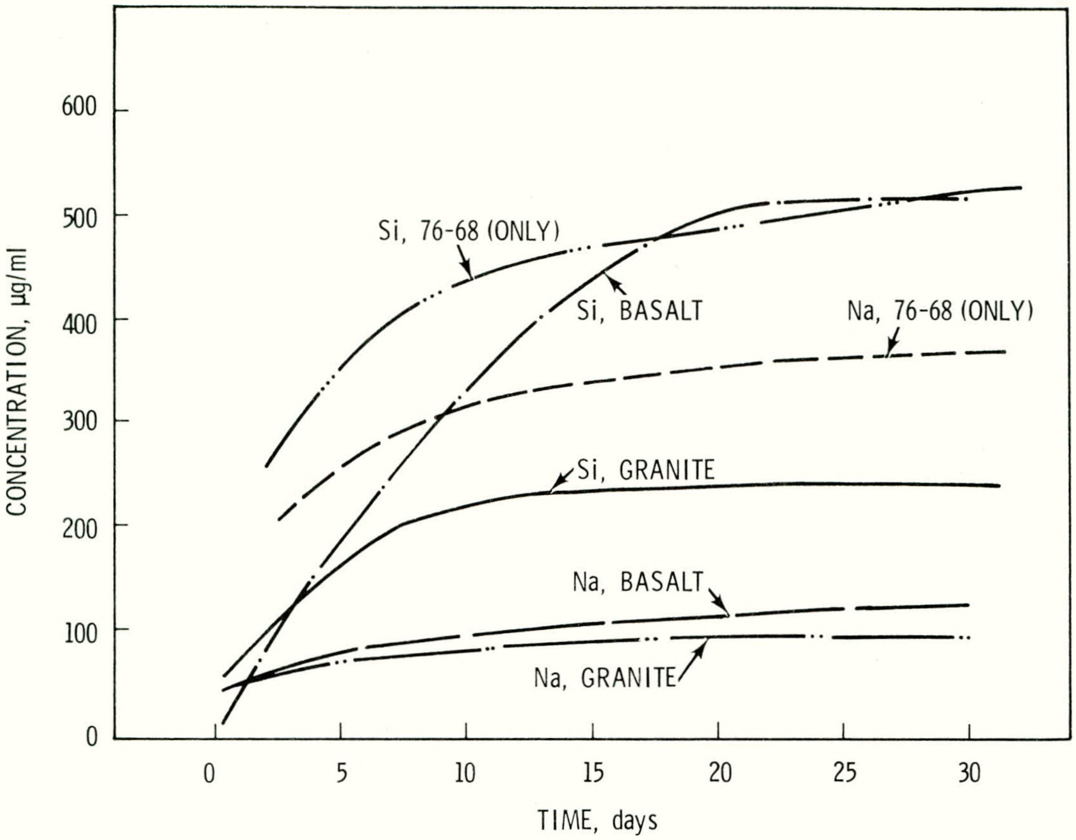

FIGURE 2. SODIUM AND SILICON SOLUTION CONCENTRATIONS AS A FUNCTION OF TIME FOR WASTE PACKAGE TESTS COMPARED WITH 76-68 GLASS WITHOUT ROCK MEDIA PRESENT

has been designed and is being fabricated. The liner will have a welded lid and will be pressurized by simultaneous internal and external pressurization to prevent soft corrosion of the autoclave.

The gold capsule welder for the spent fuel tests has been tested outside the cell. After some minor cell maintenance is completed, it will be installed in the cell. Instrumentation has been checked out for the 50-ml autoclave currently in the cell. An accurate Heise bourdon tube gage will be installed in time for use in pressure calibration.

Several informal discussions have been held with people working on the backfill-barrier program. As soon as it becomes available, a sample of an engineered-barrier material will be incorporated in the waste package tests.

TRU Leaching Studies

A new set of portland cement specimens was prepared for modified IAEA testing at Brookhaven National Laboratory. This was done with the same series of leach solutions used at PNL to ensure uniformity in preparation and curing conditions. As such, the plutonium release data reported previously provide a degree of data replication. This specimen set also included

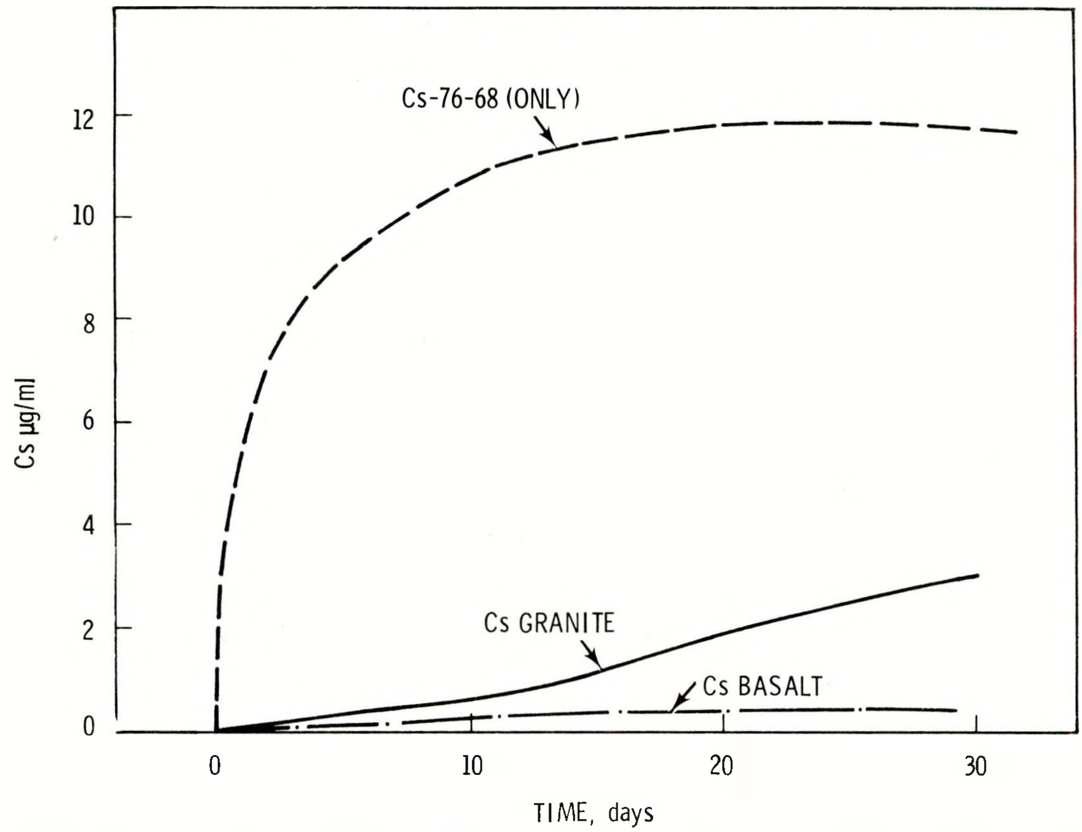

FIGURE 3. CESIUM SOLUTION CONCENTRATIONS AS A FUNCTION OF TIME FOR WASTE PACKAGE TESTS COMPARED WITH 76-68 GLASS WITHOUT THE PRESENCE OF ROCK MEDIA

a specimen for static (25 C) testing in simplified bicarbonate-dominated ground water which, with specimens currently in leaching, completed that test's leachant matrix (demineralized water, WIPP Brine B, and bicarbonate-dominated ground water) for plutonium release determination. Urea-formaldehyde and polyester-styrene specimens containing plutonium-contaminated incinerator ash were also prepared for modified IAEA leaching (in all five leachants) and for static (25 C) testing. As a result of earlier data which suggested a relatively high rate of plutonium release from urea-formaldehyde (as compared with that for other waste forms), the static 25 C test for this waste form was conducted with only demineralized water as a leachant.

The following observation can be drawn from the data taken to date from the modified IAEA TRU leach tests:

- The leach rates decrease rapidly during the first week of leaching for all waste forms.

- Plutonium release from portland cement is highest in the $NaHCO_3$ leachate and lowest in WIPP B brine. The difference is about a factor of 30 at 53 days.

- Plutonium release from urea-formaldehyde samples is substantially more (up to a factor of about 400) rapid than that from cement or polyester-styrene samples. The behavior is reversed with respect to cement, that is, in urea-formaldehyde samples, plutonium release is highest in DIW, NaCl, and CaCl simulated ground waters, and lowest in $NaHCO_3$ and WIPP B brine.

TABLE 4. SOLUTION CONCENTRATIONS DURING AUTOCLAVE COOLDOWN

	250 C	200 C	150 C	100 C	65 C	20 C	L[(a)]
				Basalt mg/ml			
Si	515	504	481	298	255	211	134
Ca	0.4	0.4	0.3	0.3	0.4	0.4	0.5
B	126	126	124	128	128	126	117
Cs	0.3	0.25	0.2	0.1	0.1	0.1	0.1
Mo	73	73	74	75	75	75	80
	250 C	**200 C**	**150 C**	**100 C**	**50 C**	L[(a)]	
				Granite mg/ml			
Si	250	250	242	240	241	193	
Ca	0.3	0.3	0.45	0.5	1.2	4.6	
B	92	92	90	90	93	93	
Cs	2.9	2.6	2.3	2.4	2.0	2.8	
Mo	18	18	17.5	17.7	18.3	19.2	

(a) L = solution remaining in autoclave after cooldown and opening - analyzed 1 week after collection.

- In polyester-styrene waste samples, plutonium release is much less affected by leach solution than are the other waste forms; only a factor of about three difference is seen in cumulative release at 30 days. The plutonium release value from these waste samples is very similar to that from cement.

Surface Science Studies

Waste glass 76-68 exposed to gamma radiation in deionized water showed strong enhancements in the leaching rates when compared with leaching rates for unirradiated samples otherwise treated identically. Increased leaching rates could be due to radiation damage to the glass structure or to the formation of reactive species by the radiolysis of water or of the air over the water. Water radiolysis can lead to the formation of H_2O_2 as well as reactive free radicals and ionic species (Burns and Moore, 1976). HNO_3 is expected from air radiolysis in the presence of water (Wright, Linacre, Marsh, and Bates, 1955). Several experiments were performed to evaluate contributions of the above possibilities to enhanced glass leaching with irradiation.

Leachate solutions were analyzed with ICP and results are reported in Table 5. The leached glasses were examined with ESCA in combination with ion sputtering.

The highest dissolution rates at a given time and temperature were found for samples irradiated while leaching in the presence of air. Lowest rates were found for the unirradiated

TABLE 5. ICP ANALYSIS OF 76-68 GLASS LEACHATES
(Parts per million by weight)

Element (NI)	90 C 13 Days DIW GI[a]	90 C 13 Days DIW NI[a]	50 C 5 Days DIW GI	50 C 5 Days DIW NI	50 C 5 Days DIW IBL[a]	50 C 5 Days HNO_3 pH = 3.5 NI	50 C 5 Days 300 PPM H_2O_2 NI	50 C 5 Days DIW GI/AE[a]	50 C 5 Days HNO_3, pH=3.5 300 PPM H_2O_2
Na	130.0	18.5	5.0	1.8	1.0	2.4	0.88	4.7	2.2
Cs	–	2.2	–	0.13	–	0.18	0.045	1.8	0.16
Ca	7.8	1.0	0.80	0.18	0.13	0.37	0.099	0.41	0.39
Ba	0.8	0.1	0.19	0.03	0.03	0.09	0.014	0.07	0.08
Sr	1.4	0.2	0.14	0.03	0.03	0.07	0.014	0.07	0.06
Si	177.1	21.0	6.5	1.44	1.9	3.54	1.53	5.47	3.13
B	31.3	4.5	1.1	0.26	0.29	0.68	0.28	0.85	0.64
Mo	7.2	2.6	0.1	0.13	0.12	0.02	0.092	0.38	0.03
Zn	37.6	0.09	2.0	0.17	0.068	0.87	0.003	0.80	0.75
Nd	–	–	–	–	0.02	0.72	0.00	0.13	0.62
Ce	–	–	–	–	0.04	0.20	0.00	0.003	0.17
Fe	–	–	–	–	–	0.30	0.00	0.015	0.36
Solution pH Before/After	5.7/4.6	5.7/8.5	5.7/3.3	5.7/7.2	5.7/7.2	3.5/3.9	5.3/7.0	5.3/6.5	5.3/4.0

(a) GI = gamma irradiated; NI = not gamma irradiated; AE = air excluded; IBL = irradiated before leach.

control, the H_2O_2 leached sample, and the sample irradiated prior to leaching. Intermediate rates were measured for samples leached in HNO_3 and for a sample irradiated while leaching in the absence of air.

The pH of the leachate for irradiated specimens, with the exception of the air-excluded sample, became acidic, as did the irradiated blank in DI water. Ion chromatographic analysis established a strong correlation between pH and the concentration of nitrate ions in solution. It can be concluded that HNO_3 is being formed under the experimental conditions where air (N_2) is present.

The effects of HNO_3 are particularly evident in the results of ESCA analysis. Figure 4 shows that the HNO_3-leached sample and the samples irradiated in the presence of air have neodymium removed from the near-surface region of the glass, while samples treated under all other conditions have enhanced neodymium at the surface. This enhancement is particularly strong in the case of the sample irradiated with air excluded. Similar results were obtained for zinc. Lanthanides and zinc may help to passivate the glass surface against further attack in slightly basic solutions. Thus, removal of these elements in acidic solutions may explain some of the enhanced leach rate. However, the effect of radiation on the leach rate cannot be explained by HNO_3 attack only. In addition, the sample irradiated in the absence of air had a release rate greater than that for the control sample but less than that for the irradiated-in-air analog, again implicating reactive species in addition to HNO_3.

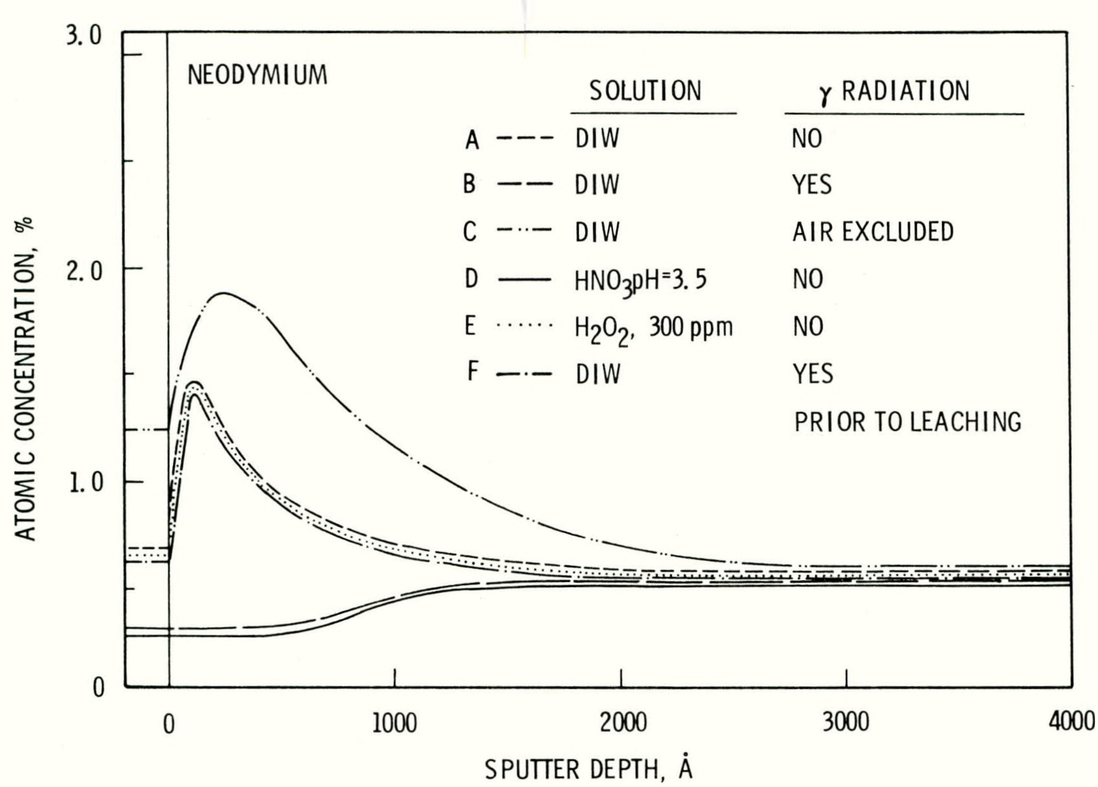

FIGURE 4. ESCA PROFILE FOR NEODYMIUM CONCENTRATION IN GLASS VERSUS SOLUTION AND RADIATION TREATMENT

ESCA profiles of iron show increased near-surface concentrations under all of the conditions employed, with the strongest effects observed for the samples irradiated (with and without air present). Sodium depletion is greatest for the samples irradiated in air. It should be noted, however, that the depletion depth of sodium cannot account for all of the sodium detected in solution. Particularly in the case of the sample irradiated in air, extensive matrix dissolution must have occurred. The depletion depth of sodium represents less than one-tenth of the total sodium release, with the balance being due to the moving glass boundary (matrix dissolution).

ESCA shows silicon has been depleted to the greatest depth in the sample irradiated in the absence of air. However, ICP analysis reveals that silicon mass release is greater for the sample irradiated in air. It is likely that the boundary of the glass is retreating more quickly in the case of the sample irradiated in air, reducing the apparent depletion depth of the silicon. The air-excluded sample showed a strong enhancement of zinc and lanthanides, slowing the rate of boundary retreat. It can be concluded that HNO_3 acid formation during irradiation in the presence of air can cause enhanced leaching because of the dissolution of the protective layer on the glass surface. However, this can account only partially for the enhanced leaching observed in a gamma field. Apparently, some of the products of water radiolysis also attack the matrix of the glass causing enhanced reaction with the aqueous solution.

Spent Fuel Special Studies

These studies are to identify leaching mechanisms and determine leachinble leaching mechanisms for spent fuel directly. The research plan is to investigate the dissolution of the UO_2 matrix materials by studying single-crystal and polycrystalline pellets of UO_2. The knowledge thus obtained will be correlated to the leaching behavior of spent fuel.

The effect of H_2O_2, which may be produced by radiolysis of water to cause the formation of UO_3-hydrate scales, was identified previously. With time, these porous scales increase in thickness and eventually crack, causing enhanced dissolution. The work this quarter was concentrated on the effects of radiation, more specifically, on identification of the radiation-induced surface activation.

Electrochemical measurement experiments this quarter have confirmed the proposed mechanism for radiation-induced dissolution of UO_2. The radiation source used in the experiments was ultraviolet radiation (UV) of 40 mW/cm^2 intensity with a wavelength of less than 300 nm (greater than 3 eV). During an electrochemical dissolution experiment with single-crystal UO_2 in solutions of DI water containing 300 ppm or 50 ppm H_2O_2, the application of this UV radiation increased the current density in the electrochemical cell twofold. This increased current density (indicating radiation-induced anodic dissolution) during electrochemical dissolution of an oxidized UO_2 surface was due to the formation of UO_3-hydrate film which is a semiconductor. Specifically, this film is an n-type semiconducting film with a bandgap near 4 to 5 eV. Single-crystal UO_2 is a p-type semiconductor and was not susceptible to radiation-induced dissolution until an oxidized film of UO_3-hydrate was formed. Currently hard x-rays are being used as the radiation source. These results will be useful in planning future experiments demonstrating radiation-induced dissolution of UO_2 and spent fuel with gamma radiation.

Work is in progress to design electrochemical cells and instrumentation for leaching spent fuel in a hot cell. A microprocessor-controlled potentiostat was purchased and received.

Testing and calibration measurements are in progress. The leaching of spent fuel in the hot cell will be monitored continuously for identification of various leaching mechanisms and determination of the leaching kinetics.

Finely powdered UO_2 (fuel grade) was contacted (with continuous agitation) with DI water, 0.015 M $CaCl_2$ solution, 0.03 M NaCl solution, 0.03 M $NaHCO_3$ solution, and with WIPP B brine in order to determine equilibrium solubilities. Solution pH values were also determined at the beginning of contact and at each sampling time. Solutions have been set up with normal air, pure oxygen, and argon as the gas phase. Solutions were thoroughly sparged with each gas to remove other dissolved gases. The solution in argon atmosphere contained iron powder or iron powder plus 0.0001 M $EuCl_3$ as an electron carrier.

The solutions in contact with air have been sampled four times over a 3-month period, and the equilibrium uranium solubilities appear to be ~10 ppm in DI water, ~90 ppm in 0.015 M $CaCl_2$, ~50 ppm in 0.03 M NaCl, ~750 ppm in 0.03 M $NaHCO_3$, and ~50 ppm in WIPP B brine at pH values of 5.7, 4.9, 5.0, 8.7, and 5.0, respectively. The DI water has shown a twofold decrease in uranium concentration with time and may not yet be at equilibrium. The $CaCl_2$, NaCl, and brine solutions all showed a drop in pH range (from 6.7–7.2 to 4.8–5.0) as the uranium dissolved. These values seem too low for just CO_2 dissolution from air. The only apparent explanation for this pH drop during UO_2 dissolution is through formation of sodium or calcium uranates or polyuranates as solid phases. A solution of 0.05 M $(C_3H_7)_4NCl$ contacted with UO_2 for 15 days showed a pH drop from 7.7 to 7.3, and it is known that uranates of $(C_3H_7)_4N^+$ are quite soluble. All this points strongly to the formation of equilibrium solid phases of sodium and calcium uranates in the Na^+- and Ca^{2+}-containing solutions. Further sampling of all solutions is planned.

GEOLOGIC MEDIA—NUCLIDE INTERACTION STUDIES

Evaluation of Experimental Methodology

Column experiments at PNL have shown a decrease in the effective porosity (as determined by tritium elution) of a column of crushed granite (12.7 cm long and 3.2 cm in inside diameter) as the flow rate increased from about 1×10^2 m/yr to 2×10^3 m/yr. The largest change in effective porosity occurred between flow rates of 530 m/yr and 1330 m/yr. The decrease in effective porosity from lowest to highest flow rates was on the order of 10 percent, which would account for only a small part of the differences often observed between batch and column Kd values. However, in finer textured materials (with corresponding smaller pores, less porosity, and fewer water pathways) or intact low porosity rocks, the decrease in effective porosity may be more pronounced with increases in flow rate. A decrease in the effective porosity of a column will result in a decrease in both the residence time for a radionuclide and the available surface area for radionuclide-rock interaction in a column experiment. Both of the above effects would confound the interpretation of the results. To generate useful data it is mandatory that flow rates in porous or fractured rock column experiments correspond to those expected in the geologic setting being investigated (on the order of 100 m/yr or less).

A comparison of batch and column methods was carried out using crushed argillite with I-131 and Tc-95m as tracers. Flow rates in these experiments were 600 to 700 m/yr which allowed a contact time of about 15 to 20 minutes between tracers and the rock. No retardation of iodine by the column was found (eluted with the tritium peak) in air or in a controlled atmosphere (<0.2 ppm O_2, <20 ppm CO_2). Technetium was retarded slightly (Kd of 0.3 to 0.4

ml/g) in both column experiments, but not nearly so much as predicted by the batch experiments (Kd = 31 ml/g in air and 175 ml/g in the controlled atmosphere). The batch Kd values were found to be strongly dependent on contact time; thus the low Kd's from column studies with short residence times are not surprising.

A comparison of 15- and 28-day batch adsorption experiments with column experiments was made using (Sentinel Gap) basalt and comparable cesium concentrations. The flow rate used in the initial column experiments was 5000 m/yr and yielded retardation factors that were an order of magnitude lower than those predicted by the batch experiments. Column experiments conducted recently at 430 m/yr yielded retardation factors that approached those found by the batch method. The maximum difference between batch and column retardation factor at the lower flow rate was only a factor of three.

It is obvious that a comparison of batch and column methods must include residence time or contact time of the radionuclide with the rock. For sorption reactions that require hours or days to reach equilibrium, short contact times in short columns or at high flow rates will preclude equilibrium conditions.

Mechanism Studies

Adsorption isotherms of strontium on argillite and basalt, neptunium on argillite, and plutonium and americium on basalt were investigated at RHO. The desorption of strontium on all three rock types was also investigated as a function of time, along with changes in the ground-water chemical composition. Several phenomena were observed.

The sorption isotherm for strontium on argillite was linear (constant Kd) over five orders of magnitude in strontium concentrations from 10^{-10} to 10^{-6} M, which may indicate the presence of a natural strontium concentration of $\sim 10^{-6}$ M maintained by the argillite. In the strontium-basalt experiment, natural or background strontium concentrations were low ($<10^{-7}$ M), and as the isotherm approached this level, the Kd increased drastically, which indicates a precipitation of strontium (probably $SrCO_3$).

The desorption studies of strontium from the three rocks indicated that strontium behavior closely follows that of calcium in argillite and granite. Over a 6-month period, strontium and calcium concentrations were found to increase linearly with time in solutions contacting the argillite. Both elements were found to decrease with time in solutions contacting granite (however magnesium increased for about 3 months and leveled off). In solutions contacting basalt, calcium concentrations increased slowly, but the scatter in strontium data was too great to say whether it really followed calcium. These results do show, however, that chemical analogs may be a useful tool in predicting behavior of some radionuclides (Sr-Ca and perhaps Ca-Sr-Ba-Ra).

The adsorption isotherms of neptunium on both basalt and argillite showed a decrease in Kd from 10^{-8} to 10^{-6} M. At concentrations above 10^{-6} M the Kd increased, which (as in the strontium-based system) probably indicated the precipitation of some solid phase containing neptunium.

Sorption experiments with Hanford basalt yielded Kd values that decreased from about 4 ml/g to 2 ml/g with increasing plutonium concentration from 10^{-14} to 10^{-12} M Pu-237. Very little plutonium sorption work has been done at concentrations that preclude precipitation of plutonium as $Pu(OH)_4$. Plutonium Kd values this small are not usually expected or found, but in a previous quarterly report, unusual behavior of plutonium on vesicular basalt was also reported at pH 4.0. The behavior of plutonium on basalt at RHO may be caused by complexation by CO_3 since the pH is 9, but carbonate complexation of plutonium is not likely at pH values of 4.0 (the pH at which sorption of plutonium was unexplainably low in previous work). The common element between the two studies at RHO and PNL is the basalt, which has a glassy phase that easily dissolves and releases silica into solution. Several studies are yet needed to determine the behavior of plutonium in rock-water systems and the possible colloid or complex formation with silicon.

An attempt by RHO researchers to study americium sorption by basalt as a function of americium solution concentration showed that americium precipitates at concentrations above 10^{-11} M if the pH is 8.5. At lower americium concentrations the Kd values were small on basalt, contrary to expectations. The behavior of plutonium and americium in solutions at high pH in contact with basalt should be investigated, as it may have importance in the near-field environment if silica complexation is the cause of low sorption rather than carbonate complexation. Silica solubility in the near field will be much higher than that in far-field situations. If silica-actinide complexes are formed and transported to a lower temperature region, mineral precipitation may be the mechanism that controls the solubility of many transuranic elements in the repository.

Sorption isotherms of strontium and cesium on granite, argillite, and tuff were made. The strontium results on all three rocks showed a constant Kd for tracer concentrations below the solution background levels of natural strontium from the rocks. At strontium tracer concentrations above the background level, Kd for strontium was found to decrease with increasing concentration. Possible precipitation of $SrCO_3$ in the granite systems gave an apparent high Kd value for strontium at $\sim 10^{-3}$ M. Behavior of cesium on argillite and granite was similar to that of strontium, except that there was no Kd increase at 10^{-3} M Cs.

NUCLIDE SOLUTION CHEMISTRY

Nuclide Solution Chemistry

The effect of $S^{=}$ and Fe(II) additions to tracer levels of $^{95M}TcO_4^-$ (10^{-13} M) was studied in a WIPP brine solution containing vermiculite suspension. Separately or together, $S^{=}$ and Fe(II) reduced the Tc(VII). The sulfide added was observed to disappear within 4 hours of mixing; however, the reduction of TcO_4^- was slow and took approximately 1 day for a 50 percent decrease in concentration. An increase in pH during the equilibration time was also observed. After 10 days equilibration, the pH values of the samples were 0.3 to 1.5 pH units higher than those measured after 4 hours of equilibration. After 10 days, a control sample with no $S^{=}$ or Fe(II) addition showed 63 percent of the technetium in solution. Addition of Fe(II) dropped the soluble technetium concentration 10 percent, and the addition of $S^{=}$ dropped this concentration to 6 to 17 percent, depending on slurry pH. Addition of both $S^{=}$ and Fe(II) reduced the soluble technetium concentration to 4.8 percent after 10 days.

To study the leachability of plutonium-containing wastes and to determine plutonium migration potential, it is important to determine the solubility of plutonium compounds. Rai, Serne, and Moore (1980) studied the solubility of ^{239}Pu(IV) oxide and hydroxide and observed a continuous decrease in sample pH with time. In response to this pH decrease, plutonium concentration increased proportionally. It was hypothesized that the decrease in pH was due to radiolysis effects of alpha radiation. The results discussed below show that the alpha radiation produced nitric acid, which was responsible for the observed pH behavior of air-equilibrated suspensions of plutonium compounds.

The hydrogen ion activity in PuO_2(c) and Pu(IV) hydroxide suspensions were plotted as a function of time. An increase of up to five orders of magnitude in H^+ activity occurred over a 3-year period for all types of plutonium suspensions. The increase in H^+ activity was also accompanied by a proportional increase in solution plutonium. The increase in H^+-ion concentration appears to be more rapid in the PuO_2(c) suspensions than in the Pu(IV) hydroxide suspensions. However, the rate of change in the H^+ activity for both of the suspensions is proportional to the H^+-ion activity.

The plutonium solids remained near the bottom of the tube or attached to the stirring bar during the slow shaking periods. If the increase in acidity were due to radiolysis from only plutonium solution species, the plutonium hydroxide suspension should have approximately 100 times the rate of H^+-ion production at a given pH value. Within experimental uncertainty, both PuO_2 and $Pu(OH)_4$ suspensions have nearly the same rate of H^+ production for a given H^+-ion activity. This indicates that the total amount of plutonium in each tube (which was approximately the same for each suspension) is involved in the radiolytic increase in H^+.

Although the effect of alpha radiation on air/water systems to produce nitric acid has not been reported, Lina and Bardwell (1929) published data showing NO_2 production from alpha radiolysis of N_2-O_2 gas mixtures. To determine whether alpha radiation was oxidizing nitrogen into nitric acid, the nitrate concentrations in some of the Pu(IV) oxide and hydroxide suspensions were determined after approximately 1000 days of contact time (Table 6). The pH and nitrate-ion concentrations were also determined for $^{238}PuO_2$ suspension initially in triply distilled water. Because the original solutions did not contain NO_3^-, its presence should be indicative of the formation of nitric acid due to radiolysis. The results show that almost equivalent amounts of H^+ and NO_3^-, and hence HNO_3, are produced in aged plutonium air-equilibrated suspensions (Table 6).

According to Wright et al (1955), the production of nitric acid is a result of the radiation energy deposited in the gas phase. The ^{239}Pu alpha particle has a range of about 35 microns in water, which is equivalent to a top surface volume of approximately 1.8×10^{-5} cm^3. If one assumes that, at most, one-half of the alpha particles escape from the surface volume and deposit their energy in the air, and that all of the NO_2 (g) produced in the gas phase is converted to HNO_3 in solution, the highest rate of H^+ production observed (2×10^{-5}M/l/day) would require over 7 grams of ^{239}Pu in 20 ml of solution used in this experiment. This estimate greatly exceeds the solubility limit of $^{239}PuO_2$(c) in a solution of pH 2 and even exceeds the total amount of plutonium compounds present in each tube. Therefore, it is concluded that the nitric acid is produced from radiolysis of dissolved N_2 and O_2 (radiolysis of water can be an additional source of O_2).

These results show that N_2 (gas) (the only source of nitrogen) was converted to HNO_3 because of alpha radiation of suspensions of plutonium compounds. The intermediate reactions for HNO_3 production were not identified. However, the final concentrations of H^+, NO_3^-, and plutonyl ions were identified as the end products.

Solubilities of Compounds

Studies are being conducted to determine whether the plutonium and neptunium concentrations in solutions contacting doped glass beads are governed by a solid phase of the elements.

TABLE 6. EFFECTS OF ALPHA RADIATION IN PLUTONIUM SOLUTIONS UNDER ATMOSPHERIC CONDITIONS

Sample	Contacting Solution	Contact Time, days	Log H^+, moles/l[(a)]	Log NO_3 moles/l[(b)]
$^{238}PuO_2$-1	Distilled Water	1	ND	ND
		1,266	-1.52	-138 ± 0.02
$^{239}PuO_2$-4	0.0015M $CaCl_2$	1	8.5	ND
		1,028	-2.65	-2.66 ± 0.04
$^{239}PuO_2$-15	0.0015M $CaCl_2$	1	5.5	ND
		1,021	-2.95	-3.14
$^{239}Pu(OH)_4$-10	0.0015M $CaCl_2$	1	-7.0	ND
		1,208	-2.15	-2.39 ± 0.03
$^{239}Pu(OH)_4$-22	0.0015M $CaCl_2$	1	-4.0	ND
		1,021	-2.10	-2.58 ± 0.13

(a) ND = not determined.

(b) Although nitrate concentrations were not determined at 1 day of contact time, the NO_3^- at this time should be absent because the starting suspensions were made in distilled water. The reported concentration for each sample is an average, along with the standard deviation, from two or three measurements. Only one measurement was made for $^{239}PuO_2$-15 sample.

Pu/Np-doped glass beads were contacted with a dilute salt solution (0.0015 M $CaCl_2$) containing quinhydrone (a redox buffer). The suspensions of crushed glass beads and the dilute solution were adjusted to pH values ranging from 3 to 8. The results on neptunium concentrations in 0.015 and 0.0018 μm filtrates were reported last quarter. It was also reported that quinhydrone effectively controlled the redox potential.

The concentration of plutonium in the 0.015 and 0.0018 μm filtrates were similar, suggesting that the colloidal particles >0.0018 μm were not present in the solutions. When PuO_2(c) was added to the suspensions (Figure 5), the concentration of plutonium in solution did not change substantially, which suggests that the plutonium concentrations in solutions contacting glass beads may be controlled by PuO_2 (c) or a solid similar in solubility to PuO_2(c).

To assess the potential environmental consequences of storage of plutonium-containing wastes in soils or geologic formations, plutonium migration rates must be estimated. These rates are affected not only by adsorption on the soils or geologic formations but also by the plutonium solubility in the hydrologic environment. Further, polymers are known to form, and their fate needs to be determined in the geosphere. Summarized below are the results of six experiments in which preformed polymer solutions were adjusted to higher pH; five experiments in which precipitated (by hydroxide) preformed polymer was contacted with fresh solution; one experiment in which precipitated (by heating) preformed polymer was

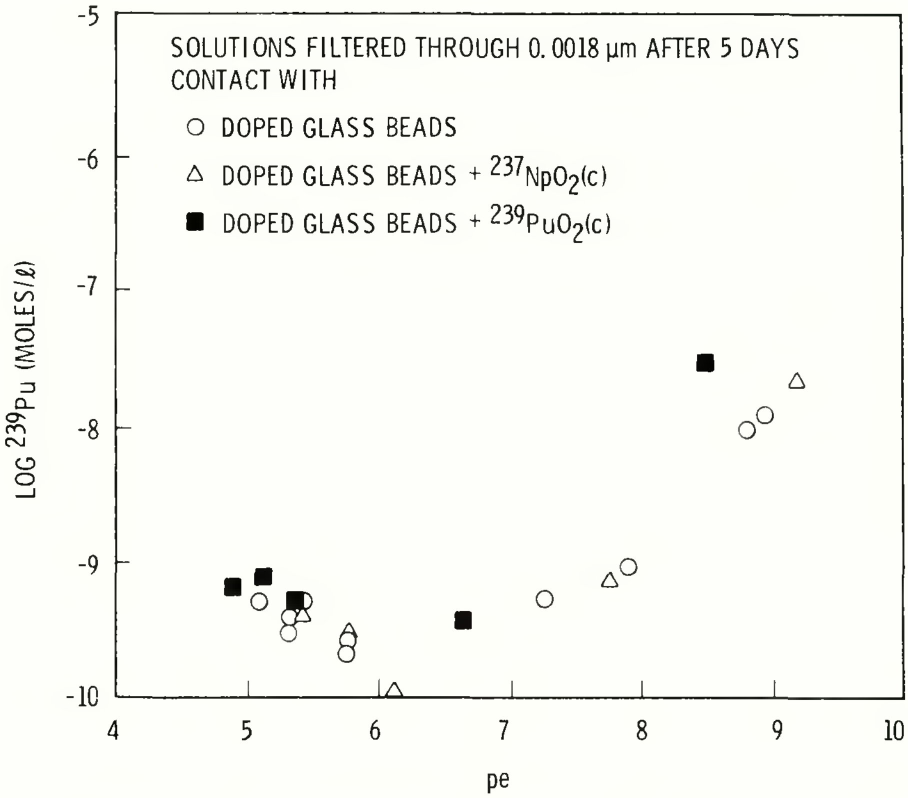

FIGURE 5. Pu CONCENTRATION IN SOLUTIONS IN CONTACT WITH CRUSHED GLASS BEADS

contacted with fresh solutions; one experiment in which precipitated (by heating) preformed polymer was contacted with fresh solutions; one experiment in which a dilute Pu(IV) monomer solution was rapidly pH adjusted; and two experiments in which rapidly precipitated Pu(IV) hydroxide was contacted with fresh solutions.

All of the data from these different types of experiments fall within a general band that is intermediate between the solubilities reported earlier for amorphous Pu(IV) hydroxide and for crystalline PuO_2. While the data are generally comparable, there do appear to be some significant differences:

1. Preformed polymer exhibits higher solubility (by a factor of about three) in nitrate solutions having ionic strengths of 0.02 to 0.04 than in dilute (10^{-3} M) chloride solutions. The nitrate solution data include approaches to equilibrium from both directions; the close agreement indicates that an equilibrium condition was indeed achieved in these experiments.

2. Preformed polymer that has been heated exhibits lower solubility than that which has not.

3. Rapidly precipitated Pu(IV) hydroxide has a higher solubility than does preformed polymer. The hydroxide solubility measured in this work is not as high as reported earlier by Rai et al (1980).

The plutonium in 2 nm filtrates from these experiments was essentially all Pu(V) and/or Pu(VI), as shown by the thenoyltrifluoroacetone (TTA) extraction tests. The test results typically indicated that 1 percent or less was Pu(III) and/or Pu(IV) and that 85 percent or more was Pu(V) and/or Pu(VI). The close agreement between the sum of the ionic species and the total plutonium indicates that plutonium polymer was not passing through the filter in significant amounts. One preformed polymer solubility solution (pH 3.2) tested by a spectrophotometric method was found to contain Pu(V) rather than Pu(VI), Pu(IV), or Pu(III). Thus, the oxidation state found for the soluble plutonium in equilibrium with plutonium polymer is in complete agreement with that found earlier for Pu(IV) hydroxide and PuO_2(c).

PREDICTIVE MODEL DEVELOPMENT

Data Banks and Data Reduction

The Sorption Information Retrieval System (SIRS) was demonstrated this past quarter, using a limited data set. Most of the debugging is finished and code validation has begun. SIRS has been divided into three packages: Data Generation (e.g., data entry), Analysis, and Auxiliary. By separating Generation from Analysis, the chances of inadvertently damaging the data base are minimized; the Generation package must be called out separately. A debugging routine has proved useful in checking candidate data for errors prior to entry.

Leach Modeling

One of the key questions pertaining to glass leaching is whether leach mechanisms are reversible, in the sense of the mechanism slowing down as released constituents concentrate at the glass interface. For reversible mechanisms, the behavior in the glass must be coupled with mass transfer behavior in a leachate in order to model the resulting release, and it implies that the release can be controlled by mass transfer in the leachate. A likely place to look for reversible release is in static leach experiments, where released constituents are allowed to accumulate in the leachate. Then reversibility implies that a limiting concentration in solution is approached asymptotically. The limit cannot be interpreted as a thermodynamic solubility, since the mechanism is not the dissolution of a simple crystalline phase but the concepts are similar.

In recent experiments, crushed 76-68 borosilicate glass (simulated commercial high-level waste glass) was leached in (initially) deionized water in a static leach test at 35 C. The solution concentrations of both sodium and molybdenum seem to be approaching a limiting concentration after 500 hours. A plot of concentration versus square root of time shows a poor fit to pure diffusion behavior, and a semilog plot shows a poor fit to exponential approach to a limiting concentration.

By assuming solid state diffusion and a proportionality between the concentration in the solid at its surface and the concentration in solution, rather than a zero surface concentration, a good fit to the data was obtained for both sodium and molybdenum. This approach is similar to that of White and Claassen (1979), who considered the case of a Freundlich isotherm relating surface and solution concentration. Assuming a linear "isotherm" and that a negligible fraction of the constituent in the solid is lost during leaching (implying that a flat concentration profile recurs at equilibrium), one gets for the solution concentration:

$$\frac{C}{C} = \frac{mC}{C_o} = 1 - E^{\phi}\,\mathrm{erfc}\sqrt{\phi}\ ,$$

where

C = solution concentration, g/cm^3

C_∞ = limiting solution concentration, g/cm^3

C_o = initial concentration in the solid, g/cm^2

m = C_o/C_∞ = proportionality constant

ϕ = m^2S^2Dt

S = solid surface area/liquid volume, cm^{-1}

D = diffusivity in the solid, cm^2/sec

t = time, sec.

The results of fitting this functional form to the data are shown in Table 7 and Figure 6. The value of S was 49 cm^{-1}.

For release controlled by diffusion only, such as for the zero surface concentration condition, the release described by

$$\frac{mC}{C_o} = \frac{2}{\sqrt{\pi}}\sqrt{\phi}$$

or equivalently

$$\frac{C}{C_o} = \frac{2}{\sqrt{\pi}}\,S\sqrt{Dt}.$$

This is shown by the dashed line in Figure 6.

The fitted diffusivities are in the right ballpark for ions in glass, but they need more scrutiny before it can be said they are accurate. It is encouraging that both sodium and molybdenum data are fit well by this functional form. The similar values of m are perhaps not unexpected since it is assumed that the molybdenum in the glass is in the Mo^{+6} state, which is rather soluble.

Analysis of Sorption Kinetics

The sorption kinetics calculations discussed in a previous Quarterly Report were reviewed, and a more revealing analysis was developed, based as before on the classical ion-exchange chromatography theory.

If migration of radionuclides in a laboratory column experiment is assumed to be controlled by linear sorption equilibrium and linear sorption/desorption kinetics, then, assuming dispersion is negligible, radionuclide migration is described by the classical equations of

TABLE 7. EMPIRICAL CONSTANTS DERIVED FROM GLASS LEACHING EXPERIMENT

Parameter	Sodium Data	Molybdenum Data
C	3.75×10^{-5} g/cm^3	4.5×10^{-6} g/cm^3
m	7500	9800
D	7×10^{-18}cm^2/sec	6×10^{-18}cm^2/sec

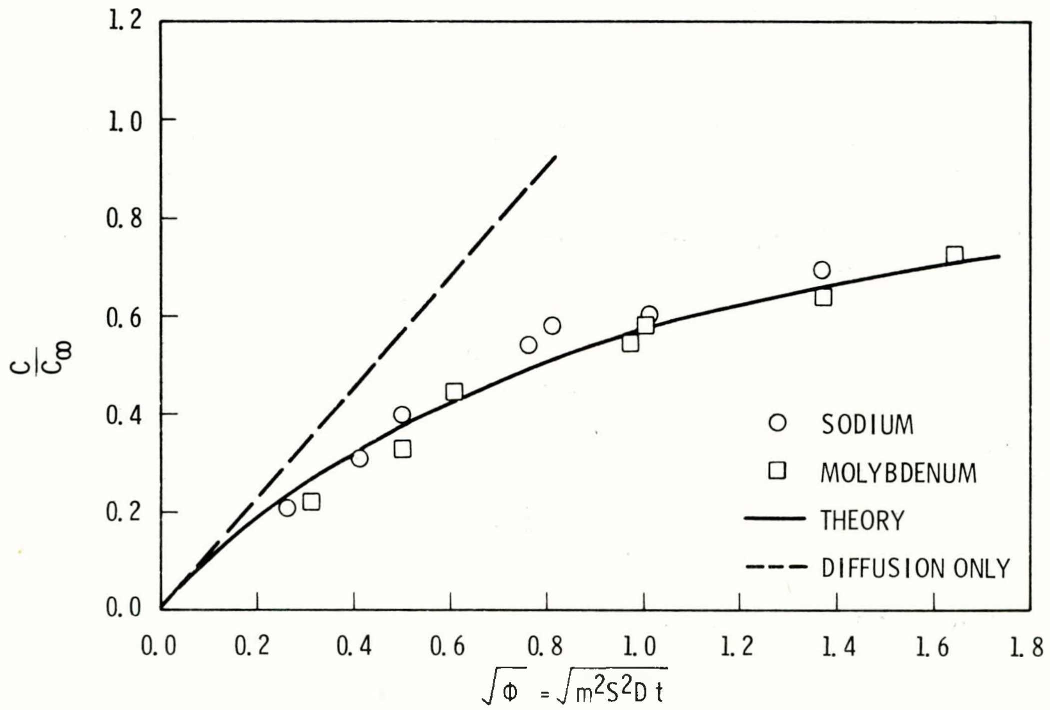

FIGURE 6. PLOT OF REDUCED CONCENTRATION DATA VERSUS DIMENSIONLESS TIME
$S = 49$ cm^{-1}

chromatography. From the equations it can be seen that a radionuclide peak at a column inlet will at first travel with the carrier velocity if sorption kinetics are not infinitely fast and eventually reforms a retarded peak traveling at the expected velocity, reduced according to the linear sorption equilibrium coefficient. The transition from one behavior to the other depends on the number of theoretical mass transfer units, n, passed by the carrier fluid, where

$n = (aK_a/E)\,(kx/v)$

a = surface area/volume in column, cm^{-1}

K_a = distribution coefficient based on area, cm

E = void fraction in column

k = sorption kinetic constant, sec^{-1}

x = distance from inlet, cm

v = carrier velocity, cm/sec.

Note that $K_a k$ is the desorption kinetic constant and aK_a is the same as the often used Kd.

Values of n = 10 are required before the reformed, retarded peak begins to take its expected position according to the sorption coefficient. This then becomes the criterion for whether kinetics are important, given the above typical assumptions, since once $n<10$ the peak assumes its "equilibrium" position. From the definition of n, it is the carrier travel time, x/v, that determines whether kinetics are important; the velocity alone should not be used as a measure. Furthermore, for $n<10$, the peak location relative to the carrier "front" (e.g., the location of a peak of a nonsorbing tracer) is not determined by the sorption coefficient alone, and the peak location seems to correspond to a smaller than actual sorption coefficient. Thus laboratory column experiments utilizing small lengths (x) and faster than realistic water velocities (v) may force n to be smaller than 10, which would elevate kinetics to an important role. Again extrapolation to probable long-term safety assessment scenarios lead to the conclusion that reaction kinetics observable in short-term laboratory experiments are fast enough to be modeled by equilibrium concepts. That is, if kinetics are important to modeling real scenarios, the rates would be so low that normal laboratory experiments could not detect the changes.

Geochemical Modeling

The chemical thermodynamic code EQ3/EQ6 was applied to model basalt/water interactions. The EQ3, or "speciation" code, was run separately to investigate the assumed initial water compositions. The deep Hanford ground-water compositions reported by Apps et al (1979) were found to be supersaturated with respect to some clay minerals. The current disagreement between "theory" and field observations could be due to slow kinetics of clay precipitation or to uncertainties in the thermodynamic data base or field ground-water measurements; as yet it is not known whether the apparent supersaturation is significant.

The EQ6, or "reaction path" code, was run to see whether a reasonable assemblage of precipitated minerals is predicted, and that is the case. This provides confidence in using EQ3/EQ6 to predict geochemical behavior in fresh fractures, to estimate changing deep ground-water composition with changing recharge rates, or to investigate other scenarios describing repository conditions.

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WBS 1.1.6

Project: Assessment of Effectiveness of Geologic Isolation Systems (AEGIS)

Principal Investigator: Pacific Northwest Laboratory (A. Brandstetter)

ONWI Project Manager: J. Kircher

Objective

The objectives of the Assessment of Effectiveness of Geologic Isolation Systems (AEGIS) Program are to: (1) develop the capabilities needed to assess the post-closure safety of geologic repositories; (2) demonstrate the assessment capabilities by performing analyses of reference sites; (3) apply the assessment methodology to assist the National Waste Terminal Storage Program in site selection; and (4) perform repository site analyses responsive to the time schedule and to the level of sophisitication required to meet the licensing needs of the National Waste Terminal Storage Program.

INTRODUCTION

In the past 3 years, the Waste Isolation Safety Assessment Program (WISAP) has been developing a methodology for assessing the long-term safety of nuclear waste storage in geologic formations. Starting with FY 80 (on 1 October 1979), WISAP was divided into two separate programs to become more responsive to the gradually changing emphasis from generic research to site-specific evaluations: The Assessment of Effectiveness of Geologic Isolation Systems (AEGIS) Program, and the Waste/Rock Interaction Technology (WRIT) Program. The AEGIS Program will continue the scenario and consequence analysis methodology development work of WISAP and will assist ONWI and DOE in site applications. The WRIT Program will continue the sorption/desorption and waste form leach studies of WISAP, will support AEGIS in the development of geochemical reaction and waste leaching models, and will provide related data as needed for site applications.

The report covers the technical activities of AEGIS for the third quarter of FY 80.

Methodology Development

Progress Reported Previously

Development work continued on improvements to the release scenario model and development of a finite-element model that couples ground-water flow as well as energy transport and solute transport. A study to determine the potential for organic compounds to influence the transport rate of radionuclides continued. Various aspects of uncertainty and geostatistics research related to the ground-water flow and contaminant transport equations were studied.

Activities During the Reporting Period

Issues Analysis

The status report on the potential for organic compounds to influence the transport rate of radionuclides was completed. An AEGIS Integrated Methodology (AIM) report was written to describe the basic components of the AEGIS approach to the general reader.

The evaluation of long-term effectiveness involves a number of distinct steps. Initially, the characteristics of the engineered components in the repository, and of the existing geologic and hydrologic systems surrounding the repository must be adequately understood. Since natural geologic processes and future human activities may alter these systems over the long time frames, an evaluation must be made to determine if there are plausible scenarios for breaching the repository. If such a scenario is identified, then the transport of radionuclides from the repository to the environment must be estimated. A final step may be added to estimate the effects of the radionuclides upon the human population. Each step of this approach is identified in Figure 1 and discussed in the report.

Work began on a study to evaluate the potential of human intrusion into bedded salt. The reference site for this study is the Paradox Basin of Utah and Colorado. The investigation involves evaluating the mineral resources contained in the Paradox Basin and determining the relative potential of human intrusion based on the exploratory and extraction techniques that may be used to obtain these minerals.

Literature searches were completed on computer chemical models and the kinetics of dissolution/mineralization reactions. A test case of the computer chemical model EQ 3/6 was evaluated using compositions of Hanford basalt and ground water. The reaction path model produced a reasonable assemblage of secondary products from the basalt dissolution and will be a useful tool in further modeling work.

Scenario Methodology Development

General development of the release scenario model continued. The submodels involved with folding and faulting were modified to reflect new theories on the origin of Columbia Plateau structures. The statistics team constructed a description of operating parameters for the release scenario model in a Monte Carlo mode. This work included altering the number and size of the time steps, identifying the best set of control variables, and identifying several additional variables that might be included in the output files to allow a more comprehensive analysis of the simulation.

Transport Methodology Development

Work continued on the development of geohydrologic response functions as a means of evaluating the overall performance of a repository site. Initial work has progressed on a distributed process control-type analysis to allow optimal placement of a repository in a known geohydrologic system.

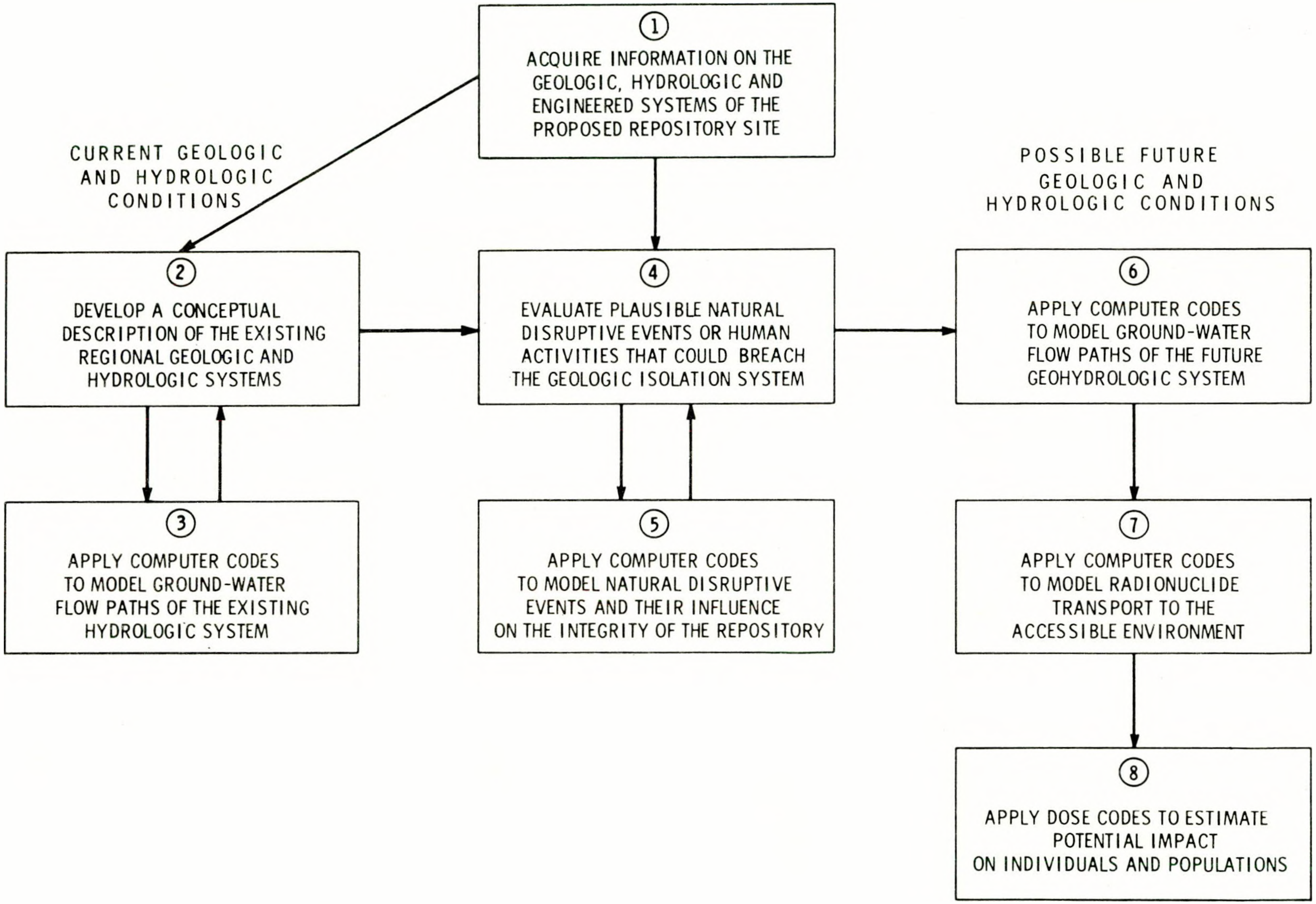

FIGURE 1. ASSESSMENT FLOW DIAGRAM

In uncertainty modeling, methods have been provided for obtaining the variance of the pore velocity when the individual variance components for the hydraulic conductivity and potential gradient have been obtained by the use of Kriging. The method for incorporating the variance of the velocity into the transport equations involves an extension of the Keller smoothing method. Initial programming to incorporate this method for use in a two-dimensional test of contaminant transport with uncertainty was begun.

Two results have been obtained that are important in effectively testing and utilizing the PNL extension of Keller's method in uncertainty analysis. The first result demonstrates that higher-order statistical parameters or moments will be required in addition to more involved expansion terms when large variances occur. If required, such higher-order moments may not be realistically determined from current field measured data. The second result provides a precise measure for the size of certain matrices that must be small if the Keller approach is to have utility. It has been shown that the measure for the matrix is an appropriate norm. Specifically, the appropriate norm is the maximum, root-mean-square, absolute row sum. This sum is used to determine whether the Keller approach will apply in any given case.

Dose Methodology Development

Documentation of computer codes ARRRG, FOOD, and PABLM has been cleared and published. The dose methodology development work has essentially been completed for this fiscal year.

Site Applications

Progress Reported Previously

The Salt Dome Reference Site Initial Assessment (RSIA) was distributed for review. Brine temperatures in the solution-mine scenario were estimated to approach the temperature of the dry host salt prior to the hypothetical breach event. However, estimation of the temperature of dry salt that surrounds a high-level-waste (HLW) inventory has proved to be more difficult than spent fuel because the available information illustrates an anomaly among repository size, quantity of stored waste, and thermal loadings.

Different modeling strategies have been selected for the regional and local hydrologic models used in the basalt RSIA. The overall approach has been to develop a regional model of the major portion of the Columbia Plateau Basalt which serves as a source of recharge waters or in other ways influences the flow of circulating ground water within the more local Pasco Basin where the hypothetical repository will be sited. The regional modeling effort will use the multiaquifer, two-dimensional VTT hydrologic code, and the local model will utilize the fully three-dimensional FE3DGW hydrologic code.

Basalt release scenarios were being developed using expert opinion based on submodel categories contained in the basalt release scenario model. Analysis of the natural disruptive phenomena suggested that only tectonic phenomena such as faulting and folding were potential natural causes for a breach of the repository host rock.

Activities During the Reporting Period

Salt Dome RSIA

The ORIGEN code is currently being used to predict, over long time periods, the full suite of radioisotopes considering both spent fuel and HLW inventories. Calculations of radiation doses from the solution-mining scenario for a repository containing spent fuel were made for mining operations commencing at 10,000, 30,000, 50,000, 100,000, 500,000, and 1,000,000 years. The calculated doses are significantly higher than natural background for all periods. New temperatures and leach rates were calculated for the solution-mining scenario for a repository containing reprocessed HLW in glass. Dose calculations for the breach scenario occurring at 100 and 1000 years after closure are in progress.

Salt Dome Site Evaluation

Four salt domes were compared for ground-water flow and radionuclide retardation capacity in the strata overlying the domes. The scenario anlayzed assumes drilling from the side of the dome into the repository that allows ground water to flow through the hole, through the repository, and up through incompletely sealed shafts. Approximate travel times of the flow were computed and the retardation capacity was evaluated qualitatively. Based upon the limited data available, Vacherie Dome appeared to be the most favorable of the four.

Basalt RSIA

Preparation of input for hydrologic models proceeded. Technical discussions with Rockwell personnel have resulted in two additional studies to be performed at Battelle to provide better estimates of recharge in (1) the higher elevations surrounding Pasco Basin and in (2) regional agricultural acreage. These studies will not be complete until the end of FY 80, but they will be used to refine input for hydrologic models on the basalt RSIA as appropriate.

A computer code for calculating the areal distribution of regional recharge for a major portion of the Columbia Plateau has been completed and tested. The code includes a subroutine to access the U.S. Topographic Data Base and obtain a topographic data file of the Columbia Plateau. Input data describing the pumping distribution for the basalt RSIA within the Pasco Basin have been prepared, and boundaries for the hydrologic model of the Pasco Basin have been established.

Initial regional basalt recharge estimates have been completed. Further sensitivity studies are being performed with the RECHARGE code in order to estimate the range in recharge that is available to the basalts.

The regional hydrologic model is currently being calibrated. Work on the local hydrologic model has been delayed while structure maps are being prepared for the Pasco Basin.

Analysis of the natural disruptive phenomena and other considerations for human intrusion have been drafted for inclusion in a working paper on release scenarios. The definition of a threshold value for ground-water flow that constitutes a "breach" received additional attention from AEGIS staff and consultants. The final value for ground-water flow will be incorporated into the scenario computer model for basalt.

WBS 1.1.6

Project: The Effects of Far-Field Inhomogeneities on Surface Temperature and Heat Transfer From a Repository

Principal Investigator: Ohio State University (F. A. Kulacki)

ONWI Project Manager: G. Raines

Objective

The primary objective is to develop analytical and semi-analytical solutions for the conduction heat transfer problem for the simple geometries often found in the stratigraphies of repository sites under consideration. Another objective is to include the temperature dependency of thermal conductivity in the solutions. A few of these solutions will be compared with the experimental results from a laboratory scale model of the repository and its subsurface surrounding, as well as with the relevant existing numerical calculations.

Activities During the Reporting Period

Solution by the Heat Balance Integral

The Heat Balance Integral (HBI) can be used to predict the temperature distribution in a semi-infinite body with an arbitrary number of sublayers. First, a differential equation is derived from each sublayer. Only three types of differential equations need to be considered when modeling a nuclear waste repository with an infinite plane between two of the sublayers. These are for (1) the case where only one thermal boundary affects the temperature distribution, i.e., the temperature distribution is the same as if the layer acted as a semi-infinite solid; (2) the case where the domain is finite, and the second thermal boundary condition is specified, say as a constant temperature; and (3) the case where the domain is a sublayer and the second boundary condition is at an interface with another subdomain. The geometries which lead to each of these cases are depicted in Figure 1. Differential equations for the first two cases have been previously reported; these are

$$\frac{d}{dt}\left[\frac{q_1\delta^2}{12\alpha(T_1)}\right] = q_1 \tag{1}$$

$$\frac{d}{dt}\left[\frac{5}{8}T_1\ell\rho c - \frac{1}{8}\frac{q_1\ell}{\alpha}\right] = \left[1 + \frac{1}{2}\frac{k(T_2)}{k(T_1)}\right] q_1 -$$

$$\frac{3}{2}\frac{k(T_2)}{\ell}(T_1 - T_2) \tag{2}$$

$$\frac{d}{dt}\left[\frac{\rho c \ell}{2}(T_1 + T_2) + \frac{\ell^2}{12}\left(\frac{q_2}{\alpha(T_2)} - \frac{q_1}{\alpha(T_1)}\right)\right] = q_1 - q_2 . \quad (3)$$

Equation 3 reduces to Equation 2 when the second boundary condition is a constant temperature and the second derivative of temperature with respect to distance is zero.

After choosing the appropriate differential equations and applying the normal (physical) boundary conditions at the interfaces, one finds that there is one more unknown than equations. It is necessary to derive another smoothing condition for the interface from the original partial differential equation for temperature and the condition that the temperature at the boundary must be the same in both sublayers (Yang, 1961). The smoothing condition is

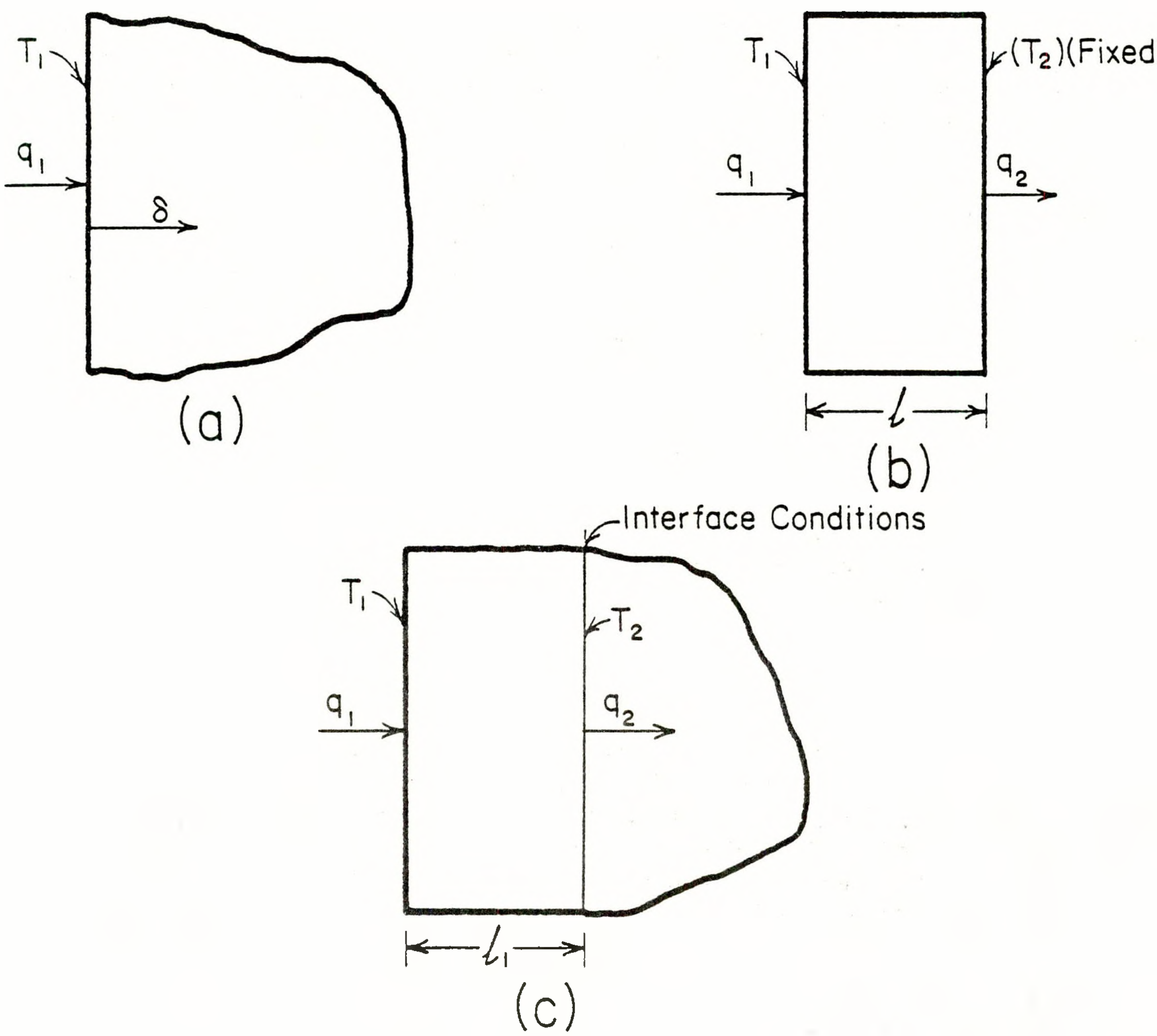

FIGURE 1. GEOMETRIES CORRESPONDING TO THE THREE BASIC DIFFERENTIAL EQUATIONS

(a) Eq. (1); (b) Eq. (2); and (c) Eq. (3).

$$\alpha_1 \left. \frac{\partial^2 T}{\partial x^2} \right|_{\ell} = \alpha_2 \left. \frac{\partial^2 T}{\partial x^2} \right|_{\ell} \tag{4}$$

Physically, this smoothing condition means that at the boundary, the temperature in both layers is changing at the same rate with respect to time. This is possible in an integral method since the dependency of the temperature on position is assumed. Therefore, the temperature depends only on time. Since this smoothing condition can be used at each interface, one has a choice between using a differential equation for each layer with one smoothing condition and using a smoothing condition at each interface and only two differential equations.

For the plane source between a finite slab and a semi-infinite body, the smoothing condition is unnecessary. When Equations 1 and 2 are solved numerically by Hamming's method (International Business Machines Corporation, 1968) with a step change in heat flux at the interface and assuming the same constant isotropic thermal properties in both bodies, the temperature at the interface is within 2 percent of the exact temperature calculated using Green's functions (Carslaw and Jaeger, 1959). When an exponentially decaying two-nuclide source, such as heat used by Beyerlein and Claiborne (1980), is assumed, the predicted interface temperature exhibits two peaks, as does the exact solution presented by Beyerlein and Claiborne, but the first peak is smaller and earlier and is followed by a large drop (see Figure 2). The reason for this error can be seen by looking at the equation for the penetration depth in a semi-infinite body with an arbitrarily varying heat source at the surface (Goodman, 1964).

$$\delta = (12\alpha)^{1/2} \; \frac{1}{q(t)} \int_0^t q(\hat{t})\, d\hat{t}. \tag{5}$$

A large time constant in an exponentially decaying heat source would produce a large penetration depth. In fact, the faster the source decays, the faster the speed of thermal disturbance moves into the solid.

Experimental Apparatus

A slab over a "semi-infinite" body was chosen as a simple experimental model of a nuclear waste repository. One reason to select this model is that it is exactly the same configuration as that used to develop the HBI model of the problem. Since the HBI method leads to results close to those of the exact solution for a step change in heat flux at the interface, the experiment would complement the analytical results. A second reason is that it is an acceptable approximation for a gulf interior salt dome (Office of Waste Isolation, 1978), which has a 100-foot-thick layer of sand, clay, and caprock over an essentially infinite body of salt.

A materials combination of interest in the present work for a waste repository is shale and salt since they often occur in nature with each other. In this case, the shale would replace the top layer. For the range 0 to 300 C, the thermal conductivity for generic salt varies from 6.1 to 2.5 W/m C and that for generic shale (axis perpendicular to bedding) varies from 1.4 to 1.25 W/m C. In the same temperature range, the thermal diffusivities vary from 3.2×10^{-6} to 1.3×10^{-6} m^2/sec for salt and from 0.68×10^{-6} to 0.55×10^{-6} m^2/sec for shale (axis perpendicular to

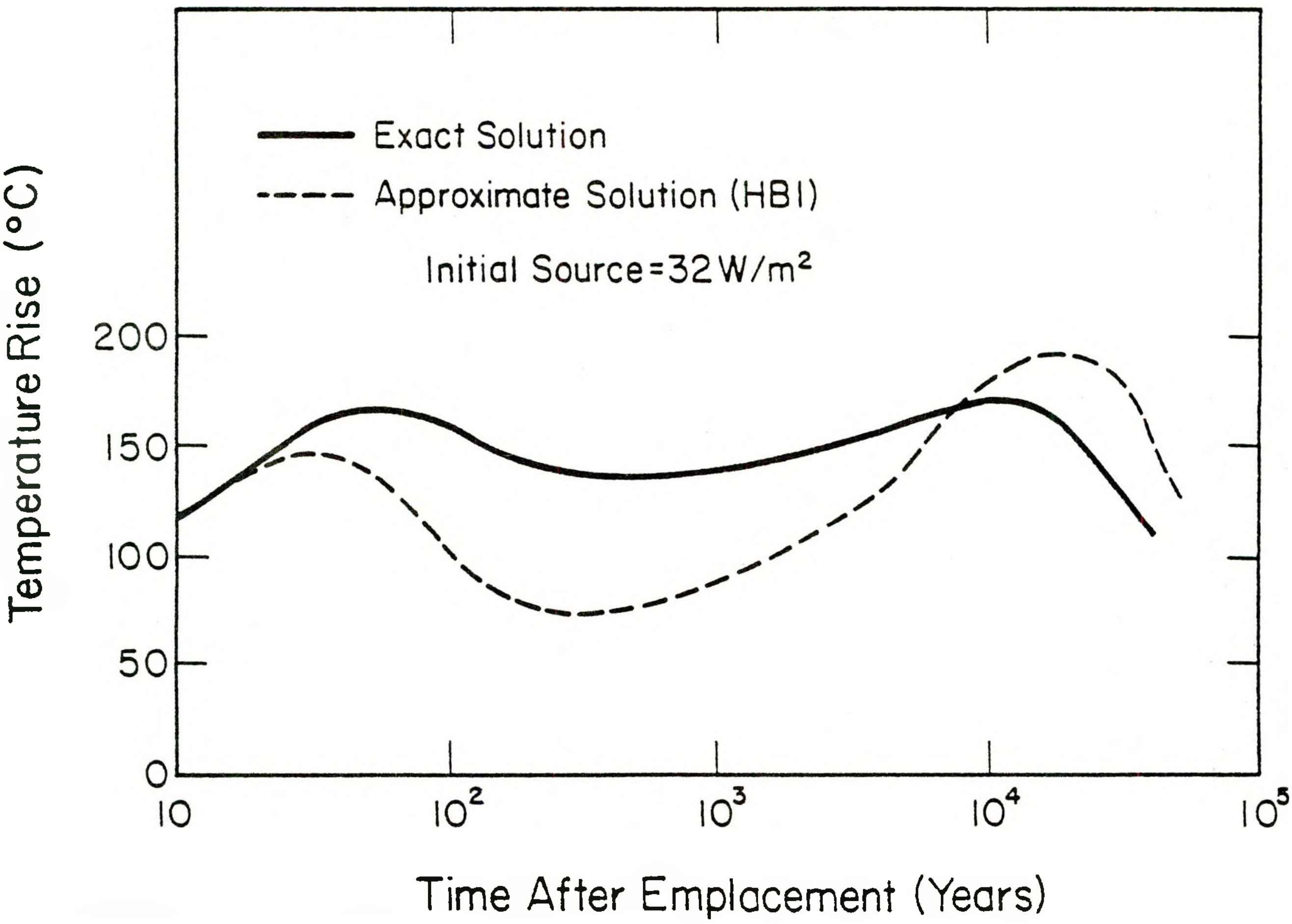

FIGURE 2. COMPARISON OF TEMPERATURE RISE AT SOURCE PREDICTED BY THE HBI METHOD AND THE EXACT SOLUTION ASSUMING A TWO-NUCLIDE SOURCE IN AN INFINITE PLANE BURIED AT 1000 METERS IN GRANITE (BEYERLEIN AND CLAIBORNE, 1980)

bedding). The best combination of materials to imitate the ratios of thermal conductivity and diffusivity for the rocks is Plexiglas and gypsum plaster. The thermal conductivities are 0.21 W/m C and 0.48 W/m C, respectively. The thermal diffusivities are 1.2×10^{-7} m^2/sec for Plexiglas and 4.0×10^{-7} m^2/sec for plaster (Baumeister, 1967). The ratio of thermal conductivity for this combination is 2.3, which is comparable to the range of ratios from 4.4 to 1.5 for salt and shale. The ratio of thermal diffusivities for the model materials also falls in the range 4.7 to 1.8 for salt and shale.

The basic dimensions and layout of the experimental apparatus are shown in Figure 3. It has a 1.5-in. (3.81-cm)-thick sheet of Plexiglas over a 1 x 1.5 x 2-ft (30.48 x 45.7 x 60.9 cm) block of gypsum plaster with a 12 x 1.5-in. (30.48 x 3.81-cm) strip heater imbedded flush with the top of the plaster block. Insulation surrounds the Plexiglas and plaster on five sides. Either an aluminum heat exchanger will be placed on the top or ambient air will be blown across the top.

A thickness of 1.5 in. (3.81 cm) was chosen for the Plexiglas, since it is the thickest available locally as a stock item. On the basis of an experimental run time of 2 hours, the plaster dimensions were determined using the HBI method. The penetration distance after 2 hours

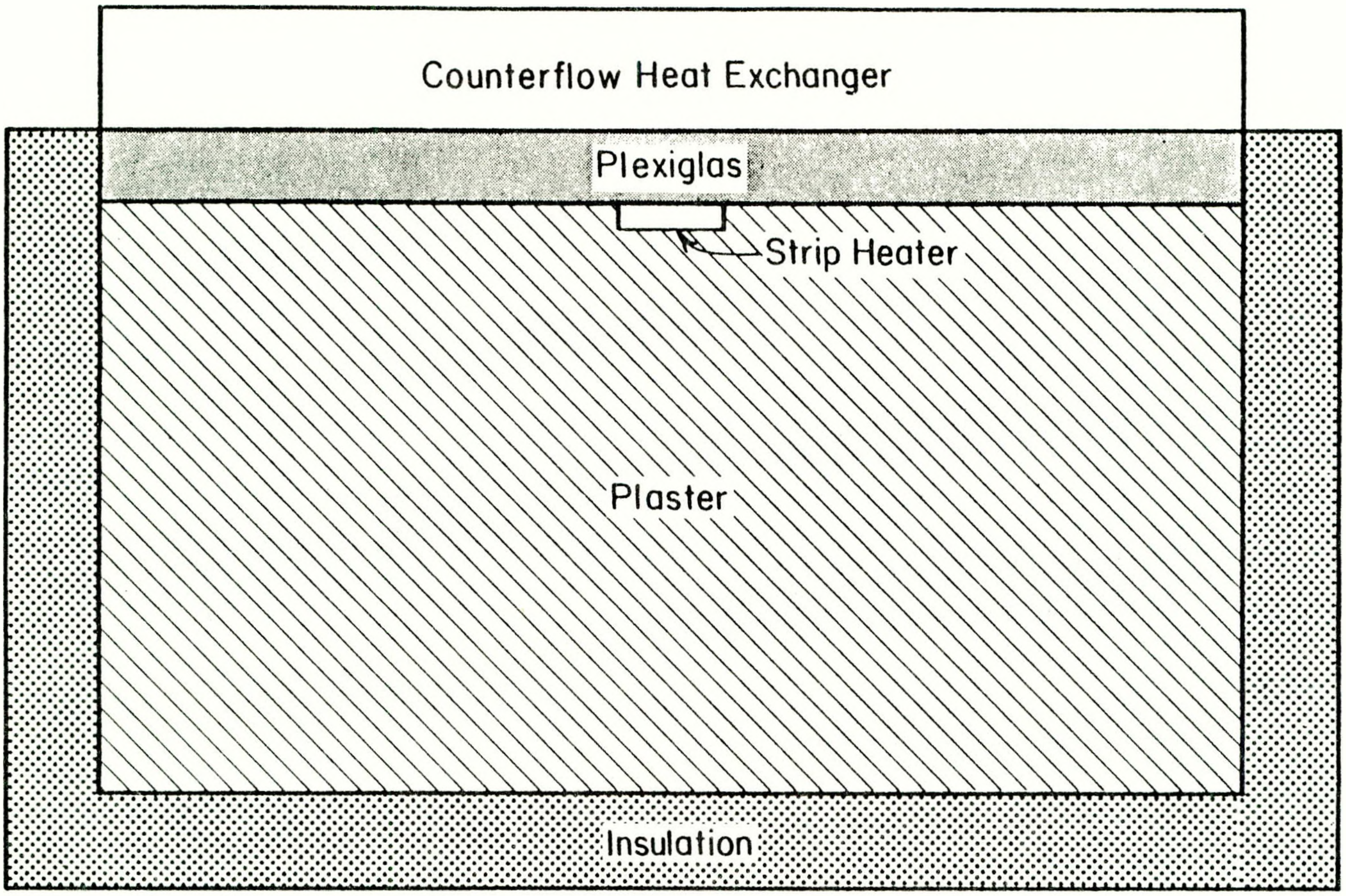

FIGURE 3. SCHEMATIC OF CROSS SECTION OF EXPERIMENTAL APPARATUS

was predicted and a safety factor was applied. This was used as the depth and assuming that the penetration depth was also applicable in the horizontal direction, a length of twice the depth was used.

The HBI method was also used to show that a heater as large as 500 watts may be necessary. For such a large power rating, a mica strip heater was selected. For runs using a lower power rating, a silicone-encased heater will be used since heaters of this type are thinner and can be easily neglected. The power in either case will be controlled with a Variac monitored with a wattmeter.

Thermocouples will be used to measure the temperature at various positions in the apparatus as a function of time. Although the actual number and locations of the thermocouples will depend on the internal configuration of the apparatus, which will vary for each test run, enough thermocouples will be used to measure the leakage of heat through the insulation in addition to determining the actual temperature field due to the heater. Since the test runs will be modeling either a one- or two-dimensional temperature field, the additional thermocouples will validate this assumption. If the leakage is too great, guard heaters will be used. Copper-constantan thermocouples will be used since they are reasonably accurate and compatible with existing instrumentation available in the Heat Transfer Research Laboratory.

Two types of boundary conditions will be modeled at the top surface. These are a constant-temperature boundary condition and a convection boundary condition. To achieve the first boundary condition, an aluminum heat exchanger will be placed in contact with the top surface of the Plexiglas. The heat exchanger will be the counterflow type and will be cooled by a constant-temperature water circulator. The convection boundary condition will be provided by blowing air across the top of the Plexiglas with a fan. The air speed will be measured with a hot-wire anemometer.

Experimental Plan

The first step in the experimental plan will confirm the temperatures predicted by the HBI model. The experiments will be used to validate the temperature rise at the interface between the Plexiglas and plaster by this model and also the usefulness of the concept of the penetration depth. The apparatus will be set up as shown in Figure 4(a), with strip heaters separating the Plexiglas and plaster and the heat exchanger on the top surface.

The next case to be considered will model a two-dimensional temperature field as shown in Figure 4(b). Runs will be made using both the constant temperature and convection boundary conditions.

The third case to be tested will provide a better model of a nuclear waste repository and its far-field region. This setup is shown in Figure 4(c). In this test, the strip heater will be imbedded 1.5 in. (3.81 cm) below the surface of the plaster. Again, both types of thermal boundary conditions will be used.

The final set of runs will consider a finite inclusion in the plaster [see Figure 4(d)]. This case is regarded as the most difficult analytically. The extra block of material will probably be sand in a suitable binder since its thermal properties lie between those of Plexiglas and those of plaster. Both the constant-temperature and convection boundary conditions will be used in this case.

Nomenclature

c	Specific heat, J/kg C
k	Thermal conductivity, W/m-C
ℓ	Layer or sublayer; thickness, meters
q	Heat flux, W/m^2
t	Time, seconds
T	Temperature, C
α	Thermal diffusivity, k/c, m^2/sec
∂	Penetration distance, meters
ρ	Density, kg/m^3

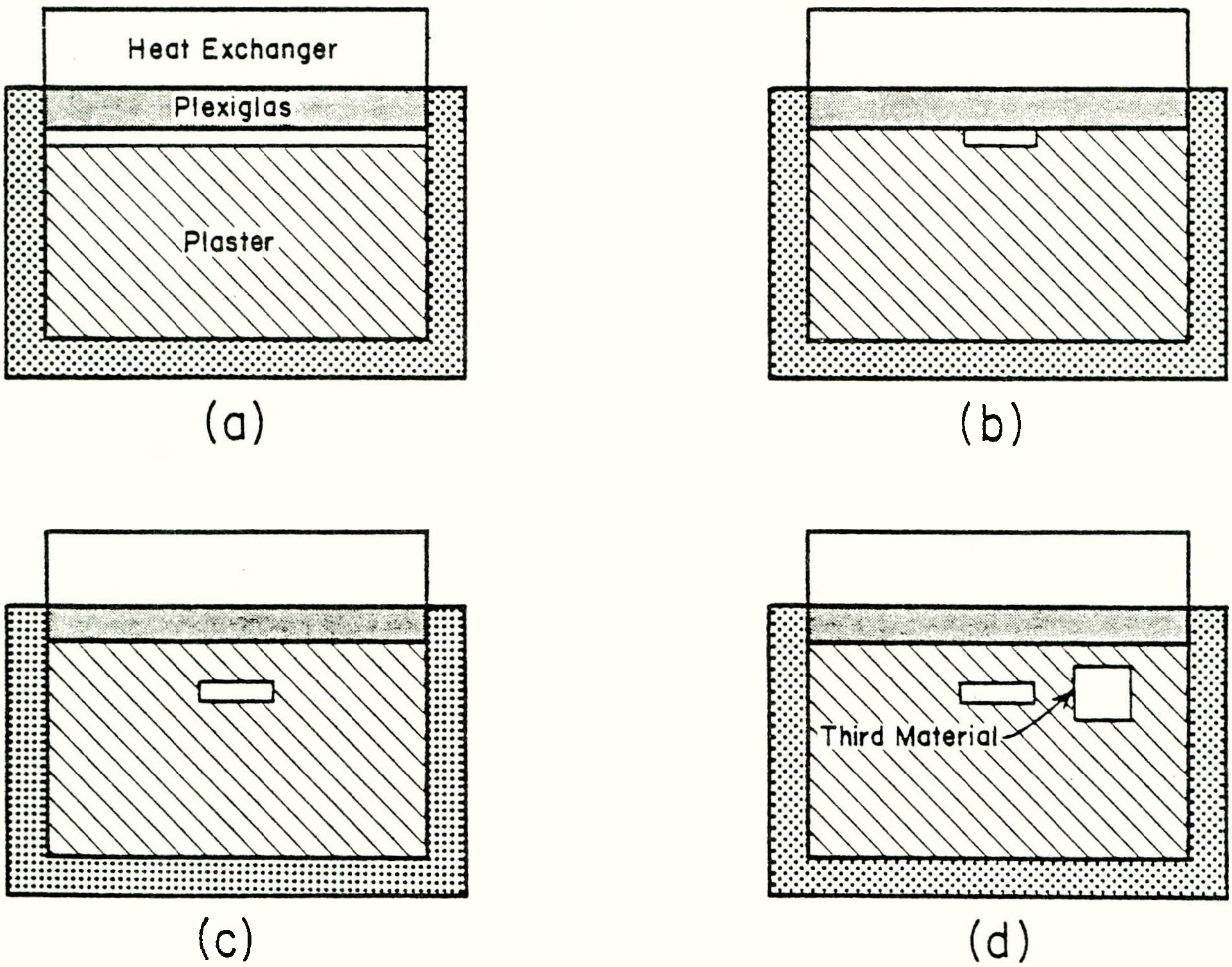

FIGURE 4. PHYSICAL CONFIGURATION FOR PLANNED EXPERIMENTS

Subscripts

1,2	Sublayer number

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WBS 1.1.6

Project: Analysis of Radionuclide Migration in Geologic Media

Principal Investigator: University of California at Berkeley (T. Pigford)

ONWI Project Manager: H. C. Burkholder

Objective

The objective is the development of analytical solutions of various problems that arise in predicting the migration of radionuclides through geologic media.

Activities During the Reporting Period

No progress report was submitted for the period.

WBS 1.1.6

Project: Systematic Comprehensive Evaluation of Performance and Total Effectiveness of Repositories (SCEPTER)

Principal Investigator: INTERA Environmental Consultants, Inc. (R. B. Lantz)

ONWI Project Manager: H. C. Burkholder

Objective

The objective of this program is the integration and development of a technology to evaluate the effectiveness of a nuclear waste isolation system in preventing adverse radiological effects to present and future human beings and their environment.

Progress Reported Previously

INTERA began work on January 2, 1980. First quarter work concentrated on two fundamental areas. These were program planning and defining the needs for the performance assessment technology to be developed and assembled during this project.

Under the program planning phase a draft management plan was submitted in February, 1980, including a milestone schedule and cost plan. A draft Quality Assurance Manual and SCEPTER QA Program Plan were submitted at the end of March.

Under program technology definition, work on developing the technology definition continued and a draft Technology Needs Definition letter report was submitted the first week in April.

Activities During the Reporting Period

Objective

Work began this quarter on reviewing and evaluating technology available for performance assessment of radiological waste disposal. The work will continue through one additional quarter. Initially, work has concentrated on review of the technology developed through past and existing ONWI work.

Procedures

In far-field technology much of the existing work has been performed by Battelle Pacific Northwest Laboratories (PNL) under the old WISAP and present AEGIS programs. During the quarter most of the far-field models (both consequence and scenario) were transferred to INTERA. Many of these models were developed and were operational on small storage computers. Conversion to large, universally available, FORTRAN-compatible machines was initiated and is currently in progress.

For near-field technology, several ONWI contractors are developing and modifying technology. Site visits were initiated and model transfer will begin next quarter.

Results

Far-field consequence models obtained from AEGIS fall into three categories. Two additional models will be obtained from the Geological Survey, and one from Oak Ridge National Laboratory. Operational status on a large-core CDC-175 machine can be summarized as follows:

Models	**Operational Status as of June 30, 1980, percent**
Hydrology	
VTT	—
FE3DGW	70
USGS3D	100
PATHS	—
Nuclide Transport	
GETOUT	100
MMT	100
Dose—Biosphere	
PABLM	100
DACRIN	30
SUBDOSA	30
KRONIC	50
LADTAP	100

The far field scenario model obtained from AEGIS was about 30 percent operational as of the quarter's end.

Conclusions

Most of the model conversions are proceeding as anticipated. The VTT (Variable Thickness Transient) Model has more specificity to the computer system for which it was developed and will take longer for conversion. However, the already operational USGS model provides the same capability for hydrology calculations as the VTT model.

SUMMARY

1.2 PROCESS/EQUIPMENT DEVELOPMENT

The scope of Applied Technology investigations covers In Situ (Field) Testing, Waste Package Design/Testing, Repository Sealing, Monitoring and Test Instrumentation, Repository Equipment, and Equipment/Testing Design Methodologies. The prime objective of this task is to carry out the necessary engineering development work and experimental performance verifications.

A repository waste package design studies program was initiated. The objective of the program is to develop initial designs.

A waste package criteria response studies program was initiated. The objective of this program is to support the development of waste package criteria responses, conformance, and predesign specification studies.

Work has been initiated at the Waterways Experiment Station to evaluate the effect of capillary action in a porous plug where an interface between brine and gas exists. Results of a threshold pressure test suggest that pressures of several hundred psi may be required to force the gas through the sample in the low-permeability regime of the grout and rock. The impact of such an effect must be included in plug design. Test results to date support the acceptability of grouts as plug materials in the short term.

An approach for the equipment reliability and maintainability (RAM) methodology guidebook that is customized to the needs of the NWTS program has been developed. The guidebook will apply a structured RAM program to assure that high availability is realized in an operating repository.

Work on the borehole cement and rock properties study continues. Potential borehole plugging and shaft-sealing materials, including cementitious formulas modified for field tests and new experimental types, are being investigated.

Excavation of the flatjack slots was completed by Terra Tek on the Heated Block Flatjack test in granitic gneiss.

Blast damage assessment technique evaluation and geologic mapping procedures were initiated at the Colorado School of Mines Experimental Mine.

Equipment procurement and installation was initiated for the extended permeability, accelerated borehole closure, and backfill consolidation tests at Avery Island.

Westinghouse produced a preliminary test plan describing a brine migration test to be implemented at the Asse Mine in the FRG.

WBS 1.2.1

Project: Swedish Cooperative Project

Principal Investigator: Lawrence Berkeley Laboratory (W. Stromdahl)

ONWI Project Manager: W. F. Ubbes

Objective

The project objective is to assure long-term containment of potential contaminants during the underground storage of nuclear waste in crystalline rock. Whether or not these conditions are met depends on the coupled interactions of heat flow, fluid flow, and rock mass properties. Lawrence Berkeley Laboratory (LBL), in conjunction with the Swedish Nuclear Fuel Safety Board (KBS), is conducting in situ heater tests, hydrologic tests, and fracture system characterization studies in granite in an iron mine at Stripa, Sweden. Additional support activities include:

(1) Defining the fracture network through the use of borehole camera logging and geophysical testing

(2) Measuring hydrological and material properties of the Stripa granite in the laboratory

(3) Macropermeability studies underground in the ventilation drift

(4) Continued development, improvement, and verification of existing mathematical models

(5) In situ stress measurements through the overcoring and hydrofracturing techniques.

Progress Reported Previously

Previously reported progress includes the completion of the cool-down phase of the heater experiments, the initiation of a systematic test program to check the calibration of instruments that were used during the experiments, an outline of the fracture hydrology field program, and early results from the macropermeability investigations.

Activities During the Reporting Period

HEATER EXPERIMENTS

Activities at Stripa

During this reporting period, recalibration of the various instruments used during the heater tests was continued.

Thermocouples. It was discovered that the resistance temperature device (RTD) which has been used as a standard for calibration of the thermocouples was self-heating; thus it introduced an error in this calibration procedure. Tests were conducted to determine the magnitude of this error and it was found that the maximum deviation from the actual temperature was of the order of 0.5 C. A correction will be applied to the calibration of the thermocouples to account for this error.

Extensometers. Analysis of the data from the recalibration of the extensometers, using a procedure which raised and lowered the head through a total height of 25 mm in steps of 5 mm, revealed that the curve of instrument output as a function of displacement was somewhat nonlinear. This nonlinearity occurred at the ends of the travel and was attributed to the behavior of the direct current differential transformer (DCDT) (Figure 1). It does not affect the interpretation of the data from these instruments since the total movements between anchor points during the heater experiments were limited to a few millimeters and care was taken at the outset of these tests to locate the DCDT at the center of its 25-mm travel.

Thus, analysis of the data from the recalibration tests was restricted to considering the linear portion of the instrument output: displacement curves in the middle of the DCDT range.

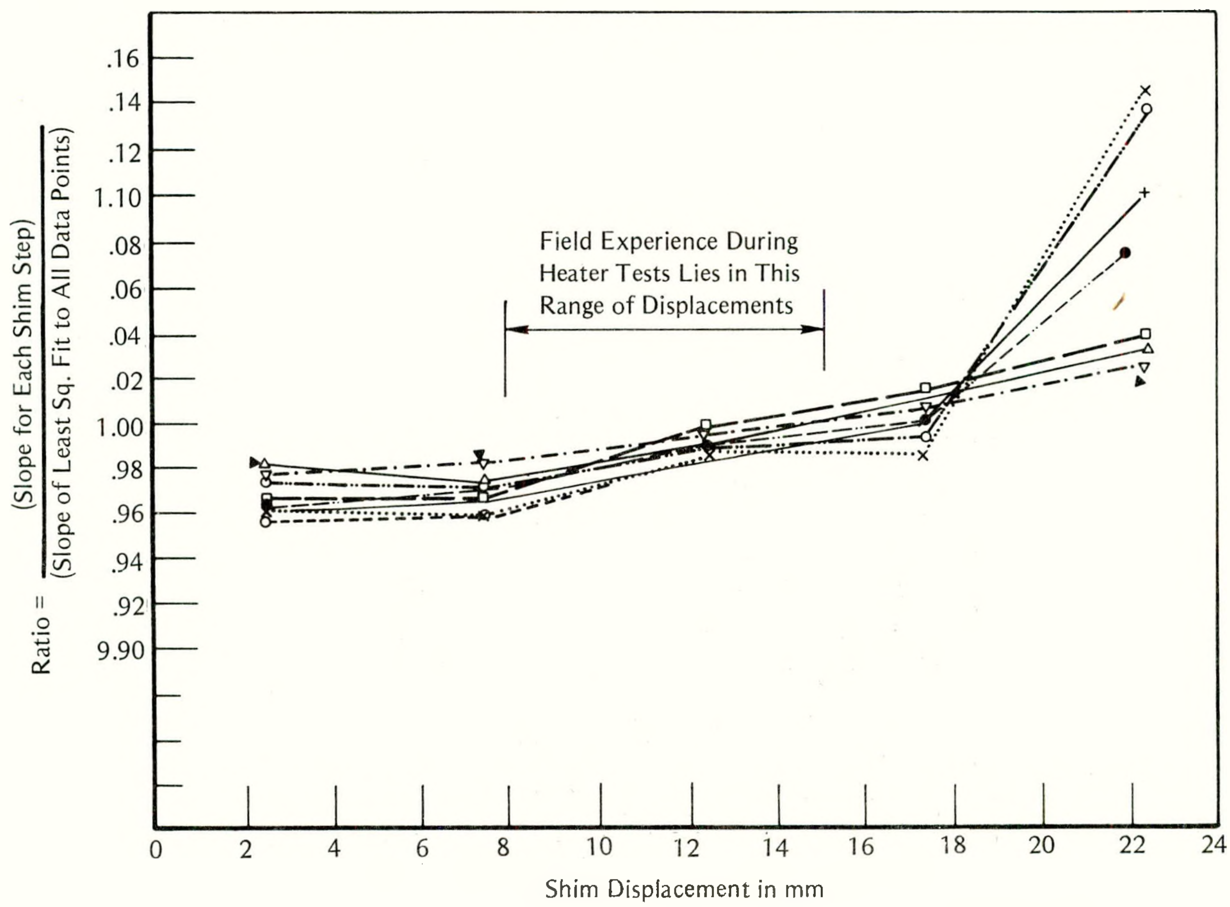


FIGURE 1. RECALIBRATION OF TIME-SCALE EXTENSOMETERS

Pull tests were conducted on individual rods of an extensometer while monitoring the DCDT output. The purpose of these tests was to verify which DCDT output was connected to which anchor. This experiment was conducted on every extensometer rod.

A circuit verification test was conducted on each extensometer DCDT to verify that data logger channels and computer channels were connected to the appropriate sensor and that the output polarity was correct in each case.

Microcalibration, moving the extensometer head by small amounts, of the order of 10 μm, was conducted for a number of these instruments. The purpose of these tests was given in the previous quarterly progress report. The results from these experiments currently are being analyzed.

Stress Gages. Field recalibration of these gages was completed during the previous reporting period. The experimental setup that was used for these tests is illustrated in Figure 2.

Activities at LBL

Laboratory Tests with Extensometer. The first phase of this test program was completed during the reporting period. The primary objective of these tests was to evaluate the effects of rod friction with this instrument on the instrument performance. The parameters that were investigated included:

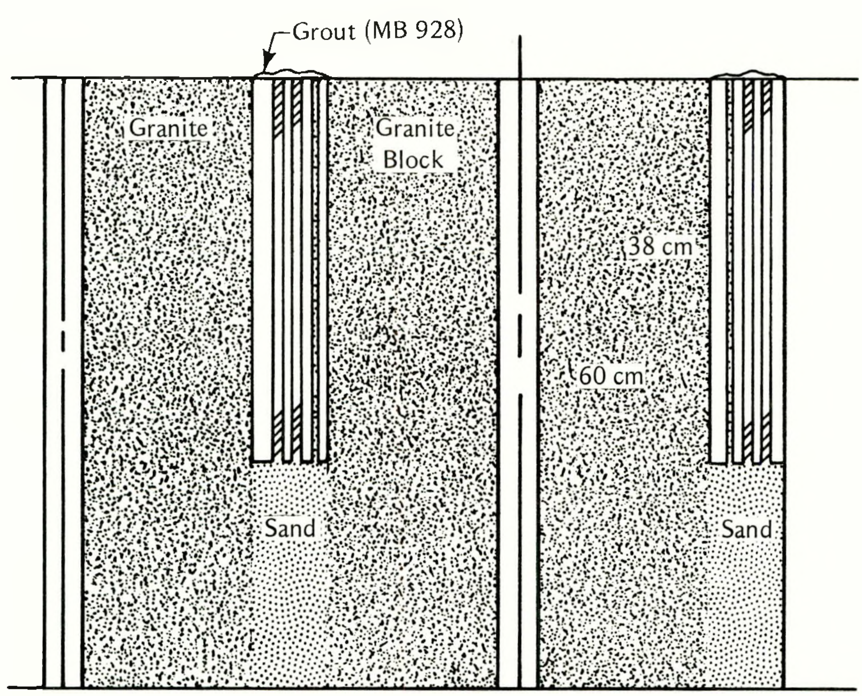


FIGURE 2. IN SITU BLOCK TEST FOR RECALIBRATION OF USBM AND IRAD GAGES

(1) Effect of conduit that was used with these instruments at Stripa to contain the grout

(2) Effect of anchor misalignment

(3) Effect of loading on the conduit

(4) Effect of rod position within the conduit

(5) Effect of vibrating the anchors and/or the head

(6) Effect of moving one rod upon the response of adjacent rods

(7) Effect of calibration by shimming the head as opposed to moving the rod anchor

(8) Effect of changing the input voltage to the DCDT sensor.

It is planned to modify the apparatus and to continue these experiments with a second phase. The objectives of this phase will be to:

(1) Investigate the instrument response when the anchors are moved by only small amounts

(2) Conduct tests moving more than one anchor

(3) Investigate the instrument response when the head is moved by only small amounts

(4) Conduct tests with the instrument in the vertical as well as the horizontal position.

Stress Gages. Four questions concerning the reliability of the data obtained using stress meters had been raised during the heater experiments and the field recalibration tests:

(1) Are the results of instrument output as a function of the applied rock stress repeatable when the gage is reset in a hole with the same initial period charge at installation?

(2) How is the instrument output affected by changing the initial period of the gage at installation?

(3) What is the scatter of the slopes of the load versus $(\text{Period})^{-2}$ curves for the gages used and recovered from the heater experiments?

(4) Was the temperature correction applied to the output from these gages during the heater tests adequate?

Of the 30 gages installed at Stripa, 27 were recovered in a working condition. Laboratory tests have been performed on these gages to answer these questions.

In answer to the first question, it has been found that repeatable results have been obtained, at least for tests with uniaxial loading. It will be necessary to conduct tests with biaxial and triaxial loading to understand this behavior more fully.

In answer to the second question, the gage output is found to vary with the initial setting load. Although the analysis of the data from these experiments is not complete, it is probable that this output varies with setting load in a predictable manner and that therefore it will be possible to interpret the stress results obtained from the heater tests.

To answer the third question, a laboratory calibration of each gage at the setting load at which it was used during the heater tests will be required. These experiments are complete and an analysis of the data is in progress.

The fourth question involves the influence of heat on gage output. This question has not been resolved adequately at this time and will require additional work.

U.S. Bureau of Mines (USBM) Gages. The recalibration work on these gages was conducted at Stripa during the previous reporting period. Activity during the current reporting period has been confined to reconstructing a master file of gage changes with their associated calibration parameters, date and time of change, etc. This file is necessary for the conversion by the computer of instrument voltages to stress readings.

Preparation of Master Data File. This computer file, together with a report, will be drafted by the end of the next reporting period. Work towards that goal that has been accomplished during this reporting period is as follows: A new computer program converting instrument voltages into temperatures, displacements, stresses, and other engineering outputs has been written. This program has been written for the LBL, CDC computer and will be used to reprocess all of the so-called "raw data" tapes obtained from the heater tests. It is a revised version of the original program that was written for the MODCOMP computer in Sweden and it removes a number of the defects that were present in the original program; these include:

- Correction for the offsets and other errors that were introduced into the data file when the wide-range boards were replaced during the heater tests
- Application of a sign error correction for the thermal expansion of the extensometer rods
- An improvement of the numerical method in correcting for the thermal expansion of the extensometer rods.

In addition, decoding and sorting the raw data tapes for processing with this new program have been completed.

FRACTURE HYDROLOGY

Computer processing of the borehole injection test data continued. To date all of the 2-meter test data from boreholes R3, R4, R5, R8, R9, R10, S1, S2, HG3, HG4, and SBH-1 have been processed. Work is progressing on the single-fracture test data from all of the boreholes and the 4-meter data from R1, R2, R6, and R7. Work has also started on the data from SBH-3.

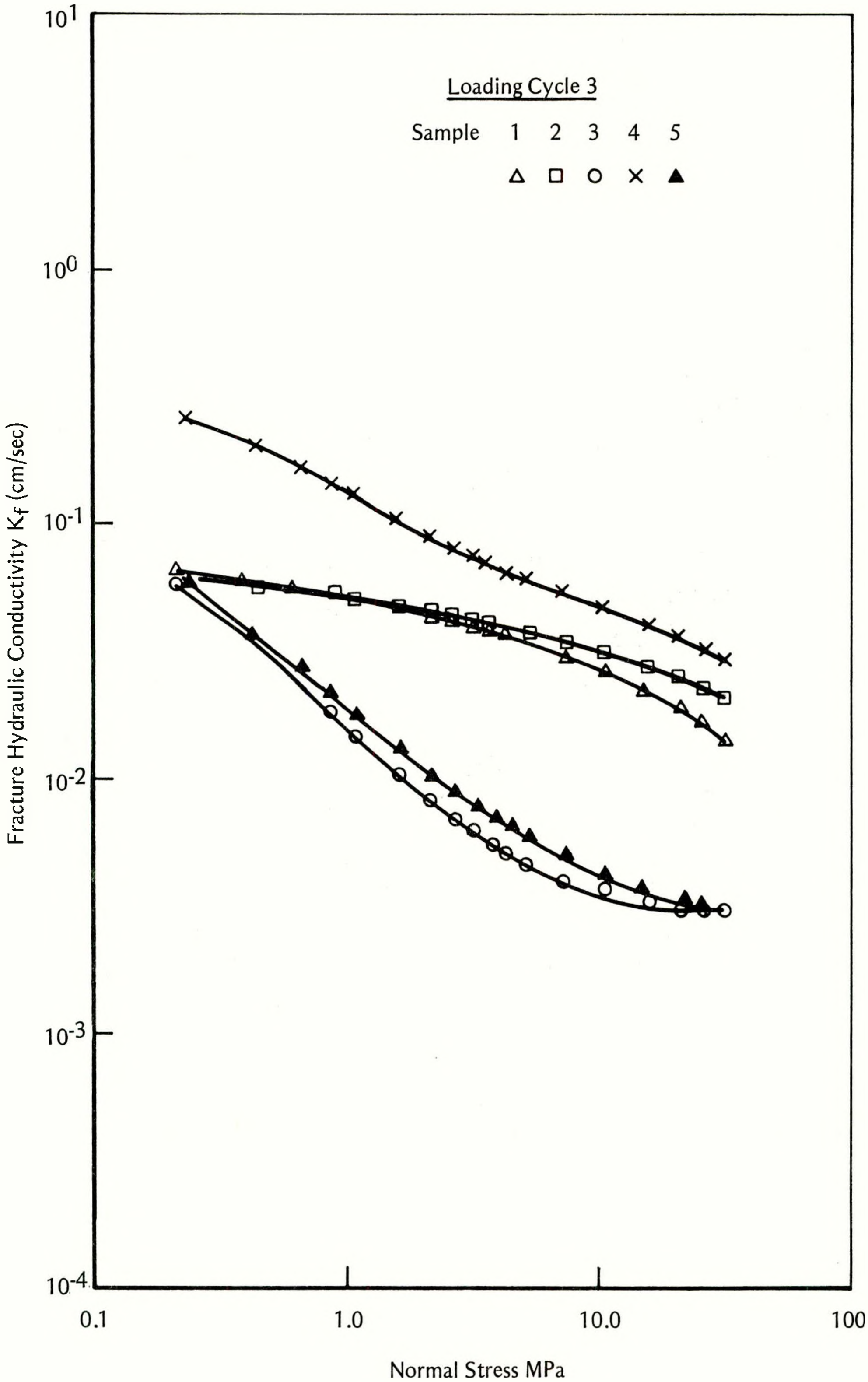


FIGURE 3. LOG-LOG PLOTS OF HYDRAULIC CONDUCTIVITY VERSUS STRESS – THIRD LOADING CYCLE

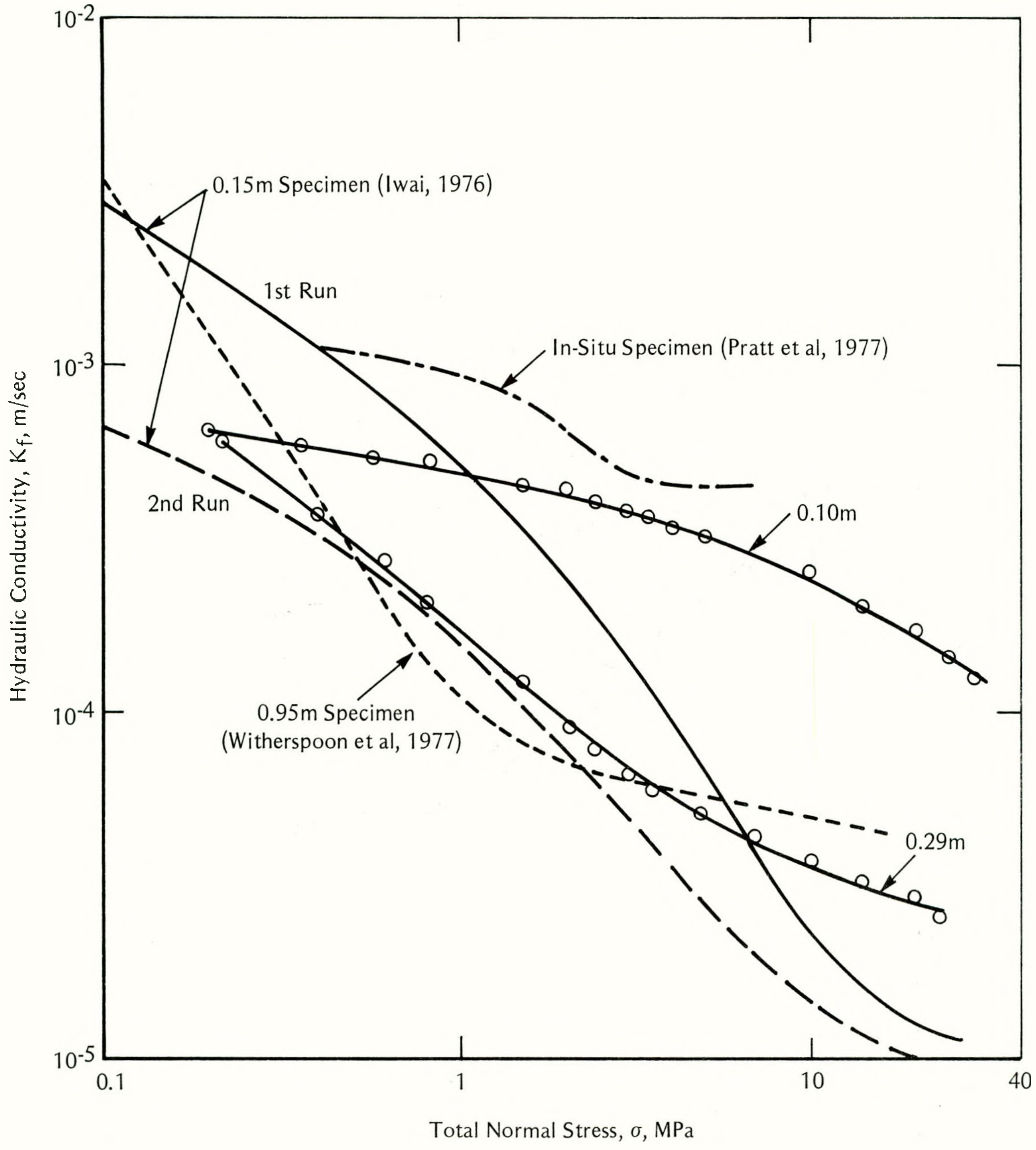


FIGURE 4. HYDRAULIC CONDUCTIVITY VERSUS STRESS – COMPARATIVE RESULTS

A draft of the report dealing with the effects of scale or sample size on fracture permeability is nearing completion. Figure 3 shows the log-log plots of hydraulic conductivity versus stress for the third loading cycle for all five samples from the same natural fracture plane that was tested. Results show that for the range of normal stresses tested, the hydraulic conductivity of the smaller sample remained greater than that of the larger sample. Earlier results, however, have indicated that a smaller sample might be expected to have a lower hydraulic conductivity than a larger sample at the upper end of the stress range tested, as shown in Figure 4. Work is progressing on analyzing the relationships between flow rate and aperture data.

The pressure-pulse laboratory study is close to completion. A review of the data showed that pressure pulse tests on single fractures gave straight-line plots of decay pressure versus decay time (Figure 5) and thus are amenable to the Brace, Walsh, and Frangos (1968) straight-line method of analysis. Figure 5 shows clear evidence of compliance effects with the water-filled packers having significantly lower decay pressure-decay time slopes than air-filled packers or the rigid steel plug seals. Also the pressure-pulse (transient) tests consistently gave lower permeability values than steady-state tests on the same samples.

A draft of the report dealing with the comparison of pressure-pulse and steady-state tests in the HG and R holes at Stripa is about 50 percent complete. Initial data reduction has shown

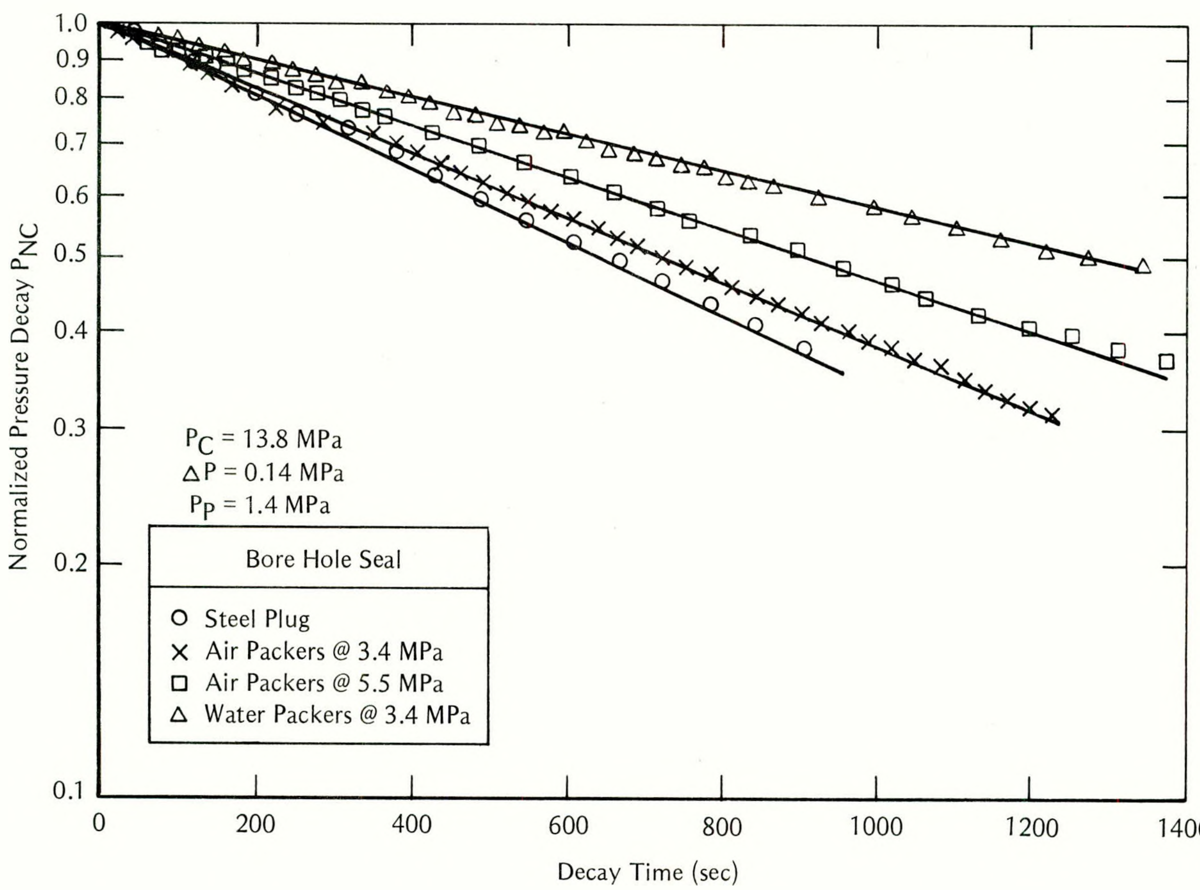


FIGURE 5. SINGLE-FRACTURE GRANITE CYCLE 4

that, in the field situation in which the tests were conducted, for borehole packer tests of multiple fractures there is not a one-to-one correlation between steady-state permeabilities and the time for a pressure pulse to decay in the same borehole packer cavity. This is clearly shown in Figure 6, where the steady-state hydraulic conductivities for each cavity are identified along with the pressure-pulse decay curves for the same cavity.

MACROPERMEABILITY INVESTIGATIONS

Following the conclusion of the ambient temperature test in late March, a saline tracer was injected into zone 6 of borehole HG3. Monitoring for tracer movement is accomplished by electrodes installed in all zones of the HG holes to measure the conductance of the water. The purpose of the test is to determine the direction of movement of the tracer under the hydraulic gradients established around the drift. It is also of interest to see whether the tracer could easily bypass the packers in the borehole, indicating a poor packer seal. Twenty liters of a 50,000 mg/l NaCl solution was cycled through zone 6 on 31 March, using the dual tube system that had been installed for that purpose. At the end of the injection period, tracer concentration in the zone was about 80 percent of feed concentration. As of the end of June, no movement of the tracer had been detected in any other zone.

Heater power was increased on 2 April to raise the room temperature to 30 C for the second constant-temperature run. The target room temperature was reached by 16 April, but the increase in temperature was accompanied by a decrease in net water inflow into the room of about 16 percent, dropping from about 50 ml/min under the ambient temperature run to about 42 ml/min at 30 C. This run was interrupted from 22 April to 13 May to modify the equipment to permit a more precise monitoring of net water inflow. The heater unit was modified to recirculate air within the room, and the air-flow monitor was modified to measure considerably lower air-flow rates. Calibration accuracy was also improved by replacing the 380-mm-diameter calibration duct with a 165-mm-diameter duct. Measurements recommenced for the 30 C run on 14 May and were ended on 11 June.

Net water inflow measurements are shown in Figure 7 for the period 1 February through mid-July. It can be seen that, following equipment modifications, the water inflow again stabilized at about 42 ml/min. Water-pressure measurements at the end of the 30 C run are shown in Figures 8 and 9; these have been plotted to permit direct comparison with the pressure data at the end of the ambient temperature run presented previously. Pressures were observed to increase in nearly all zones in a manner which strongly suggests that the observed decrease in net water inflow with increasing room temperature was caused by a decrease in the hydraulic conductivity of a "skin" of rock less than 2½-meters thick surrounding the drift.

Figure 10 shows the R-hole pressure data for the ambient test plotted as head of water against the log of radial distance away from the drift. On such a plot, purely radial, porous-media-type flow will appear as a straight line. These, with correlation coefficients on the order of 0.9 or better, are shown as dashed lines in Figure 10. The weighted average of all pressure data plots very well as a straight line, with a correlation coefficient of 0.98. Assuming that 80 percent of the observed 50-ml/min net water inflow occurred as radial flow (as determined from a Fourier analysis of total inflow), the average hydraulic conductivity of the monitored rock mass is about 1.0×10^{-10} m/sec.

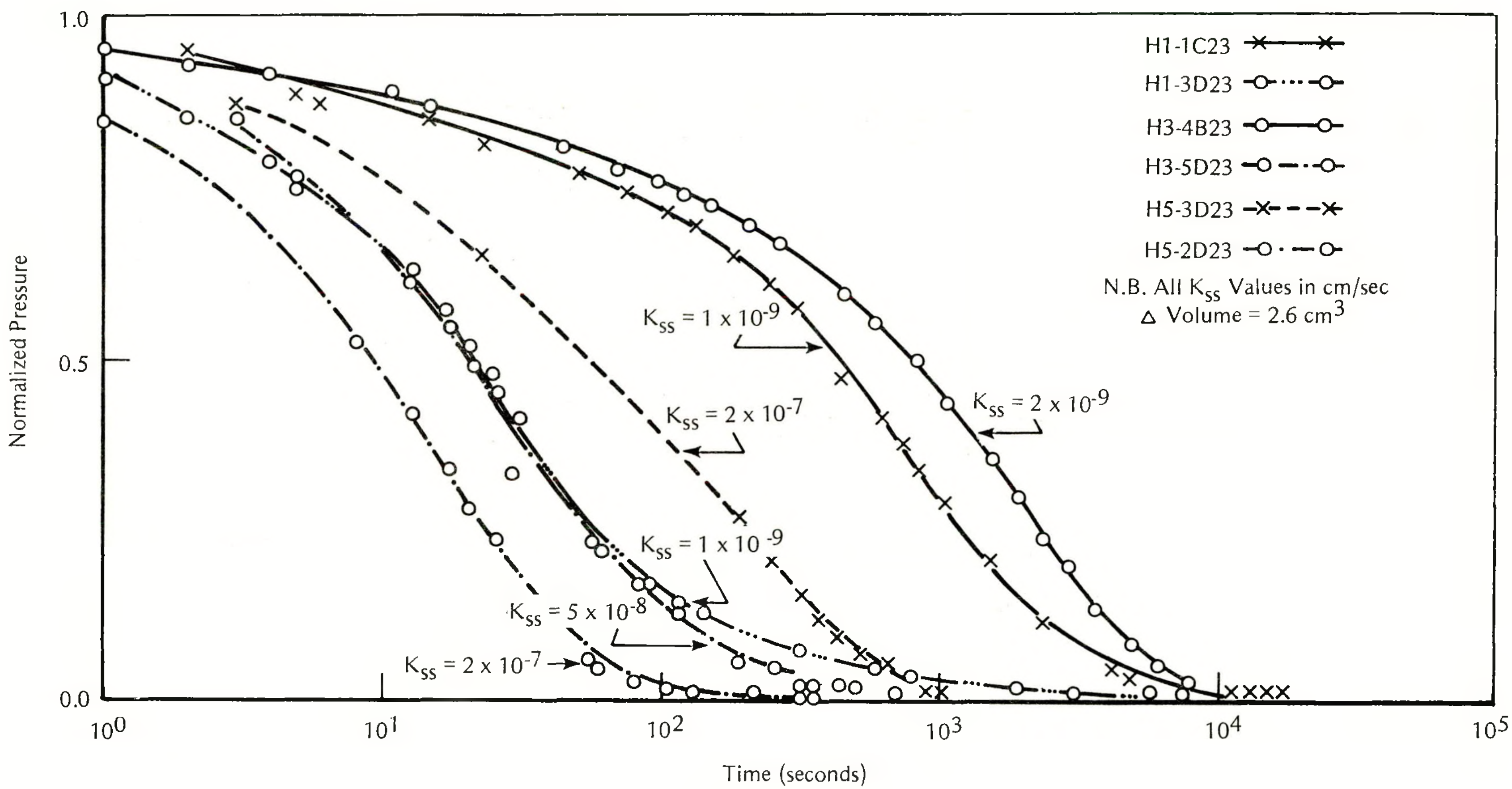


FIGURE 6. STEADY-STATE HYDRAULIC CONDUCTIVITIES AND PRESSURE-PULSE DECAY CURVES

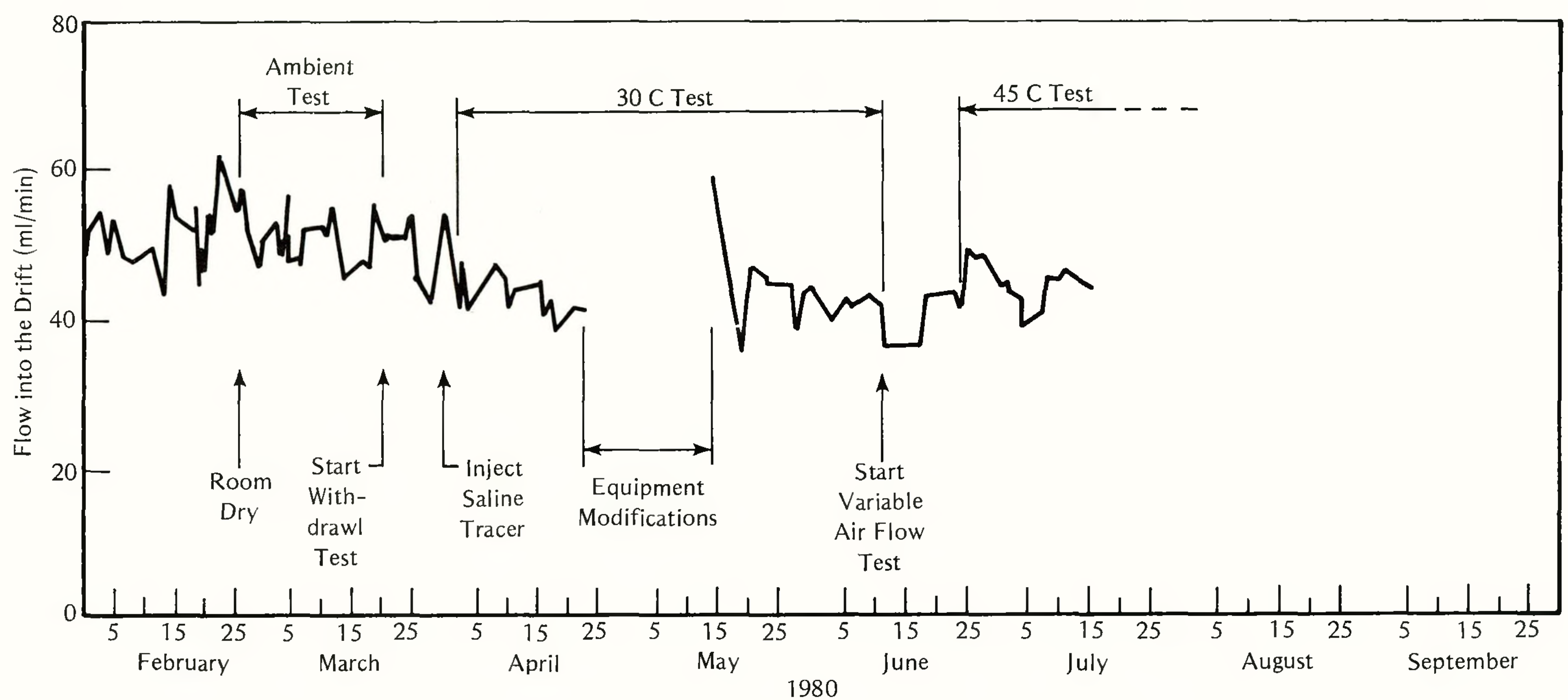


FIGURE 7. NET MOISTURE PICKUP BY VENTILATION SYSTEM FOR PERIOD 1 FEBRUARY THROUGH 15 JULY

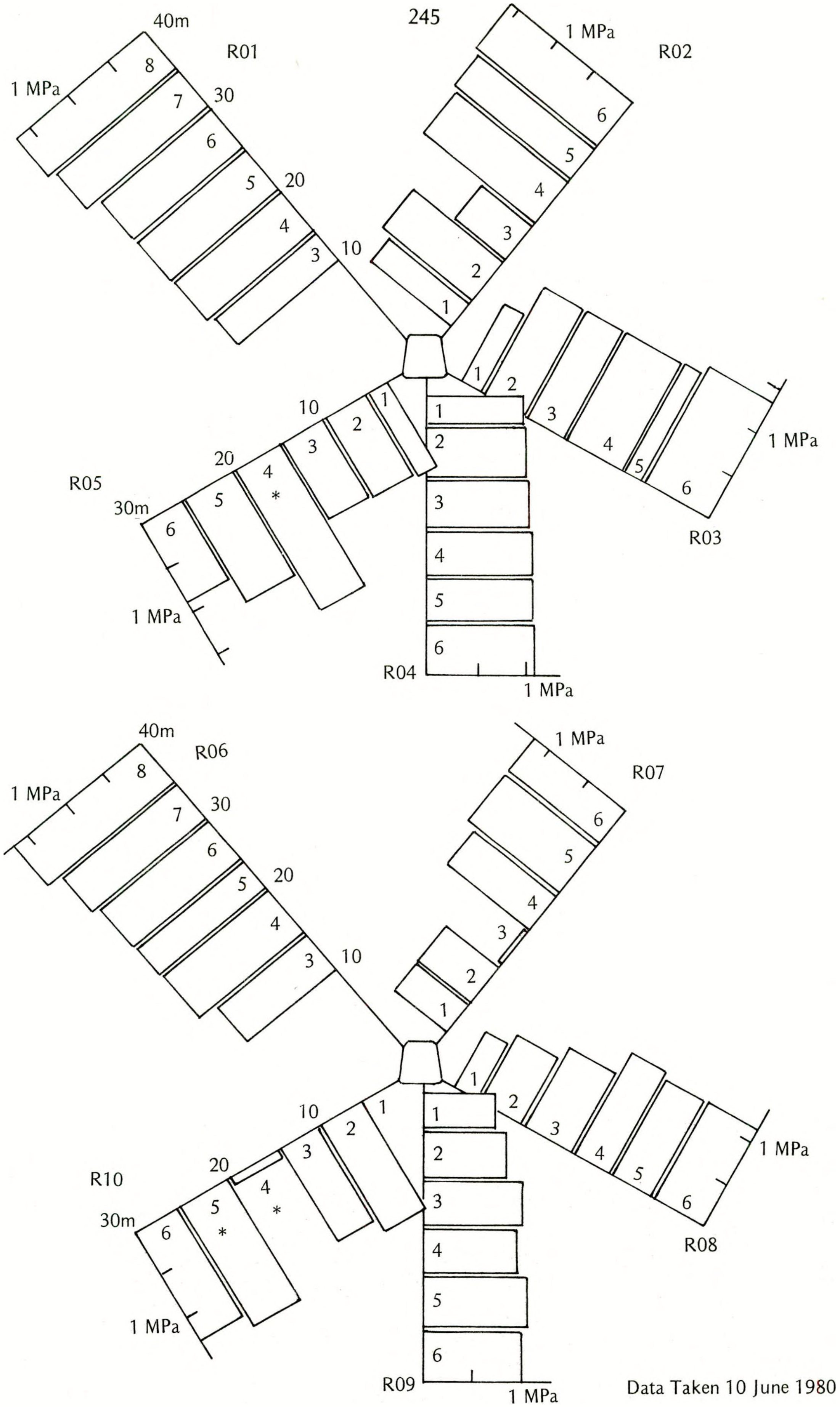
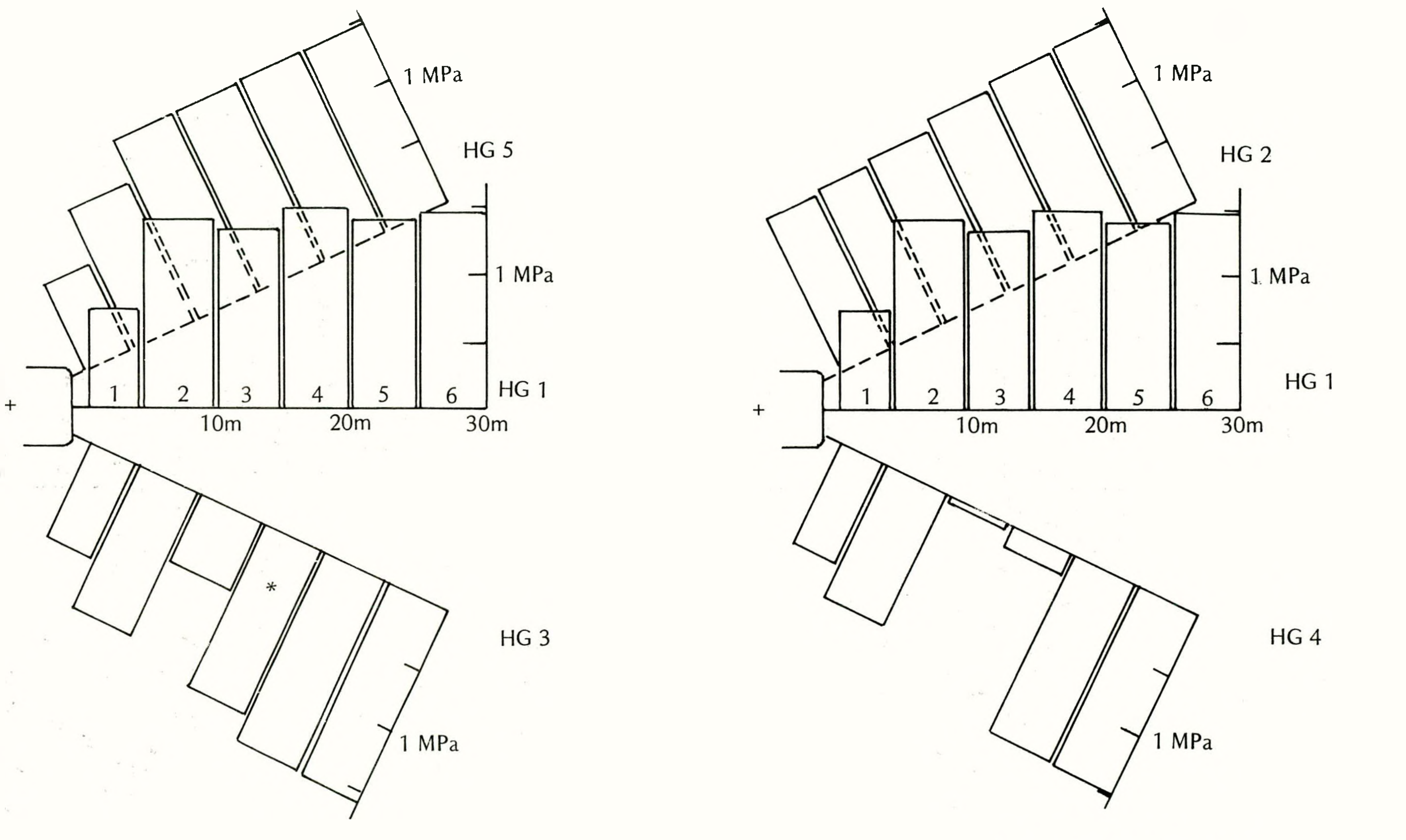


FIGURE 8. PRESSURE DISTRIBUTION IN THE R-HOLES AT THE END OF THE 30 C TEMPERATURE EXPERIMENT



Data Taken 10 June 1980

FIGURE 9. PRESSURE DISTRIBUTION IN THE HG-HOLES AT THE END OF THE 30 C TEMPERATURE EXPERIMENT

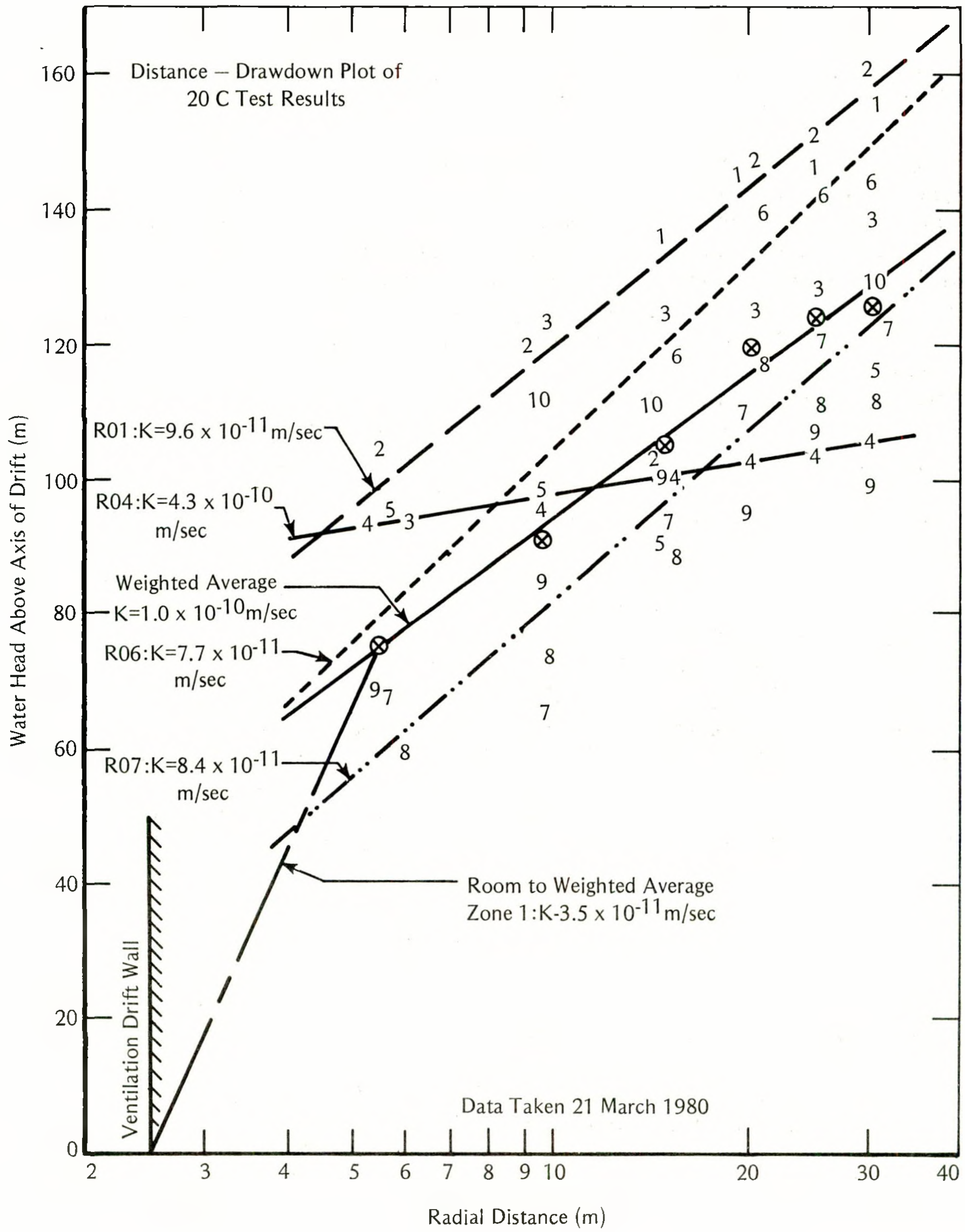


FIGURE 10. DISTANCE-DRAWDOWN PLOT OF PRESSURE DATA AT END OF 20 C TEMPERATURE EXPERIMENT

It may be noted in Figure 10 that the weighted average line and the individual borehole lines would indicate a water head significantly higher than the actual head if projected to the ventilation drift wall. This indicates that a skin of lower permeability rock exists between the drift wall and the zone 1 measurements. If this skin is assumed to be homogeneous and about 2½-meters thick, its hydraulic conductivity would be about 3.5×10^{-11} m/sec, or about one-third of the average conductivity of the rock mass. If the skin were thinner, its conductivity would be even smaller.

Figure 11 shows the R-hole pressure data for the 30 C test plotted against the log of radial distance. Comparison with Figure 10 indicates that pressures are generally higher than those for the ambient test, with the greatest increases occurring nearest the drift. These pressures reacted in a manner which tends to compensate for the observed drop in net water inflow, such that the computed rock mass permeability tends to remain stable. On the basis of the weighted average values of all pressure data and an observed net water inflow of 42 ml/min, the computed rock mass hydraulic conductivity of the 30 C run is 9.4×10^{-11} m/sec. Thus, although the drop in observed inflow was on the order of 16 percent, the compensating increase in water pressure resulted in a drop in computed hydraulic conductivity of only 6 percent. This was interpreted to indicate that the conductivity of the rock mass remained essentially unchanged, while the conductivity of the skin around the drift decreased. It should be noted, however, that the above data and interpretations are all considered to be preliminary, and may be changed when the complete experimental results become available.

The reasons for the existence of the apparent skin of lower permeability rock around the drift and for its change in hydraulic conductivity as a function of room temperatures are not known but these are probably due to thermal expansion of the rock and/or chemical precipitation left in the rock from the evaporating water. The supposition that evaporation is occurring within the rock mass rather than only on its surface was verified by a series of short experiments with varying air-flow rates and temperatures conducted in late June. Because of the potential importance of this skin effect to nuclear waste disposal, an agreement was reached between LBL and ONWI to extend the experiment an additional 3 months to permit a third test at 45 C and a cooldown test to ambient conditions. The 45 C test was started on 24 June and by the end of the month room temperature had increased to 39 C.

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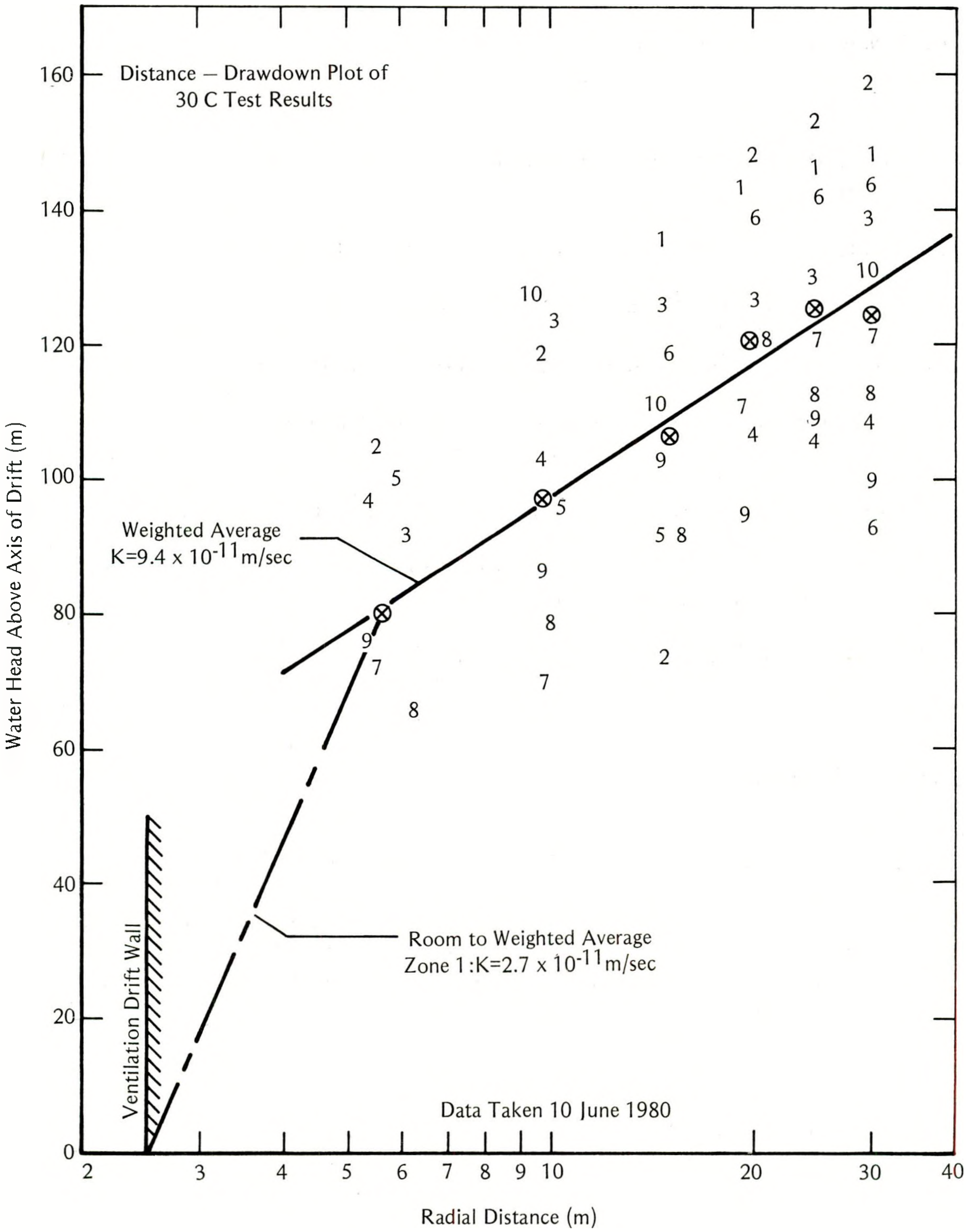


FIGURE 11. DISTANCE-DRAWDOWN PLOT OF PRESSURE DATA AT END OF 30 C TEMPERATURE EXPERIMENT

WBS 1.2.1

Project: Long-Term Monitoring and Analysis of the Avery Island Heater Experiments

Principal Investigator: RE/SPEC, Inc. (L. L. Van Sambeek)

ONWI Project Manager: R. A. Robinson

Objective

The objective of the Avery Island in situ heater tests is to provide quantitative data that can be used to evaluate whether:

- Bedded and domal salt will behave similarly in response to heating
- Laboratory-determined material properties adequately represent in situ properties
- Numerical analysis methods can adequately predict in situ effects
- The present understanding of salt and sleeve/waste canister interaction concerning corrosion, retrievability, and emplacement is representative of actual occurrence.

The objectives of the Avery Island in situ brine movement experiments are to:

- Conduct in situ, exploratory, or scoping experiments to examine both natural and synthetic brine movements in Avery Island salt
- Develop experimental methods for conducting more sophisticated brine migration experiments.

Progress Reported Previously

RE/SPEC has installed three in situ heater tests in the Avery Island salt mine. The design and fabrication/procurements for the heater tests were performed during FY 77 by Oak Ridge National Laboratory. The heater tests were installed beginning in January, 1978. The tests were in operation by 1 June 1978. The design of the brine movement experiments began in February, 1979; the experiments were installed during the summer of 1979 and were in operation by 1 October 1979. Specifications and designs for the additional studies have been developed and the installations are being made at this time. The duration of the additional studies will span the remainder of this fiscal year and part of FY 81.

Activities During the Reporting Period

OBJECTIVES

The emphasis during the quarter was to initiate the installation of the accelerated borehole closure tests and to finalize the engineering test plans for the backfill consolidation test and the post-test evaluation of the brine movement experiment.

PROCEDURES

Heater Tests

The data-gathering activities in the mine continued as scheduled. The concept of what should be included in the post-test evaluations for the Site A and Site B heater tests was developed.

Brine Movement

The engineering test plan was finalized for the post-test evaluation of the Site SB brine movement test. The data-gathering process continued at each of the sites during the quarter. A moisture-collection system has been added to the Site AB (ambient temperature) experiment to determine whether a very rapid collection of brine during early times would also be observed at that site.

Additional Studies

The fabrications, procurements, and preliminary testings of the components were completed for the accelerated borehole closure tests and nearly completed for the backfill consolidation tests. A special neoprene hose for use in the extended permeability measurements was received. The hose will be used in the construction of improved packers. The large (in excess of 1 cubic meter) blocks of salt for the South Dakota School of Mines and Technology have been delivered for finishing. These blocks will be used in a series of uniaxial and biaxial block tests by the School of Mines.

RESULTS

In Situ Heater Tests

The period of heating for the three in situ heater tests exceeds 750 days. Each of the three heater tests has now reached steady-state operating conditions. In that regard, post-test evaluation test plans are being prepared for the eventual decommissioning of the heater tests. The following six points are the prime considerations included in the post-test evaluations:

(a) Obtaining cool-down temperature and displacement data to extend the "test case" for validation of the numerical modeling methods. The apparent lack of agreement between the in situ- and laboratory-determined thermal conductivities can be studied in additional detail using the cool-down temperature data. The displacement data will allow for a determination of the elastic/inelastic proportion of the measured displacement during heating.

(b) Removal of the simulated waste canisters (heater) and sleeves for detailed examination by Oak Ridge National Laboratories, the fabricator of these components. The components will be inspected for corrosion and thermal stress cracking, corrosion in general, and other long-term heating effects.

(c) Retrieval of the corrosion coupons attached to the sleeves for a quantitative determination of the corrosion of six different alloys. Twenty-seven corrosion coupons were attached to each of the sleeves. The coupons will have been exposed to a range of environmental conditions during the period of heating and should provide a reasonable measurement of the degree of corrosion expected in actual repositories.

(d) Inspection of the heater boreholes for changes from their original condition. The heater boreholes were initially large nondescript boreholes in the salt mine floor. Nothing unusual was noted concerning the condition of the salt after drilling the boreholes. The walls were smooth and readily reflected a light shown onto them. It is expected that the heater borehole wall at Site A will now be crusted over with some form of recrystallized salt. This salt will be sampled and inspected to determine the possible mechanisms for its emplacement process. The borehole wall at Site B is not expected to be significantly changed. The bottom of the heater borehole at Site A was filled with dry sand to a depth of about 8 inches prior to insertion of the sleeve. This sand will be recovered and analyzed for foreign compositions. Some portion of the heater borehole wall will be overcored to provide a sample of the salt for radial-distance-dependent inspections and analyses. Particular attention will be devoted to that portion of salt immediately above the heater where recrystallization occurred and to the salt at the midheight of the heater where the highest temperature and gradients occurred.

(e) Recovery of the instrumentation used in the heater tests. The locations, orientations, and calibration of the instrumentation will be checked as appropriate. If any deviations are noted, these deviations will be considered in the final data analysis for the heater tests. Inspection of the physical condition of the instrumentation will be made and probable causes of failure determined (where appropriate) to judge the long-term suitability of the instrumentation in a salt environment.

(f) Collection of representative samples of salt at various radial distances and depths for comparison of mechanical, chemical, and petrographic characteristics with those of the unheated salt samples procured during installation. Some of the samples would be characterized during the post-test evaluation; others would be archived for future reference work.

Brine Movement Studies

An engineering test plan covering the post-test evaluation of the Site SB brine movement experiment was prepared during the quarter. The post-test evaluation is confined to the Site SB experiment because of the presence of the synthetic brine in this test. During the post-test evaluation, the heater borehole and two of the boreholes that contained synthetic brine will be overcored. The overcore will be inspected for evidence of movement of the tagged brine from the brine boreholes. Other aspects of the post-test evaluation include:

(a) Recovery of the synthetic tagged brine from the brine boreholes

(b) Permeability testing of the brine boreholes for comparison of results with preheating permeabilities

(c) Recovery of the heaters and instrumentation for inspection and possible characterization of corrosion effects

(d) Recovery of precipitate material found in the heater, brine, or thermocouple boreholes which might be indicative of brine movement and evaporation.

The post-test evaluation of the brine movement experiments was confined to Site SB because of the presence of the tagged synthetic brine. The Site NB test will be continued for an indefinite period of time to obtain additional data. The primary measurement being performed in the brine movement tests is the weighing of moisture in the heater boreholes. The cumulative amount of brine collected in each of the three tests is plotted in Figure 1. As shown, the collection was started after about 100 days of heating at Sites NB and SB and 200 days after sealing the Site AB test borehole (Site AB is not heated and consists merely of a borehole configuration identical to that of the other two tests). As reported previously the amount of brine collected at both Site NB and Site SB was quite significant during the first 50 days of the collection period. After this early period, the collection rate reduced substantially

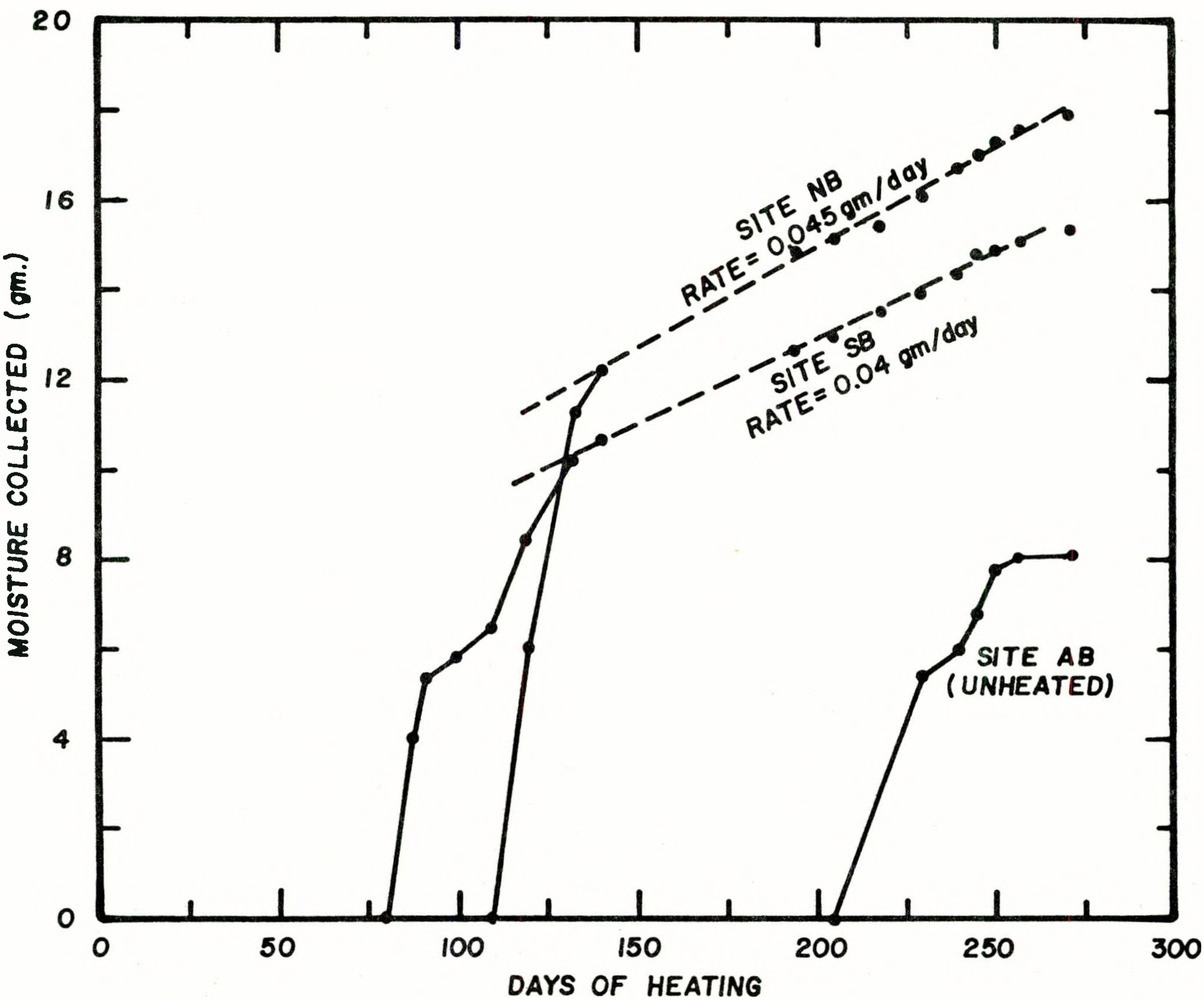


FIGURE 1. CUMULATIVE MOISTURE COLLECTED DURING THE OPERATION OF THE BRINE MOVEMENT EXPERIMENTS

and became nearly constant. A similar pattern has been observed at Site AB for the first 50 days. This rapid pickup of moisture has been attributed to removal of the residual moisture present on the borehole walls and the sleeve of the heater and included in the air when the heater borehole was sealed. If this explanation is correct, the cumulative moisture collection plot for Site AB should eventually level off to a collection rate approaching zero.

The collection rates currently being experienced at Sites NB and SB are in virtual agreement with the inflow rate which would be obtained using a method for predicting inflow into a borehole containing a heat source. In the prediction, it is necessary to know the fractional volume of brine present in the salt; if a fractional volume of 0.19 to 0.21 percent is used, the predicted and measured collection rates are in agreement for Sites SB and NB, respectively. The difference between these fractional volumes is insignificant and within the bounds of an assumed moisture content of 0.1 percent (by weight) for the Avery Island salt. The Site NB test will continue for an indefinite period of heating to provide additional moisture collection data and to see whether the present trends are sustained.

Additional Studies

Accelerated Borehole Closure Studies. The drilling to create the 1-meter-diameter core for these studies was performed without major difficulty. The ambient borehole closure test, which consists of measuring the closure of a 0.2-meter-diameter borehole drilled into the floor but without flatjack loading, has been installed and the closure of the borehole is being measured. The measurements have not been made for a sufficient length of time to allow the presentation of borehole closure data or to establish a rate of closure.

Backfill Consolidation. Two backfill consolidation tests will be performed at Avery Island. The tests will be similar to the accelerated borehole closure tests. Appropriate modifications in the instrumentation will allow for the measurement of borehole closure in a borehole filled with crushed salt (backfill). The backfilled borehole will be included in a 1-meter-diameter core surrounded by flatjacks. The operating pressure of the flatjacks will be 14.8 MPa. One of the tests will be operated at ambient temperature (27 C); for the other test the borehole will be heated to 60 C using electrical heaters incorporated in the flatjacks. The crushed salt used for backfill will be sieved using a No. 6 screen (3.38 mm). The instrumentation in the borehole will include four displacement transducers to measure the borehole closure and two earth pressure cells to measure the consolidation stress developed in the backfill.

If the backfill was not present in the borehole, closures of about 8 mm and 24 mm would be expected for the ambient temperature and heated tests, respectively. The backfill will, however, provide some resistance to closure because of the consolidation stress that develops. The magnitude of this resistance is presently unknown. A suite of laboratory tests will be performed to develop an estimate of the relationship between the consolidation stress and volumetric strain. This relationship will then be used in a thermo-viscoelastic finite element analysis to predict the reduction in borehole closure due to the presence of backfill. The tests conducted in the field will provide a test case for judging the suitability of the laboratory-determined relationship. It is expected that a time-dependent effect may well be observed in the field tests which will not be matched in the laboratory tests. Essentially, the strain rate (consolidation rate) in the laboratory will probably be up to two orders of magnitude higher than the strain rates in the field tests. The consolidation stresses developed in the samples in the laboratory testing will, therefore, probably be higher than those developed in the backfill borehole in the field tests.

WBS 1.2.1

Project: Heated Block Test in Granitic Gneiss

Principal Investigator: Terra Tek, Inc. (M. D. Voegele)

ONWI Project Manager: W. F. Ubbes

Objective

The project objective is to determine the in situ mechanical, thermal, and hydrologic properties of a jointed crystalline rock under conditions of varying temperature and stress.

Progress Reported Previously

The heated flatjack test series program began at Terra Tek, Inc. on July 15, 1979; the fourth quarter of an originally proposed six-quarter project time length has just been completed. To date the work completed remains primarily of a preliminary nature in preparation for the beginning of the actual test series. The activities specifically undertaken by Terra Tek personnel included the specification and subsequent acquisition and calibration of instrumentation to measure stress, strain, displacement, temperature, velocity, and joint permeability coefficients within the rock mass. Basic laboratory tests were performed to determine several intrinsic material properties and some computer modeling was undertaken as an aid to the design of the heaters and instrumentation. In-house manufacturing and testing of flatjacks, pressure/permeability equipment, and ultrasonic equipment were completed. The site for the block test was selected and all instrumentation boreholes were core drilled.

Preliminary in situ property testing consisting of ultrasonic and permeability measurements was completed and several types of instruments were installed to allow observance of the block response as the flatjack slots were excavated.

Activities During the Reporting Period

The original objectives of this quarter's work were to complete the excavation of the flatjack slots, install the flatjacks and all remaining instrumentation, and begin the test sequences of load and temperature cycles. Problems encountered during the flatjack excavation activities caused a reduction in scope of the projected work for this quarter. The revised objective for this quarter was to complete the excavation of the major portion of the flatjack slots.

The excavation of the flatjack slots is perhaps the most crucial aspect of the test series as a whole, since the test depends entirely upon the installation of the flatjacks. The proposed test series cannot be initiated until the flatjack slots are completed.

No technical conclusions are possible at this time since the test series has not yet begun. The progress now being obtained in the slot drilling activities suggests that the test series will be well under way in the upcoming quarter.

WBS 1.2.1

Project: Crystalline Rock Mining Technology

Principal Investigator: Colorado School of Mines (CSM) (W. Hustrulid)

ONWI Project Manager: W. F. Ubbes

Objective

The overall objectives of the program are (a) to develop excavation techniques and site evaluation procedures for application to potential nuclear repositories in hard rock and (b) to establish a hard rock test facility that can be used for future gathering of hard rock geomechanical data, development of techniques and procedures, and instrumentation evaluation.

Progress Reported Previously

The program began on 1 July, 1979. An experimental room was driven in granitic gneiss at the CSM Experimental Mine at Idaho Springs, Colorado, using careful blasting techniques. This room, which is 5 meters wide, 3 meters high, and 30 meters long, was completed in November, 1979. The principal purpose of this task was to develop excavation techniques (drill and blast) that could be used for driving the openings required for a hard rock repository. As the room was driven, the geology was carefully mapped and the rock response was measured. Upon completion of the room, a site at the end of the room was selected for the large heated block test to be carried out by Terra Tek. An instrumentation house has been constructed to house the required data acquisition equipment. Two patterns of diamond drill holes—(a) three holes 30 meters long located parallel to the long axis of the room and (b) rings of holes located at six positions along the length of the room—have been drilled for use in assessing the degree of damage done to the rock surrounding the drift in the process of excavation.

The logging of the core obtained and the borehole wall will provide a visual indication of the fractures. Various geophysical, geotechnical, and hydrologic techniques are being used in these borehole sites to provide other quantitative measures of the nature and extent of the disturbance.

Mapping the structural geology of the experimental room and the surrounding openings continues for the purposes of:

1. Development of techniques that might be used at an actual repository

2. Evaluation of the lengths over which the structural geology can be projected in this type of rock

3. Construction of a 3-D geologic model.

During the previous quarter, the drilling of the blast-damage-assessment holes was completed, logging of the cores was initiated, the structural mapping continued, development of the fracture permeability equipment continued, the NX version of the CSM borehole was finished, and the Terra Tek cross-hole ultrasonic device was tested in the laboratory and the mine.

Activities During the Reporting Period

Objectives

The principal objectives of this reporting period were: (a) development of equipment and procedures for the collection of field data from the experimental room site and (b) the collection of data from the site. Specifically, this included:

- Logging of the cores from the diamond drill holes
- Visual examination of the borehole walls using the South African-developed petroscope
- Development of an air permeability procedure and use of that procedure in the radial holes
- Determination of the stress field using the CSIRO technique
- Use of the Terra Tek ultrasonic system in the radial boreholes
- Continuation of the structural mapping of the experimental room and completion of the computer programs.

Procedures

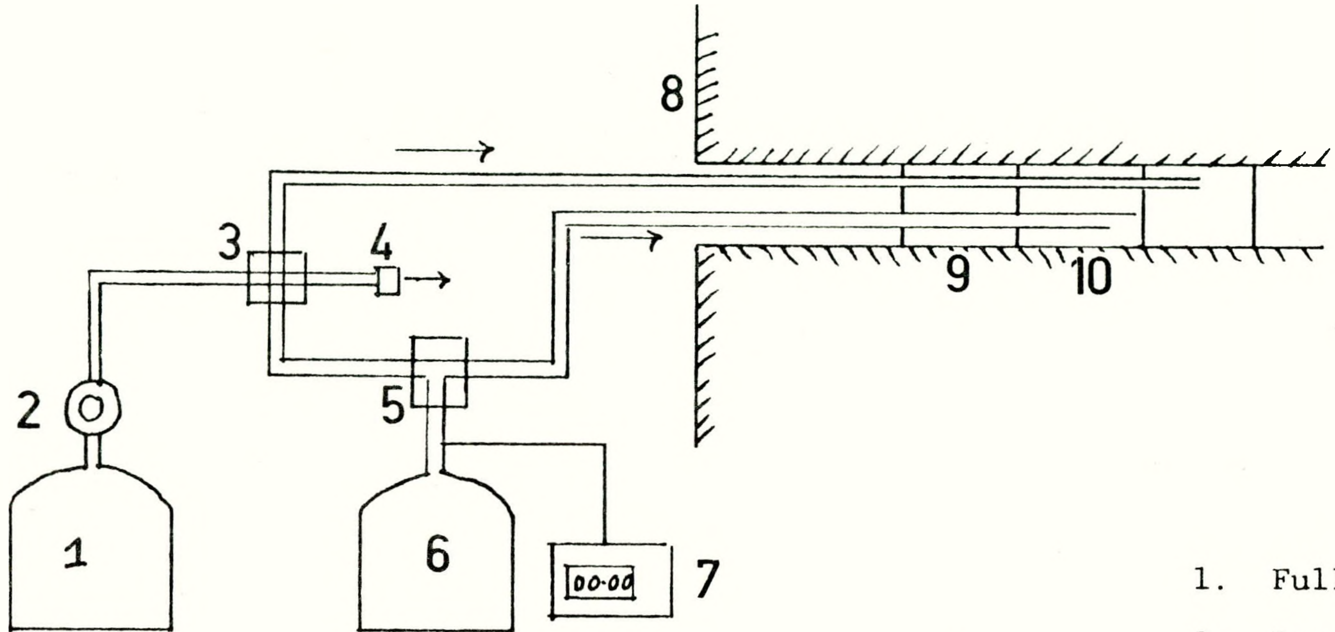
The diamond core (NX diameter) is layed out in special troughs which facilitate the identification of the fractures (both natural and induced), the measurement of their orientation, the description of the surfaces, and the identification of the rock types. These parameters are all entered onto special forms for easy analysis.

The Petroscope is a special optical borescope, developed by the South African Chamber of Mines, which is being lent to the project. It contains a built-in light source and a specially oriented scribed mirror which is viewed using a transit. The width and orientation of the fractures can be measured using this technique. By comparing these results with those from the cores, one can separate the natural and induced (drilling or blasting) fractures.

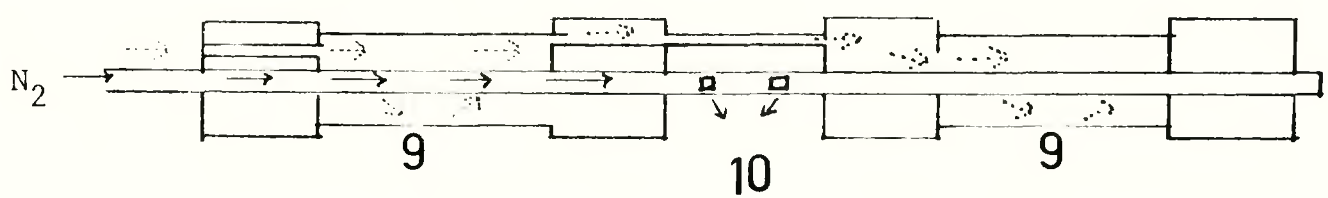
An air permeability borehole technique has been developed for evaluating the relative fracturing as a function of distance away from the opening.

The method is relatively simple, inexpensive, and quick. It is based on the principle that when pressurized air is injected into rock, the rate of air leakage will be greater in fractured or stress-relieved rock than in relatively competent or highly stressed rock.

The apparatus shown in Figure 1 consists of a constant volume container from which nitrogen, N_2, is released under pressure into a sealed measuring section of an NX borehole. The rate of air pressure decay is timed using a stop watch, and pressures after 15, 30, 45, etc., seconds are read from either a digital pressure meter (using a pressure transducer) or from an accurate pressure gage.



a. Air Injection Apparatus



b. Inflatable Packers

FIGURE 1. AIR INJECTION APPARATUS AND INFLATABLE PACKERS

1. Full N_2 Tank
2. Regulator
3. Four-Way Valve
4. To Bleeder
5. Three-Way Valve
6. Empty Tank
7. Digital Pressure Recorder
8. NX - Borehole
9. Inflatable Packer
10. Measuring Section

The fracture index (I) is based on the evaluation of measured pressures after 15, 30, 45, 60, 90, 105, and 120 seconds. A high value of I would indicate a relatively unfractured rock, whereas a low value would indicate the opposite.

The technique takes two operators and the measurement cycle, including refilling the air cylinder, moving the packers, and running two tests in each section, takes approximately 10 minutes.

The CSIRO stress gage and measurement technique was developed in Australia. Although it has been used extensively there, its use outside of Australia has been very limited. The gage itself consists of a thin epoxy cylinder in which nine strain gages at carefully controlled orientations have been embedded. This gage is glued into an NX (1-1/2 inch-diameter) borehole and, after it has set, is overcored using a 6-inch-(OD) bit. Strain readings are taken while overcoring. The core containing the stress gage is inserted into a biaxial chamber and the strain readings from the different gages are read as a function of pressure. In this way, the appropriate elastic constants to be used in data reduction can be obtained and the sensitivity of the gages checked. The three principal stresses and their directions can be calculated using any six of the readings.

The Terra Tek ultrasonic system is being used to evaluate the nature and extent of the blast damage surrounding the room. The device is a pulse-type instrument with a driver in one hole and a receiver in another. Initially, only the P and S wave velocities are being examined. In the future, wave attenuation may also be evaluated. Each transducer (driver/receiver) is split lengthwise so that it can be expanded using a cam device to press against the sides of the borehole. A torque wrench is used to ensure that the recommended value of 21 in-lb is not exceeded. The crystals are driven using a special pulse generator capable of applying a maximum 8,000 volts. The frequency of the crystals is 200 kHz. The received signals are amplified and viewed on a Nicolet digital oscilloscope.

The efforts on the structural geology program were divided into three areas: (1) continued mapping of the walls, floor, and back of the experimental room; (2) development of computer programs for analysis of the collected orientation data; and (3) selection of samples for detailed petrographic and structural analysis.

At present, the mapping of the walls of the room is about 55 percent completed. Mapping of the floor and the back of the experimental room was begun and is presently 20 percent completed. A package of computer-assisted routines for data handling, plotting, and statistical analysis of the collected structural data is being assembled. In general, preexisting, published programs are being used; however, many modifications have been required because of: (a) detection and correction of errors, (b) machine differences, and (c) variations in data inputs required (quadrant, azimuthal, and dip direction, for example).

Twenty-four core samples were chosen for uniaxial compressive strength testing and detailed structural analysis. The compression tests have been completed and ten thin sections are being prepared to examine the reasons for strength variations, structural influence in failure mode, and variations of strength values with rock type.

The three holes drilled parallel to the axis of the experimental room are presently being used for fracture permeability testing. The main injection probe consists of four packers spaced to create three cavities inside the borehole. Each cavity is connected to a pressure transducer through tygon tubing. Water or air is injected into the central chamber in one borehole. After a single characteristic fracture (joint, for example) is located, a test can be performed by injecting fluid in one borehole and observing the pressure along the same fracture in the other two holes.

Monitoring of the pressure in the adjacent two chambers indicates whether: (a) there is any leakage around the packers or (b) there are connected fractures striking parallel to the borehole. Four devices have been designed for flow measurements. These will be used simultaneously to observe and compare the applicability of each system. The outputs from all transducers are fed into a data logger which is interfaced with a cassette tape recorder compatible with the CSM computer.

No standard testing procedure has been adopted at this point. Various methods of testing will be tried until optimum results are obtained.

Results

The stress measurement program using the CSIRO gage has been completed and the computer program for analyzing the results is debugged. The elastic modulii and Poisson's ratios have been determined using a biaxial cell in the field. Very preliminary results suggest that the stress field is as expected from gravity loading.

The air permeability tests of the radial holes has been completed. The data have been entered into a computer data file and the plots should be forthcoming very shortly. One example of the results is given in Figure 2.

Some core logging results are available but these have not been transferred to the master sections. These results also have to be checked.

A report describing the details and testing procedures for fracture hydrology has been prepared. The equipment is operating properly and the preliminary results appear to be excellent. Several zones have been tested using both air and water injections. A wide range of flow rates and pressures can be measured.

The results of the uniaxial compression tests carried out on 24 core samples selected from the NX cores belonging to the six rings in the room suggest that the elastic modulii vary from 5×10^6 to 12×10^6 psi. Poisson's ratios vary from 0.16 to 0.32.

Conclusions

It is too early to make conclusions regarding the nature and extent of blast damage at the present time, although a good deal of information upon which to make such a judgment has and is being assembled.

The other data-gathering programs are well under way and one conclusion that can be made is that the procedures appear to be providing good, reproducible data.

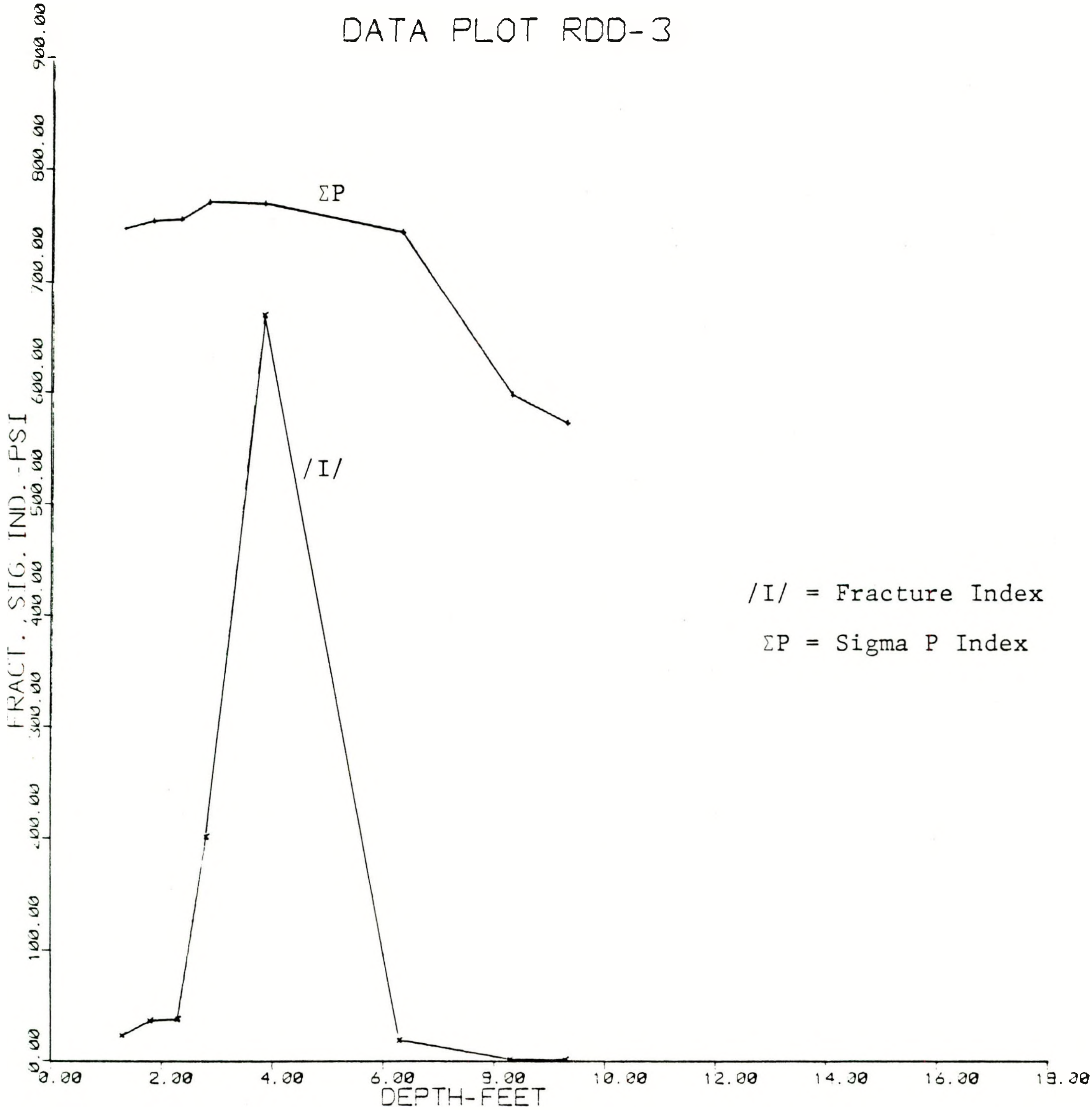


FIGURE 2. EXAMPLE OF FRACTURE INDEX DETERMINATIONS USING AIR INJECTION TECHNIQUE

WBS 1.2.1

Project: Experiment Development to Support Field Testing

Principal Investigators: Westinghouse (F. F. Klein, G. R. Kilp) and D'Appolonia (L. Jarolimek, C. Shubart)

ONWI Project Manager: W. F. Ubbes

Objectives

The principal objectives of the program are to develop test plans for future field tests on the phenomenon of brine migration in salt under simulated nuclear waste repository conditions, and to investigate waste-to-rock interactions under simulated conditions of future degradation.

The first objective is to develop a plan for the post-test evaluation of the brine migration test being conducted under a separate contract in the Avery Island salt dome.

Progress Reported Previously

BRINE MIGRATION (AVERY ISLAND)

A plan for post-test evaluation of the brine migration test at Avery Island was issued. This plan recommended activities to be conducted following the heating phase of the test to collect samples and evaluate the test and equipment performance.

BRINE MIGRATION (FRG ASSE MINE)

Work was initiated on initial definition of test needs for a brine migration test to be conducted in the Asse mine in West Germany. This included a literature survey and contact with investigators in the field of brine migration. The recognized models of brine migration were identified and characterized, and objectives were developed for the brine migration test.

These objectives are basically that the test should provide information for confirmation of the brine migration models and that at least a part of the test should accurately simulate actual repository conditions to observe unexpected phenomena. The tests should include the effects of radiation.

WASTE/ROCK INTERACTION

The initial review of waste/rock interaction technology continued. Additional pertinent literature not available previously was ordered. This initial review covered the following general areas:

- Potential waste forms
- Potential repository site characteristics

- Function and alternative materials of the elements comprising a representative waste package design
- Key licensing issues
- Preliminary concepts for field test of waste/rock interaction phenomena.

Activities During the Reporting Period

BRINE MIGRATION (AVERY ISLAND)

Objective

The objective is to participate in a workshop to be organized by ONWI to develop a final Post-Test Evaluation Plan for Avery Island.

Procedures

The draft Post-Test Evaluation Plan for the Avery Island brine migration test was presented before a workshop and comments were offered.

Results

The plan was found to be sound but some of the planned activities were to be delayed until test results on the synthetic brine were evaluated. The test was to be continued for at least 60 more days to determine whether the water collection rate continues to decrease or whether a steady production rate becomes established. Subsequently, a final test plan was issued and was found to be acceptable.

BRINE MIGRATION (FRG ASSE MINE)

Objectives

The objectives were to:

- Visit FRG to discuss objectives, plans, and capabilities for brine migration testing at Asse
- Develop detailed brine migration test objectives and conceptual test designs for the Asse brine migration test; also, identify developmental tests required to support the Asse test
- Characterize the Asse mine (as needed for the test planning and interpretation of the results) and determine geological configurations of the planned tests.

Procedures

After meeting with officials at the FRG Asse mine, Westinghouse produced a preliminary test plan describing the basic concept of a brine migration test. The FRG provided additional information regarding their facilities.

Results

Objectives were established for the brine migration test and for the basic outline of the test design. The design would be based upon cylindrical containers in boreholes in the salt which would produce conditions simulating a repository environment and with variations of significant parameters to determine information relating to brine migration phenomena. An important factor identified is that a radiation source, if present, must be easily and quickly retrievable.

With this background, a preliminary test plan describing the brine migration experiment concept was developed. This would consist of about nine individual test sites, each of which would be geometrically identical but would have different conditions and parameters. The parameters that would be varied include:

- Radiation - present or absent
- Temperature
- Temperature gradient
- Borehole atmosphere.

The gap in the borehole between the salt and the experiment container may affect the rate of brine migration, depending upon the sensitivity of brine migration to borehole gas pressure. This gap will be filled with a porous, nonreactive material which will allow collection of water vapor by passing a gas through this gap. Two conditions will be maintained for different test sites. In one, the gases produced by the test will be sealed with this gap and any moisture produced will be collected at the end of the test. In the other, moisture will be continuously collected during the test to observe any threshold behavior.

The experiment will involve electric heaters placed in the borehole and a ring of guard heaters at a radius of about 0.5 meter around the borehole. The heat will be adjusted to provide a variety of maximum salt temperatures ranging from 120 to 200 C and thermal gradients ranging from 0 to 3 C/cm. These are selected to cover the anticipated range of repository conditions.

A radiation source designed to simulate the dose rate from HLW will be included in most test sites. Some sites will be without radiation to determine the effect of radiation on brine migration by comparison. The radiation source will be ^{60}CO with about 16,000 curies per test site.

The experiment apparatus consists of a metal cylinder about 24 feet long with a 6-foot-long heated length 16 feet below the floor of the mine (Figure 1). The test area will be isolated

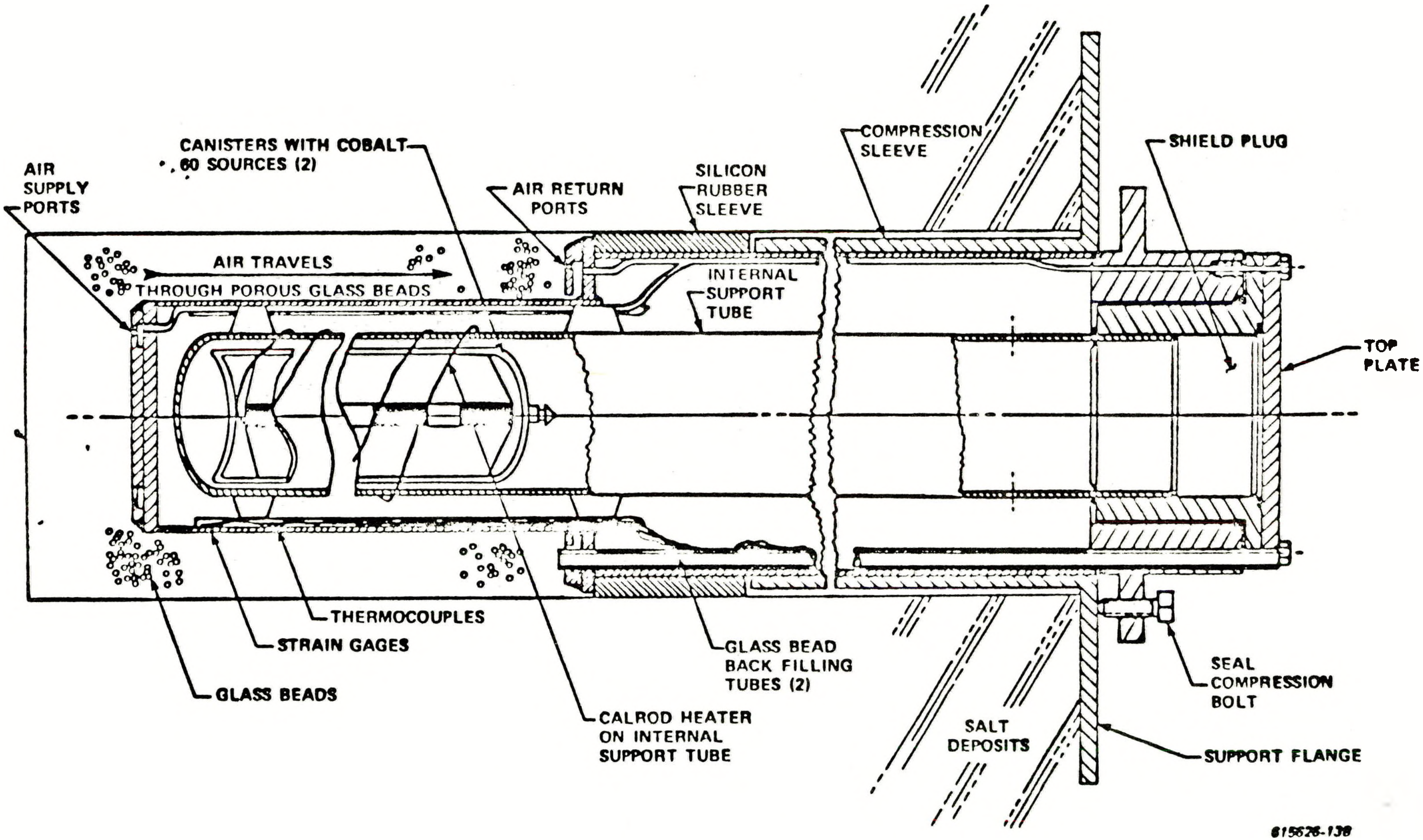


FIGURE 1. SECTION VIEW OF TEST ASSEMBLY INSTALLED IN SALT DEPOSIT

from the mine environment by an elastomeric seal above the active length. The test section was originally described as being 20 cm in diameter, but this may be increased because of the 30-cm diameter of the FRG radioactive materials handler which must fit inside the test section.

The test section will be surrounded by a porous material in the gap between the source and the salt to support the salt against closure by creep and to provide access for instrumentation.

The test data will be composed primarily of the amount of water collected and local temperatures. Consideration is being given to utilizing a data acquisition system which is currently installed at Asse, but it would appear that there is insufficient capacity available in that system; therefore, a conventional data logger system will likely be employed. Other parameters will be measured but these have not yet been identified.

WASTE/ROCK INTERACTION

Objectives

Objectives were to:

- Continue to review relevant waste/rock interaction technology
- Continue to develop a matrix for nuclide/rock direct contact interaction tests
- Initiate test plans for waste/rock direct contact tests without presence of ground-water oxidation products.

Procedures

The objectives of the waste/rock interaction task were carefully reviewed in terms of the issues derived from a status review of waste/rock interaction technology. In this manner, the specific objectives, concerns, and issues for the first test plan were identified and a "focused" test matrix was initiated.

Concepts for a test series covering the interaction between nuclides and salt (specifically in the Asse mine) without the presence of degraded barrier materials were developed through consideration of the test matrix elements previously identified. A test plan schedule and associated milestones, along with relatively detailed descriptions of the milestone definitions, were prepared for this first test plan. This plan includes provisions for defining any associated instrument development and the bench testing required for executing and evaluating the test series.

Results

Review of a large number of literature references and other relevant documents was completed. In addition, direct contacts were made with technical experts working in areas expected to have the greatest impact on waste/rock interaction testing. Visits were made to the Pennsylvania State University, the Hanford Engineering Development Laboratory, and the Pacific Northwest Laboratory to review ongoing programs with emphasis on waste-form degradation, testing and modeling, waste-form development, modeling of nuclide migration, barrier-material selection and testing, and bench-test methods. Summaries were prepared on the state of the art for waste forms, barrier materials, modeling of nuclide liberation and migration, and salt deposit sites with repository potential.

For the disposal of nuclear waste, it is desirable to employ a "top-down" systems engineering approach to rigorously define test programs. In this manner, the probability of identifying all the proper objectives, test matrices, issues, and test requirements is enhanced. Selected elements for the initial waste/rock interaction test plan were determined using engineering judgment as a means to expedite this first plan. Follow-on plans will utilize the systems approach to the maximum extent possible.

The basic concepts of the first test plan were defined as follows:

(1) Use the Asse mine of the Federal Republic of Germany as the test site.

(2) Use of an artificial brine made from Asse salt containing the nuclides or surrogate nuclides (if possible) in direct contact with the salt test hole. No simulated barrier degradation products will be present.

(3) Emphasis on the 1,000 to 10,000-year postemplacement period to guide nuclide selection and test conditions.

Pertinent test parameters such as temperature, pressure, nuclide concentration, etc., are to be selected as part of the specific test plan matrix development. Instrumentation and control requirements and any supporting (nonfield) test needs are also to be defined. On a somewhat later schedule, a comparable test plan for waste/rock interaction studies with the presence of simulated barrier degradation products will be initiated.

In developing the first test plan, a list of specific objectives and test concerns were derived.

The basic objective of the first test is to show whether and how nuclide migration is retarded by salt under simulated repository conditions. Ideally, this would involve determination of the respective distribution coefficients (Kd's) for each of the nuclides of interest for comparison with bench-test data and use in nuclide migration models.

WBS 1.2.2

Project: Commercial Waste and Spent Fuel Packaging Program

Principal Investigator: Rockwell Hanford Operations (RHO) (R. E. Smith)

ONWI Project Manager: J. A. Carr

Objective

The objectives are to: support the National Waste Terminal Storage (NWTS) Program, managed by the Office of Nuclear Waste Isolation (ONWI), by developing performance, acceptance and design criteria for waste packages for geologic storage or disposal; support geological demonstrations of spent fuel; develop a standard experimental demonstration package for spent fuel suitable for use in various geologic demonstrations; provide technical guidance and evaluation of dry surface storage demonstrations and spent fuel tests.

Activities During the Reporting Period

No progress report was submitted for the period.

WBS 1.2.2

Project: Spent Fuel Studies

Principal Investigator: Hanford Engineering Development Laboratory (HEDL) (D. A. Cantley)

ONWI Project Manager: E. F. Benz

Spent Fuel Characterization Equipment

Objectives

The objectives are to document work completed on nondestructive fuel rod and assembly characterization equipment formerly intended for use at the Engine Maintenance Assembly and Disassembly (EMAD) facility, and to design, construct, and test a spent fuel calorimeter for direct, accurate measurement of assembly decay heat to support assessment of thermal effects in demonstration geologies.

Progress Reported Previously

Installation of the calorimeter system was completed at the Engine Maintenance Assembly and Disassembly (EMAD) facility. Calibration and acceptance testing of the calorimeter system was completed indicating system performance in close agreement with design calculations. Calorimetry of Turkey Point Reactor spent fuel assembly D34 indicated a decay heat level of 1615 watts.

Activities During the Reporting Period

Objectives

The objectives of the present quarter's work were to perform calorimetry on Climax Spent Fuel Test (CSFT) assemblies being held in EMAD lag storage and characterize the performance of the calorimeter.

Procedures

Several reference measurements were made with the calorimeter to determine thermal performance and operating characteristics without spent fuel. Procedures, equipment, and techniques were developed to minimize EMAD hot-bay contamination when inserting and removing spent fuel for calorimetry in the boiling water vessel. Spent fuel assembly D04 was measured for decay heat level.

Results

The heat loss from the calorimeter is a function of ambient temperature and pressure and the nominal level is 520 watts. A nominal assembly decay heat value of 1580 watts was measured from assembly D04.

Conclusions

Minimal hot-bay contamination occurred during calorimetry of D04. Contamination was isolated to the fuel handling area around the calorimeter. The measured decay heat value is within 2 percent of the 1540 watts predicted by the ORIGEN code.

Spent Fuel Characterization

Objective

The objective of this program is to quantify the effects of geologic disposal tests on the physical, mechanical, and chemical condition of spent fuel rods and assemblies. Particular attention is directed to evaluation of the effects on integrity with regard to radionuclide containment.

Progress Reported Previously

The nondestructive examinations data from the Turkey Point spent fuel assemblies and rods used in the CSFT were received from Battelle-Columbus Laboratories (BCL) and analyzed in total to support the conclusion reported previously that the spent fuel is in good condition with no cladding breaches or other gross anomalies.

The destructive examinations on the companion rods from the Turkey Point CSFT assemblies were completed. These examinations included fission-gas analysis, burnup analysis, cladding-impurity analysis, and detailed metallography of the cladding and fuel. Reduction and analyses of these data were in progress.

Efforts were initiated to procure stainless-steel-clad spent fuel rods from Northeast Utilities (Connecticut Yankee). These rods were to be characterized and laboratory tested to assess behavior under disposal conditions.

Activities During the Reporting Period

The objectives of the work performed this quarter were to continue analysis of the destructive data from the Turkey Point CSFT fuel rods and to coordinate efforts to obtain data from the examinations of Connecticut Yankee and Browns Ferry spent fuel.

All data from the destructive examination of five fuel rods pulled from the CSFT assemblies were received from BCL. The data are currently being reduced and analyzed to provide a description of the pretest condition for the CSFT.

Fuel hot cell examinations were identified as a key area of mutual interest in programs being conducted by EPRI (LWR fuel performance), Pacific Northwest Laboratories (PNL) (AFR storage), and HEDL (dry geologic disposal). Agreement was reached among these organizations to coordinate future fuel procurement, shipment, and examination activities, and to exchange data obtained from the examinations. Connecticut Yankee fuel examinations were identified as being of near-term interest. Efforts by EPRI and Northeast Utilities to provide stainless-steel-clad fuel rods from Connecticut Yankee for characterization continued.

Contact was made with Oak Ridge concerning the availability of BWR fuel rods from a Browns Ferry fuel assembly. One fuel assembly, discharged January, 1980, will be shipped the week of August 4 to BCL where 15 rods will be examined for fission-gas data, sectioned, and sent to Oak Ridge for reprocessing studies. The remaining rods will be available for HEDL use. Preliminary plans call for nondestructive examinations on 17 of the rods and destructive examination of 5 rods to include fission-gas analysis, burnup and hydrogen analysis, and metallography.

Spent Fuel Package Performance

Objectives

The objectives are to develop the data, methodology, and analytic capabilities to predict the performance of spent fuel and package components (e.g., stabilizer, canister, and buffer) during the disposal cycle for the purpose of (1) evaluating and selecting materials for waste packages, (2) characterizing spent fuel as a waste form, (3) establishing the degree to which the package components serve as radionuclide containment barriers in a multibarrier package, and (4) validating the performance of the multibarrier package final design.

Progress Reported Previously

A proposed program plan for evaluating the effects of normal transport environments on spent fuel arrival condition and subsequent disposal integrity was forwarded to the working group on normal transport. The whole rod test at 482 C was stopped for an interim examination. No rod failure was observed, but there was approximately 1.8 percent cladding creep strain, resulting in a hoop stress reduction of 31 percent. Modifications were made to the STAFF-5 two-dimensional fuel performance model to simulate thermowells, fuel assembly support structure, and other features of the Fuel Temperature Test (FTT) facility. The STAFF-5 model was documented. Fabrication and assembly of the Climax Materials Interaction Test (CMIT) was completed. A study examining uncertainties in decay heat calculations for spent fuel was completed. The calculated decay heat values and the results of a calorimeter measurement for a spent Turkey Point fuel assembly were compared. Initial activities associated with the materials screening phase of the Spent Fuel Filler/Stabilizer Program were reported. A framework for identifying potential filler materials and relevant material characteristics was established by generating a list of possible filler performance functions and other possible screening considerations. Corresponding material properties and attributes pertinent to these performance functions and potential filler materials with favorable properties were then identified. A compilation of the pertinent material properties and attributes for each of the fillers was initiated.

Activities During the Reporting Period

Structural Analysis and Evaluation

This quarter's objectives were (1) to complete a finite element structural analysis of various fuel assembly types; (2) input static and dynamic loadings to assess component stress levels for use in fracture mechanics analyses; and (3) support Transportation Technology Center (TTC) working groups on matters pertaining to spent fuel performance in transit.

Static and response spectra loadings were applied to elastic finite element models of both BWR and PWR fuel assembly configurations. The sensitivity of these structures to grid spacer coupling and boundary condition effects was examined. Fracture mechanics analyses were initiated to assess cladding crack growth rates under applied loadings.

Modal analysis results show, in general, fuel assembly fundamental frequency responses in the 1 to 2 Hertz range (pinned end conditions). The fuel assembly modal participation is dominated by the fundamental modal response with 98 percent of the energy of vibration resident in this mode. The fuel assembly structures will sustain large bending deflections (i.e., deflections on the order of 10 percent of the assembly length when pinned end conditions are applied) prior to the onset of yielding in the guide tube structure. Cladding stresses are low, lagging guide tube stress levels typically by 50 percent.

Fuel stiffness and thus resistance deflection under dynamic loading is low. Case studies of deflection-limited (e.g., canistered) fuel will be completed to further evaluate cladding stresses and fracture potential.

Elevated-Temperature Whole Rod Tests

The main thrust of activities in the whole rod tests this quarter was nondestructive and destructive post-test examination of rods removed from Tests 2 and 2b during interim examinations.

The destructive examination of the two rods removed from the 900 F whole rod test is almost complete, although only a rough assessment of the data has been made. Metallographic samples were examined for changes in pellet condition, oxide or fuel cladding chemical interaction (FCCI) thickness, and hydride concentration. There was no qualitative change in pellet condition. The external oxide width on the rods annealed in air was somewhat increased, as expected. Prior to the test, there was an axial hydride gradient. After the anneal, the gradient no longer existed and the hydride concentration was approximately the same as the highest pretest concentration. At this time, no explanation is offered for the increased hydriding.

A zone of material much harder than the base Zircaloy cladding was found in the cladding adjacent to both the OD oxide and ID FCCI zones. Both the oxide layer and FCCI zone exhibited axial cracks. When the cladding was etched, it was observed that the sharper of the cracks extended the full width of the hard zone. The blunt cracks in the FCCI zone did not propagate into the hard zone. The zirconium concentrations in the cladding and hard zone determined by Scanning Electron Microscope—Energy Dispersive Analyses by X-ray (SEM EDAX) were indicative of an oxide solid solution observed by others (Ocken, 1980), were at much higher temperatures, leading one to believe that this hard zone may be oxygen-stabilized alpha-zirconium. Ion microprobe examinations are planned to confirm the nature of this zone. However, it appears that since the oxide/FCCI zone is well bonded to the cladding, the cracks initiating in the oxide/FCCI zone propagate rapidly through the brittle zone as the cladding creeps and are stopped when they reach the ductile Zircaloy.

The nondestructive interim examination of the rods from the 1060 F whole rod test has been completed. A comparison of pre- and post-test profilometry indicated more creep in the three-cycle rod than in the two-cycle rod. This difference agreed with the difference in the starting internal pressures of the two rods as evaluated with the Exxon creep equation (Merckx, 1974). There was no difference in creep strain between the two-cycle rods which had been only at 1060 F and those rods which had been at 482 C and at 571 C. There was a small increase in the creep strain at elevations corresponding to the locations of most grid spaces. The cause of these strain peaks is being investigated further. In addition, the examinations of these rods indicated no additional release of fission gas from the fuel nor any axial migration of fission products.

Whole rod tests are continuing at 510 C and 571 C with only minor shutdowns for equipment or power outages. Design was initiated for new test hardware to provide the capability to test whole rods at elevated pressures.

The formulation of the program plan to determine the performance of spent fuel under disposal conditions continues. No mechanisms have been identified which will change the physical condition of the fuel. The cladding degradation mechanisms all appear to be amenable to a conservative phenomenological representation. The characterization distributions of pertinent performance variables has, so far, yielded little information. The vendors and utilities are being pursued for their fuel performance data.

A detailed analysis of the role fission gas will play during disposal continues. It appears that the Office of Airborne Waste Management identifies only four important isotopes which have biological effects. The inventories of gas, volatiles, and fission products as a function of fuel burnup and disposal duration have been determined. The multitude of models that predict the magnitude of gas release are also being evaluated.

Performance Modeling

Validation of the STAFF-5 model results against FTT experimental results continues. STAFF-5 results show very good agreement with results of FTT Test 2 (evacuated canister, no external heaters). Validation against results for helium-filled canister tests continues and is approaching completion.

Material Interaction Tests

Three electric test furnaces, each with four independently heated and controlled zones for conducting the thermal control test portion of the CMIT, were installed. System operation and calibration were verified and completed.

Nuclear Modeling

During a previous reporting period, a calculated decay heat value of 1.86 kW was obtained for Turkey Point spent fuel assembly D34 after a 2.4 year cooling time. This value was 15 percent higher than a recent calorimeter measurement of 1.615 kW. This discrepancy has been traced to outdated decay energies in the ORIGEN library that was used. The use of decay energies obtained from the Evaluated Nuclear Data File (ENDF/B-V) reduced the discrepancy to 10 percent, a difference not inconsistent with previous sensitivity studies.

During this reporting period, a new version of the ORIGEN decay heat code (ORIGEN 2) was obtained from the Oak Ridge National Laboratory and converted to run on the Richland UNIVAC computer. Heat decay values calculated using this code and its associated nuclear data library are in excellent agreement (approximately 2 percent high) with measured heat values obtained for assembly D34. The values calculated for assembly D04 also agree to within about 2 percent (low) with recent measured values. The principal difference between the new and old calculations, other than the use of newer decay energies, is the ^{133}Cs capture cross section. Sensitivity studies had earlier identified this cross section as the largest contributor to decay heat uncertainties that arise from nuclear data. This sensitivity becomes much smaller for cooling times beyond 10 years.

The ORIGEN2 calculations were further validated by comparing them with calculations made by Savannah River Laboratories. With the exception of ^{106}Ru and ^{134}Cs, calculated inventories for actinides and fission products are in good agreement. The ^{134}Cs discrepancy is not unexpected; however, the ^{106}Ru is not understood.

Spent Fuel/Filler Material Interaction Studies

The two objectives of the work performed this quarter were to complete the compilation of the filler materials attributes and perform preliminary interaction evaluations, including criticality, radiation attenuation, and thermal and mechanical interaction calculations.

Attribute compilation efforts continued for the initial list of potential spent fuel filler materials. This compilation effort was completed during the quarter to the extent that information was available. Criticality calculations for the filler materials were completed. These calculations were used to evaluate the relative criticality concern associated with the use of the filler materials. The largest K_{eff} calculated was 0.21, indicating that none of the candidate filler materials interact with the spent fuel assembly neutron flux in a manner that would create a criticality concern. The calculations assumed that the filler effectively maintained the original geometry of the fuel assembly and that the assembly was unirradiated. Radiation attenuation calculations to evaluate the shielding effectiveness of the filler materials were 90 percent completed.

An evaluation of the spent fuel filler materials thermal performance was completed. The thermal conductivity of the filler materials was related to the resulting temperature differential between the cladding and the canister wall. Comparison of the temperature differentials produced by the various filler materials provided insight into the heat transfer effectiveness of these materials. The metal alloys and graphite offered the most favorable heat transfer characteristics having a $\Delta T \leq 10$ C. The calculated ΔT was 10 to 50 C for glasses and concrete and 50 to 100 C for crushed repository geologic media and helium. Calculations assumed a decay heat level for the spent fuel assembly of 0.964 kW.

Mechanical interaction evaluations were also completed. Both thermal gradient and differential thermal expansion effects on the tensile stresses induced in the spent fuel filler were evaluated. The evaluation of tensile stresses induced in the filler materials by spent fuel canister temperature gradients showed that spent fuel having a decay heat of 0.964 kW will induce stresses in excess of the tensile strength for concrete and most of the glass fillers. Thermal gradient stresses induced in the metal alloy fillers are insignificant compared with their respective strength levels. The analysis of the filler tensile stresses developed during cooldown from the fill process because of differential thermal expansion of the spent fuel cladding and filler material (glasses and metal) shows that glasses must not have thermal expansion coefficients in excess of 7×10^{-6} C^{-1} for use with Zircaloy-4 cladding and coefficients of less than 16×10^{-6} C^{-1} for use with 304 stainless steel cladding based on a criteria of tensile stress limit of 1000 psi for glasses. Because of the good strength and ductility properties exhibited by the metal filler materials, the analysis indicated that no significant problem arises from stresses developed during cooldown for most of the metals.

Experimental plans were developed for initial testing of spent fuel cladding/filler materials compatibility. Specimens were designed to simulate PWR and BWR fuel rods from the standpoint of gas volume to fuel column volume ratio. A 416 stainless steel mandrel inside the cladding specimen will occupy the volume and simulate the thermal expansion characteristics typical of fuel in a fuel rod. Calculations were performed to confirm the design using an Exxon (Merckx, 1974) equation to describe the Zircaloy strain behavior and a Larson-Miller Parameter life-fraction approach to estimate failure time. The materials compatibility tests will be conducted under conditions expected to exist prior to canister breach. Temperature limit tests are planned to determine the maximum allowable temperature for fuel rod cladding during the short term fill process. A furnace was obtained and specimen fabrication was initiated for the temperature limit tests. Fill process tests will be conducted to establish cladding-filler interactions for fill processes requiring melting or fusing of the filler material. Disposal condition tests are being planned to establish material interactions as a function of time and temperature in unbreached canisters.

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Ocken, H., 1980. "An Improved Evaluation Model for Zircaloy Oxidation", *Nucl. Tech.*, 47:343 February.

Merckx, K., 1974. "Calculational Procedure for Determining Creep Collapse of LWR Fuel Rods", *Nucl. Des. & Eng.*, 31:95-101.

WBS 1.2.2

Project: Waste Package Criteria Response Studies

Principal Investigator: Battelle Columbus Laboratories (N. E. Miller)

ONWI Project Manager: J. Carr

Objective

The objective of this program is to support the development of waste package criteria responses, conformance, and predesign specification studies.

Progress Reported Previously

This is the first quarterly report on the project.

Activities During the Reporting Period

Four of the six tasks planned for this study were active during this quarter. The activities of each task are described below:

Task 1

The objective of the first task is to review and interpret the ONWI criteria documents and to develop waste package design responses to each criterion. The objective for this quarter was to review the ONWI criteria documents and to develop an outline which shows the relationship of all the criteria. This outline will subsequently be used in determining the parameters of the waste package design which must respond to the criteria.

The criteria documents were carefully reviewed and a criteria-relationship outline in matrix form was developed including a description of each relationship. The relationships uncovered among the various policies/criteria affecting waste package design will enable the identification of specific parameters of importance in waste package design to be carried out much more efficiently.

Task 2

The objective of the second task is to assemble an annotated bibliography of documents which will be of use to a waste package designer. The objective for this quarter was to organize the staff, to develop a methodology for review of the documents, to identify documents for review, and to begin review and abstraction of the collected reports.

Approximately 700 reports have been identified as potentially containing information which may be of use to a waste package designer, and approximately 100 of these reports have been abstracted. The reports were identified from the computerized literature searches, from a manual search of the ONWI library, from the personal libraries of the project staff, from information gathered at the recent technical meetings, and from the reference lists of each report that has been abstracted.

By cross checking the report reference lists and by keeping current on newly published reports, it is expected that the bibliography will contain most technical reports which will be of use to the waste package designer.

Task 3

The objective of this third task is to develop a dictionary of waste-package-related terms for use by the ONWI waste package development staff and contractors for more accurate communications. The objective for this quarter was to compile terms and to review the definitions.

The first draft of the dictionary has been completed.

Task 4

The objective of the fourth task is to develop broad guidelines to the waste package design describing aspects of the waste management systems which interface the waste package. The objective of the task for this quarter was to identify the organizations active in studying and/or designing equipment, procedures, and methods for packaging, transporting, and emplacement of high-level waste; to obtain a list of all potentially pertinent reports, and to visit the key facilities.

Visits to several facilities were arranged. In addition, a list of reports was obtained. The reports available in house were identified and procured; others were ordered.

WBS 1.2.2

Project: Repository Waste Package Design Studies

Principal Investigator: Westinghouse Electric Corp.

ONWI Project Manager: J. Carr

Objective

The objective of the program is to develop the preliminary designs for practical, easy-to-handle waste packages that will retain nuclear wastes for long periods of time and then effectively retard their release so that the natural barriers provided by the geology can reduce their transport to the point where they pose no threat to man and his environment.

Progress Reported Previously

This is the first quarterly report for the project.

Activities During the Reporting Period

Objectives

The objectives are to:

- Formulate design specifications based on ONWI criteria and requirements, and on NRC and EPA regulations
- Perform concept bases assessment to identify missing information which may impede the preliminary design efforts
- Prepare and submit a Quality Assurance Plan.

Procedures

Based on ONWI-supplied criteria and requirements documents, a top-down systems engineering approach was used to develop design specifications. This approach also identified the needed input design data and required interface control information.

Information and data needed for design were identified during the development of the Design Specification. This information was assembled for the first waste form/geology combinations. Where these data sets were incomplete, the missing data were identified to ONWI. Data values which are missing and which may impede design progress will be estimated based on sound engineering judgment.

Results

A system specification tree shown in Figure 1 was developed from various criteria, requirements, and regulatory documents. This tree depicts the interrelationship among the aspects of the geologic repository system The block defined as the "waste package" was subjected to a systems engineering approach to determine major operations functions and to develop functional requirements from which a design specification was generated. Functional flow diagrams were developed starting with the major program operations functions and extending down to third-level functions for some major aspects. These functional flow diagrams are shown in Figures 2, 3, 4, and 5.

Requirements Allocation Sheets were completed for each of the functional blocks shown in Figures 2 through 5. This resulted in a detailed list of design requirements, facilities requirements, and other interface requirements related to the waste package.

A comprehensive design specification was then drafted using the outline shown in Figure 6. This specification, along with its developmental history, was submitted to ONWI.

The design specification document developed for Waste Package Design will subsequently be reviewed and matured as conceptual design studies proceed.

One of the results of the Waste Package Design specification, using the systems engineering approach, was the identification of specific design values and data needed to proceed with waste package design. These data were generated for spent fuel and commercial high-level waste forms and for salt and basalt geological media. Sources for these data included existing reports and research efforts. Over 200 individual reference items were reviewed relative to geologic disposal of nuclear wastes. From this assessment of design concept data bases, certain missing data were identified. These generally fell into three categories:

(1) Data which are site specific

(2) Data which do not exist

(3) Data which are in development but are not yet available.

Data in Category 1 cannot be generated exactly until a specific repository site is chosen. However, generic data can be and will be utilized which encompasses a variety of sites in similar rock material. Generic values will be chosen as the worst case or upper limit values for each parameter needed.

Category 2 data will have to be allocated by ONWI to the waste package based on overall repository requirements and specifications.

Data in Category 3 may become available as more interfacing occurs between contractors, or as current research is documented and published.

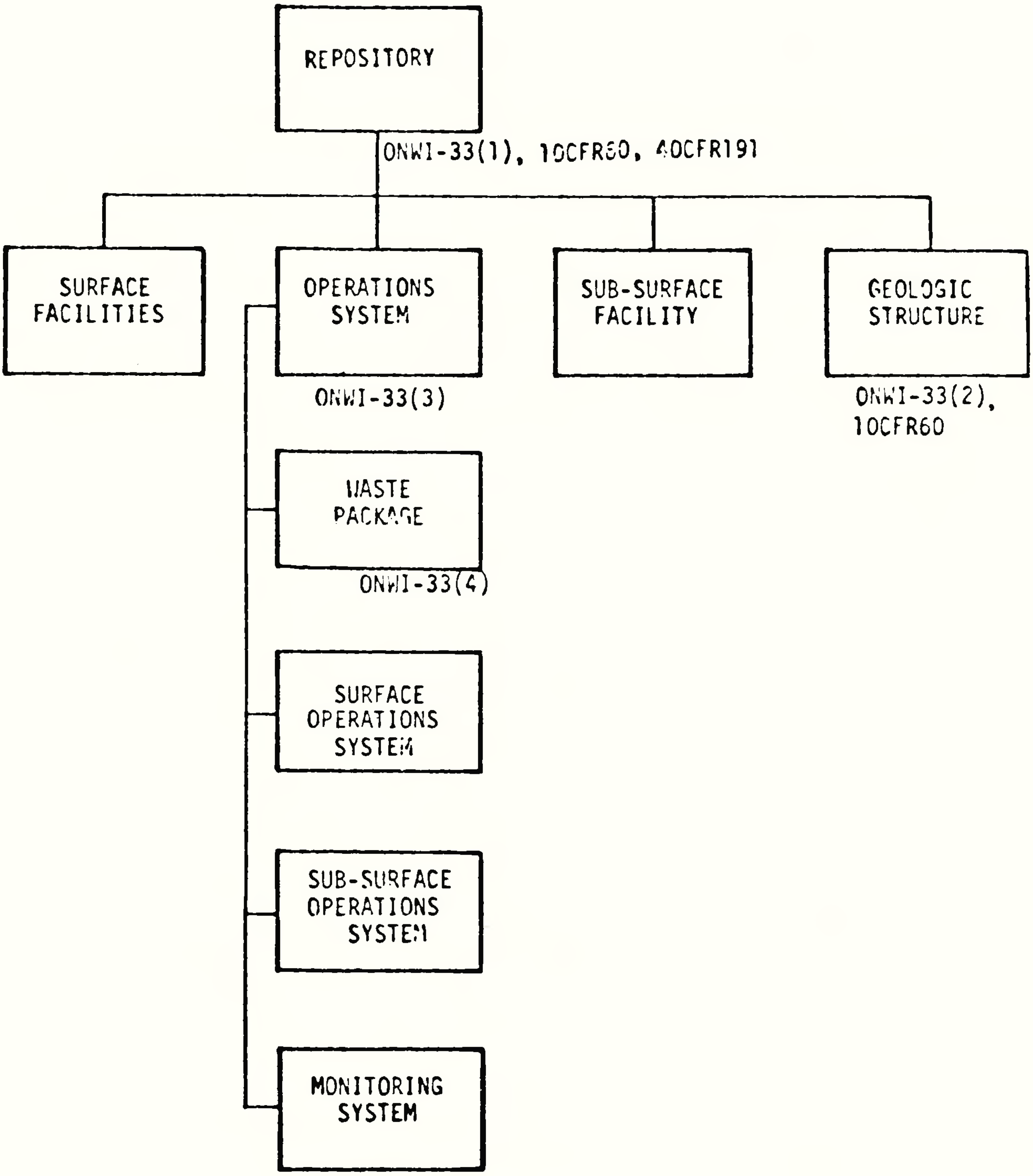


FIGURE 1. SYSTEMS SPECIFICATION TREE

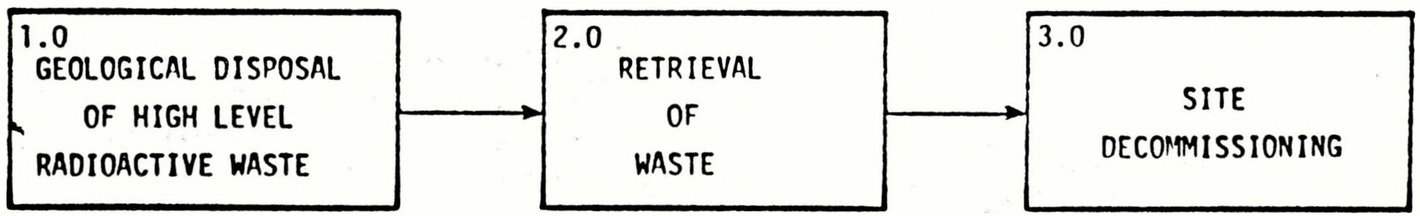
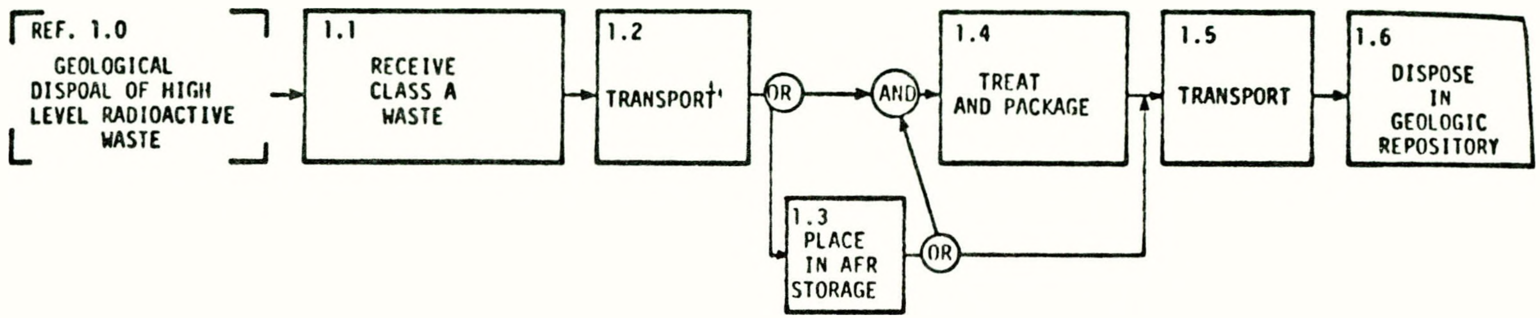
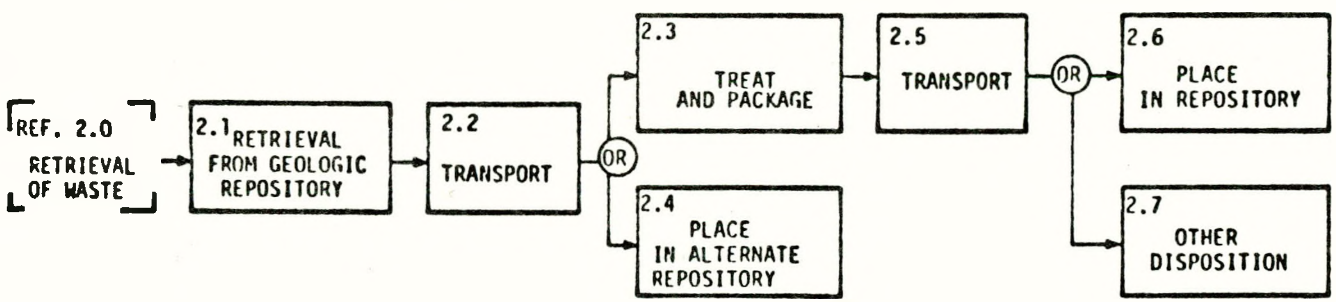


FIGURE 2. MAJOR PROGRAM OPERATIONS FUNCTIONS



FIRST LEVEL OPERATIONS FUNCTIONAL FLOW CHART - PROGRAM FUNCTION 2.0



FIRST LEVEL OPERATIONS FUNCTIONAL FLOW CHART - PROGRAM FUNCTION 3.0

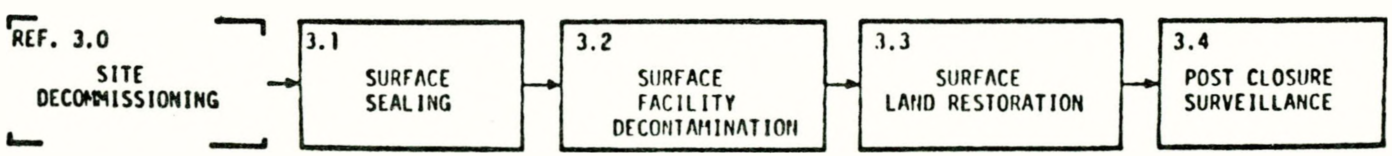


FIGURE 3. FIRST LEVEL FUNCTIONAL FLOW CHARTS OPERATIONS

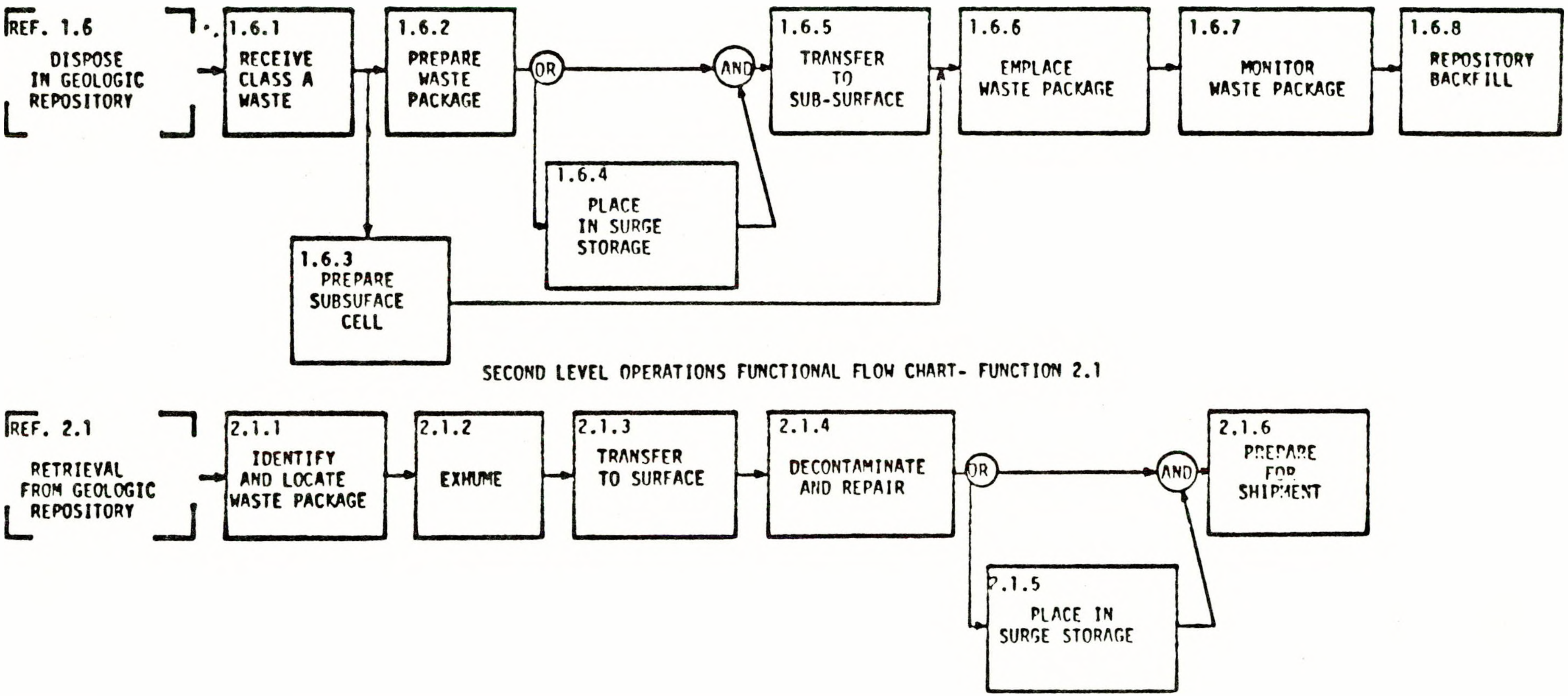
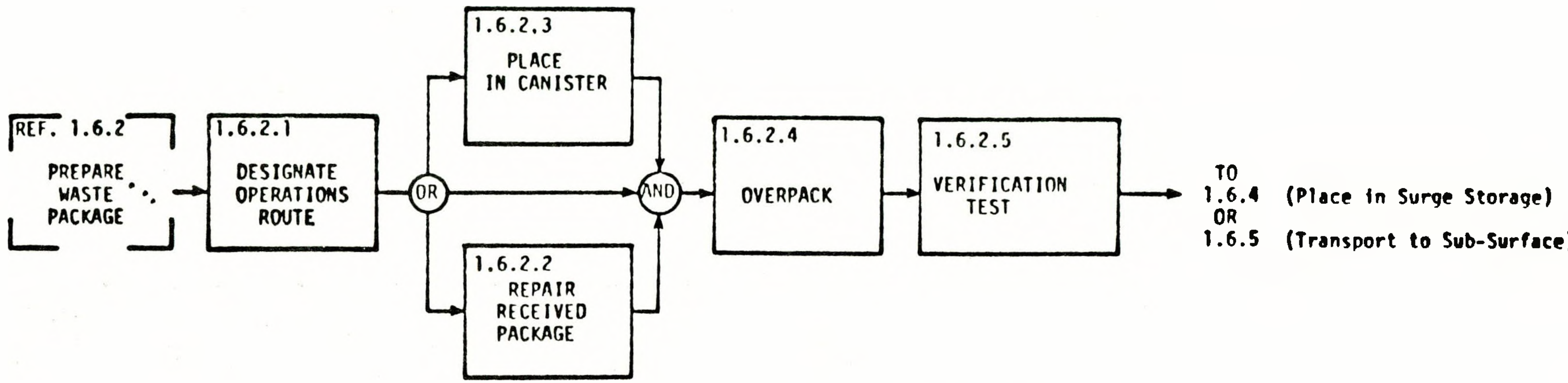
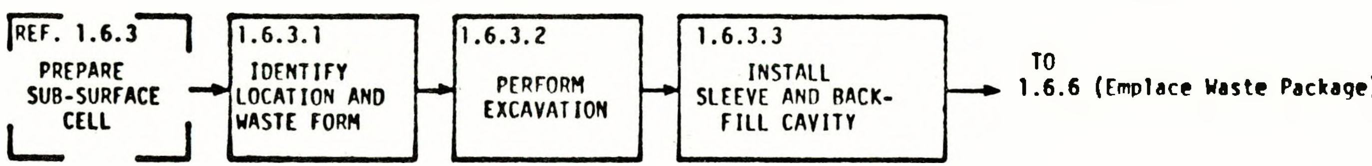


FIGURE 4. SECOND LEVEL OPERATIONS FUNCTIONAL FLOW CHARTS



THIRD LEVEL OPERATIONS FUNCTIONAL FLOW CHART - PROGRAM FUNCTION 1.6.3



THIRD LEVEL OPERATIONS FUNCTIONAL FLOW CHART - PROGRAM FUNCTION 1.6.6

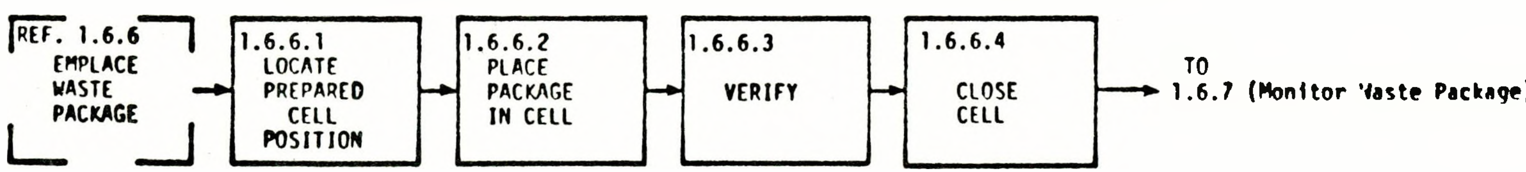


FIGURE 5. THIRD LEVEL OPERATIONS FUNCTIONAL FLOW CHARTS

PERFORMANCE, DESIGN AND PRODUCT CONFIRMATION SPECIFICATION
ENGINEERED WASTE PACKAGE SYSTEM FOR GEOLOGIC DISPOSAL

1.0 SCOPE

2.0 PROGRAM DOCUMENTS
- 2.1 APPLICABLE DOCUMENTS
- 2.2 SOURCE DOCUMENTS
- 2.3 REFERENCED DOCUMENTS
- 2.4 COMPANION DOCUMENTS

3.0 REQUIREMENTS
- 3.1 PERFORMANCE
  - 3.1.1 Functional Characteristics
    - 3.1.1.1 Primary Performance Characteristics
    - 3.1.1.2 Secondary Performance Characteristics
  - 3.1.2 Operability
    - 3.1.2.1 Reliability
    - 3.1.2.2 Maintainability
    - 3.1.2.3 Useful Life
    - 3.1.2.4 Environment
    - 3.1.2.5 Transportability and Handling
    - 3.1.2.6 Standardization
    - 3.1.2.7 Safety
- 3.2 WASTE PACKAGE DEFINITION
  - 3.2.1 Component Definition
    - 3.2.1.1 Waste Form
    - 3.2.1.2 Waste Package Components
  - 3.2.2 Interface Requirements
- 3.3 DESIGN AND CONSTRUCTION
  - 3.3.1 General Design Features
  - 3.3.2 Codes and Standards
  - 3.3.3 Materials, Parts and Processes
  - 3.3.4 Corrosion Resistance
  - 3.3.5 Interchangeability
  - 3.3.6 Identification and Marking
  - 3.3.7 Storage

4.0 QUALITY ASSURANCE PROVISIONS
- 4.1 ENGINEERING TEST AND EVALUATION
- 4.2 QUALIFICATION TEST
- 4.3 RELIABILITY TEST OR ANALYSIS

5.0 NOTES

6.0 APPENDIX
- 6.1 TABLES

FIGURE 6. OUTLINE FOR WASTE PACKAGE DESIGN SPECIFICATION DOCUMENT

WBS 1.2.3

Project: Borehole Cement and Rock Properties Study
Task 1. Borehole Plugging Cement Studies

Principal Investigator: Pennsylvania State University (D. M. Roy)

ONWI Project Manager: F. L. Burns

Objective

This project is oriented toward the development of improved technology in cements and cementitious materials in conjunction with their specific role in borehole plugging, grouting, and shaft sealing of various natural repositories for radioactive waste isolation.

The problems of processing, emplacement, reliability, and long-term stability are addressed through: (1) establishing the effects of compositional variables upon the rheological properties, (2) investigating volume stability, (3) modifying the nature of cement hydrate, (4) investigating the interface/bond between cement and host rock, (5) studying accelerated reaction kinetics, and (6) identifying various mechanical/physical properties as determinants in predicting long-term performance.

Geochemistry of Cement-Based Systems

The objective of these studies is to examine those factors related to longevity of cement-based and related repository plugging and sealing materials. The goal is to generate cementitious composite plugging and sealing materials that have high potential of approaching thermodynamic stability, or if not achieving full stability, then undergoing changes with time that would not compromise their properties. This research includes studies of specific cement-based and related seal materials, alone and in combinations with rocks (both generic and site specific), to determine their compatibility. The studies involve assessing and generating essential thermodynamic data, performing control studies, characterizing starting materials and products; characterizing ancient cements and concretes, determining reaction rates, and examining certain other special factors impacting longevity of seal materials. Combinations of these results will be used to project anticipated changes and assess reliability and degree of assurance of repository borehole plugging and shaft sealing materials' performance.

THERMODYNAMIC PROPERTIES OF CEMENT AND MINERAL PHASES

The objective of this subtask is to determine the most thermodynamically stable phases from a total chemistry consisting of (1) seal (cementing) materials and (2) seal materials in combination with host mineral and rock components. Thermodynamic parameters, both calculated and experimentally derived, may be used to define stable end products.

An assessment of available thermodynamic data on portland cement-related phases, including both starting materials and final end products, is in progress. This includes details of stabilities within the basic cement system, lime-alumina-silica-water, which also encompasses a variety of natural mineral phases. In the current period, investigations of the effects with salts added to the system were initiated.

Calcium Silicates

Because they constitute some 80 to 85 percent of the total constituents, calcium silicates are by far the most important cementitious materials in commercially available portland cement-based materials. Study has been concentrated on these phases, particularly on tricalcium silicate (Ca_3Si) because it has the most negative free energy of hydration to form noncrystalline Ca-Si-H gel plus calcium hydroxide. A comprehensive thermodynamic treatment is required to determine the driving force for the transformation of early formed Ca-Si-H gel to a more stable crystalline product (Roy, 1980). The free energy of formation for each candidate phase, or free energy of reaction between sets of phases, is the principal quantity required to assess their relative stabilities. The Gibbs free energy of formation, $\Delta G^{\circ}_{f,t_o}$ (at T_o = 298.15 K, 1 atm pressure, standard state), is given by the following relationship:

$$\Delta G^{\circ}_{f,T_o} = \Delta H^{\circ}_{f,T_o} - T_o \Delta S^{\circ}_{T_o} . \qquad (1)$$

If the free energies of formation (derived from the enthalpies of formation ($\Delta H^{\circ}_{f,T_o}$) and entropies of formation ($\Delta S^{\circ}_{T_o}$)) are known for each candidate phase, then the most stable individual phase or combination of phases from a given total chemistry (i.e., that combination which has the most negative free energy of reaction) can be determined.

With certain assumptions, the free energy of hydration (ΔG) of Ca_3Si to form noncrystalline gel (Ca-Si-H) has been calculated according to the following reaction to be

$$\begin{aligned} Ca_3Si + 3H_2O &= \frac{1}{2}(Ca_3Si_2O_7 \cdot 3H_2O) + \frac{3}{2}Ca(OH)_2 \\ &\quad \text{(gel, noncrystalline)} \\ \Delta G &= -16.0 \text{ kcal/mole } Ca_3Si. \end{aligned} \qquad (2)$$

A more favorable reaction is the transformation

$$Ca_3Si + \frac{18.5}{6} H_2O = \frac{1}{6}(5CaO{\cdot}6SiO_2{\cdot}5.5H_2O) + \frac{13}{6} Ca(OH)_2 \qquad (3)$$

(tobermorite, crystalline)

$$\Delta G = -24.14 \text{ kcal/mole } Ca_3Si,$$

which yields crystalline hydration products, including the crystalline calcium silicate hydrate, tobermorite. Finally, if the excess calcium hydroxide is consumed by reacting with silica to form additional tobermorite, the ΔG change is even more favorable:

$$\begin{aligned} Ca_3Si + \frac{13}{5}SiO_2 + \frac{16.5}{5}H_2O &= \frac{3}{5}(5CaO{\cdot}6SiO_2{\cdot}5.5H_2O) \\ \Delta G &= -39.92 \text{ kcal/mole } Ca_3Si. \end{aligned} \qquad (4)$$

Calcium Aluminates

Tricalcium aluminate (Ca_3Al) is normally present in varying amounts in portland cements, and its stable hydration behavior is important, particularly for seal materials used in the presence of salts such as in the Los Medaños area. The free energy of hydration at 298 K to form the sulfate-containing salt ettringite, known for its expansive characteristics, has been calculated using values of the heat of formation of ettringite, National Bureau of Standards (NBS) values for heat of formation, and entropies. The basic reaction considered is:

$$Ca_3Al + 3Ca^{+2} + 3SO_4^{-2} + 32H_2O \leftrightarrows Ca_6Al_2(SO_4)_3(OH)_{12}\cdot 26H_2O, \quad (1)$$

and the relevant ionic concentrations in solution of ground water of the Los Medaños area are considered to be: 0.155 M Na_2SO_4 and Ca^{++} = 0.003 M. For reaction (1), the $\Delta G = \sim -37$ kcal/mole, which is energetically very favorable, the precision depending upon certain assumptions. However, when compared with the stable hydrate, hydrogarnet (Ca_3AlH_6), according to the following reaction:

$$Ca_3AlH_6 + 3Ca^{++} + 3SO_4^{-2} + 26H_2O \leftrightarrows Ca_6Al_2(SO_4)_3(OH)_{12}\cdot 26H_2O, \quad (2)$$

the net free energy of reaction to form ettringite is approximately 2 kcal/mole, which is barely energetically favorable, considering limits of error. Thus the supply of sulfate as well as temperature are important controlling factors in stabilizing the expansive component ettringite.

The precision of the data and validity of assumptions will continue to be assessed in greater detail.

Detailed examination of the data upon which these calculations are based is in progress, in addition to generating new experimental measurements to help assess the validity of the underlying assumptions.

STABLE CEMENT COMPOSITES

The major objective of this part of the program is the design and evaluation of cement and cement composites that have potential for thermodynamic stability.

General

Work has continued on several sets of portland cement-based mixtures using either Class C (C-6) or Class H (H-4) cements with compositional modifications formulated to explore relative long-term stability at temperatures up to 90 C. Experiments are also planned at higher temperatures.

Various additional reactive additive components have been obtained and are currently being evaluated. Two recent silica fumes which have very high surface areas, as expected, were found to require use of high water-to-cement (w/c) ratios or a superplasticizer to make them workable. Both silica fumes demonstrated pozzolanic behavior when reacted with lime.

X-Ray Diffraction Characterization

During this quarter X-ray diffraction characterization studies were carried out on four mixes at various stages of curing.

X-ray diffraction data for the Class C + slag + fly ash samples demonstrated that the starting material reactivity increases with temperature. Peaks of residual cement phases (β-C_2S) tended to decrease in intensity, as did the amount of $Ca(OH)_2$ produced during the reaction. Small amounts of calcium silicate hydrate (C-S-H) were detected at 60 and 90 C in the 7-day samples. In addition, at 14 and 28 days, C-S-H was also present at lower temperatuers (27 and 45 C).

X-ray diffraction studies of the Class C + slag + quartz mixes showed decreasing quartz, residual anhydrous cement phases (β-C_2S), and $Ca(OH)_2$ with increasing temperature. Unique to this mix among the series, however, is the fact that the $Ca(OH)_2$ had reacted completely and was not evident in the 7- and 14-day samples cured at 90 C. At 28 days, the $Ca(OH)_2$ had reacted and was not found in either the 60 or 90 C samples. Reactivity in these mixes is generally high, resulting in rapid development of high compressive strengths. This mix appears to have considerable potential for longevity-durability since, at least at higher temperatures, the $Ca(OH)_2$ reacts nearly as rapidly as it is formed. In addition, significant C-S-H is present at all temperatures and times.

The major trends in phase changes for the Class C + ferrosilicon dust + quartz mix determined from X-ray diffraction data were the general decreases in the amounts of residual cement phases (β-C_2S), quartz, and $Ca(OH)_2$ with increasing temperature. The latter was absent from samples cured at 90 C at all curing times (7, 14, 28 days). C-S-H material was present at all times and temperatures, apparently increasing with length of cure. Permeability values for this mix ranged from 10^{-5} to 10^{-8} darcys. Work is continuing on this mixture.

X-ray diffraction data for the Class H + ferrosilicon dust + quartz mix once again indicated a relatively constant, slightly decreasing quantity of quartz and residual cement phases with increasing temperature. Once again the $Ca(OH)_2$ decreased with temperature in each of the 7-, 14-, and 28-day determinations and was absent in all of the 90 C samples. C-S-H was present at all temperatures except 27 C and 7- and 14-day curing.

Results for the cements tested confirmed that the reduction of free lime is achieved and, implicitly, more of the strength-generating phase, C-S-H, is formed with the addition of various reactive silica materials. Also, the study demonstrated that certain additives or combinations of additives were more effective than others.

STUDIES OF CEMENT/ROCK (MINERAL) INTERFACE AND BONDING

Knowledge of the interface or zone of contact between the plugging material and the host rock is critical in considerations of borehole plugging. This zone has the potential to be the weakest link in the multiple-barrier chain, a possible path of fracturing and ground-water transport after sealing of a repository. Certainty of the permanence of a cement-based repository seal requires full knowledge of physical and chemical interaction between the cement and the host rock, and the rate at which changes may take place.

Cement and Rock Experiments

These studies were carried out with two types of rock: a quartzitic sandstone and grains of slag, a "reactive rock" prototype, in order to contrast different interfacial zones.

Tensile tests and subsequent scanning electron microscope (SEM) examination of the interface region of a Class H + ferrosilicon dust + quartz mix cured in place on top of a polished disk of quartzite for 7 days at 60 C plus 21 additional days at 90 C showed that the cement/rock parts were pulled apart along the interfacial region, giving a tensile bond strength of about 200 psi.

After separation of the cement/rock parts, some material is left behind as random patches on both the quartzite and cement faces. The interfacial material, different from either "cement" or "rock", appears solid with little associated porosity or crystallinity. The material is rich in calcium and also is more silicon-rich than the cement itself.

Substantial differences in reactivity between 27 C and 90 C were shown in SEM studies of Class C + slag + quartz mixtures hydrated for 14 days. The 27 C sample had sharp interfacial areas between the slag and the adjacent matrix material. The matrix/slag bond was not yet strong enough to break slag grains during compressive strength testing. The 90 C sample was more massive with very little evidence of voids. The slag tended to fracture through the grain and did not show interface separation, which indicates a significant increase in strength with temperature. Reaction rims were not sharp, but graded one into the other. This appears related to the observed increase in compressive strength with temperature.

Kinetics of Cement/Mineral Interactions

Details of reaction kinetics for predicting interface reactions can be more easily understood from single-material experiments. Samples of pure cement phases (Ca_3Si or alite) with single crystals of natural minerals (quartz, calcite, and halite) have been prepared and cured at 90 and 180 C. Some SEM observations have been completed and X-ray diffraction analyses are in progress.

DIFFUSION STUDIES

Ion Diffusion Through Hardened Cement

The results of ion diffusion measurements obtained before this reporting period show that the apparent diffusion coefficient is independent of the w/c ratio of the paste (w/c = 0.35 to 0.45), that is, of porosity of the samples for samples cured a relatively short time (7 days). During the current period, the temperature dependence of the diffusion coefficient is being measured to establish the mechanisms of diffusion. The ionic diffusion through quartzite (dominantly SiO_2 body) is being measured to compare with that through cement hydrate. The effects of electrical potential on the ionic diffusion are also being measured.

Ion Diffusion/Permeability Experiments

In addition to the passage of fluid, it is necessary to know the extent of transport of ionic species via permeating liquids. The fluid which had passed through a given sample at the conclusion of a permeability measurement of cementitious composite/rock core samples (limestone and quartzite) was analyzed. At this point the analytical data are too few and thus the values seem very similar, except for one case, where samples were cured in a limestone core which appeared to have leaked. The analysis of this liquid showed relatively higher calcium than in the low-permeability samples in limestone cores (1050 ppm versus 50 to 200 ppm); concentrations of minor Mg, Si, Al, and SO_4, and low K and Na. An argument can be made that if this sample leaked it probably leaked along the limestone/cement interface. SEM work on a cement/quartzite interface showed that this interface material was of different composition from the cementitious mix or rock. It is possible that this material along the interface is more soluble than the C-S-H matrix material. Examination of such data will continue.

SPECIAL STUDIES

Bacteria Deterioration of Cementitious and Related Materials

Work has continued on collecting and compiling the literature on microbial deterioration of cement and related building materials. The literature has been categorized according to the following topics: corrosion of cement, concrete, and mortar; corrosion of building stones and rocks; corrosion of other building materials; and environmental specializations such as thermophiles and barophiles.

Ancient Cements, Mortars, Concrete

The study of performance of ancient cements, mortars, and concrete provides one important line of evidence regarding long-term, man-made materials performance. Photographic documentation of ancient cement and concrete samples was completed prior to any additional destructive study of these specimens. Differential thermal analysis (DTA) and thermal gravimetric analysis (TGA) of these samples (15 including certain rocks which may have been used as raw materials) are presently being conducted. All samples have been X-rayed using a computerized Phillips diffractometer; analysis of the data will follow some software modifications. Initial microprobe analyses of selected samples were inconclusive because of the difficulty in producing the required highly polished surfaces for quantitative analyses. Additional studies are in progress.

Los Medaños Area Cores

Cores from the Los Medaños area (AEC-7 and AEC-8 holes) have been installed in the permanent core storage and archiving facility of the Materials Research Laboratory. Eighteen samples have been taken from two intervals of the AEC-7 core. These intervals correspond to depths of 1685 to 1692 feet and 2998 to 3018 feet. X-ray diffraction of these samples has been completed.

The major mineral of the upper interval is halite (NaCl, PDF 5-628). Albite [$Na(AlSi_3O_8)$ PDF 20-554], a detrital mineral in evaporites, was identified in one sample. Clay minerals and iron oxides also may be present, but identification of other accessory minerals will be accomplished when they are isolated in the water-insoluble fraction of the samples.

The lower interval (2998 to 3018 feet) studied to date is composed of two major minerals in two distinct lithologies. These are: halite in coarsely recrystallized clear rock salt beds and anhydrite ($CaSO_4$, PDF 6-266) in finely crystalline beds, with apparent stringers (thin discontinuous interbeds) present in the halite. Accessory magnesite ($MgCO_3$, PDF 8-479) was identified in several samples from this interval.

Materials Selection and Evaluation

The objective of these studies is the improvement of technology for use of cementitious materials for repository sealing applications. Potential borehole plugging and shaft-sealing materials, including cementitious formulas modified for field tests, and new experimental types are being investigated. The problems of processing emplacement, reliability, and long-term stability are addressed in research to establish the effects of composition and particle characteristics of components upon the rheological properties, to investigate volume stability, and to determine various mechanical, physical, and thermal properties as both indicators of early suitability and predictors of longer term performance.

MIXING/PLACING CHARACTERISTICS: RHEOLOGY

Assurance of placeability is one of the major factors in a new mix design. A joint effort under way involves collaboration of the Pennsylvania State University Materials Research Laboratory (PSU-MRL) and Waterways Experiment Station (WES) personnel and concerns the investigation of a new dense cementitious mix suitable for use in borehole sealing/plugging in the Los Medaños area. The mix proposed by PSU-MRL personnel utilized a coarse American Petroleum Institute (API) Class H cement, fly ash, calcium sulfate, a superplasticizer, defoaming agent, salt, and water. Subsequently, a modification was suggested by WES personnel involving a change in the mixing water to a saturated $CaSO_4$ solution. Viscometric measurements were undertaken to investigate the effect of the modifications upon the rheological properties and consequent pumpability.

A systematic study of variations to the mix was carried out. All mixtures produced within the range of variations tried were sufficiently fluid for pumpability, but the use of the modified mixing water resulted in an early separation of liquid and solid fractions during testing, causing settling. A series of viscometric studies therefore was made, in which ingredients were systematically removed to determine the cause of settling. Table 1 summarizes the combinations of materials, the components deleted in each experiment, observations on the settling time, and the flow pattern.

A complex interaction occurs among the several components of the mix, but it was found that the more favorable rheological characteristics were evident in the mix as originally conceived, with use of deionized mixing water rather than calcium sulfate-saturated water for mixing. A second alternative, yielding mixes with a higher viscosity, but within suitable range, is to delete the defoaming agent as well as the dissolved sulfate from the mixing water. Two shipments (received about 1 month apart) of the same type of cement from the same plant were compared. However, no differences due to irregularities or irreproducibility in the cement itself were observed. For reference, measurements of zeta potential will also be made in the future for more complete diagnosis of the apparent rheological differences observed.

TABLE 1. SUMMARY OF OBSERVATIONS AND COMPONENT VARIATIONS FOR PROPOSED LOS MEDAÑOS MIX

Cement (H-7)	Gypseal (A31)	Fly Ash (B26)	Defoamer (A27)	NaCl (B8)	Plasticizer (A28)	Mixing Water		Thixotropic	Antithixotropic	Settling Time, min	Flow Pattern	
						$CaSO_4$ Sat.	Deionized				Irreg.	Reg.
X	X	X	X	X	X	X		X		5	X	
X	X	X		X	X	X		X		5		X
X	X	X			X	X		Low rpm	High rpm	5		X
X			X	X	X	X		High rpm	Low rpm	5		X
X			X		X	X		Newtonian	Newtonian	5	Slight	
X						X		High rpm	Low rpm	5	Slight	
X	X	X	X	X	X		X	X		∼5		X
X	X	X		X	X		X	X		15		X
X	X	X			X		X	Low rpm	High rpm	15		X

VOLUME STABILITY OF HARDENING AND HARDENED COMPOSITES

These studies primarily involve determining the early hardening and volume change characteristics, which are expected to have significant effects on controlling long-range properties. Measurements were made on pastes prepared with three different Class C and Class H cements. Cement C-6 had a specific surface (Blaine) of 3800 cm^2/g, while the others, cement C-7 and cement H-6, have not yet been measured.

In general, C-6 and C-7 were found to behave very similarly. Small differences in the rate of shrinkage were observed during the first 4 hours using a w/c ratio of 0.30, C-7 showing a higher rate of shrinkage than C-6 during that period. After 4 hours, both cements reached a similar rate of shrinkage; at the end of 24 hours the overall shrinkage for C-6 was 0.83 percent, while that for C-7 was 0.76 percent.

As expected, there was a big difference between the results from the coarser cement H-6 and the two Class C cements, C-6 and C-7, when prepared at the same water-to-cement (w/c) ratio. At the end of 24 hours, cement H-6 showed a shrinkage of 2.26 percent, a total difference of about 1.47 percent between H-6 and the Class C cements. This difference was attributed to the lower surface area of the Class H cement. According to the API recommended specifications, Class C and Class H cements should be used with a water percent by weight of cement of 56 and 38, respectively. Possibly, the Class C cement also combines more water in hydration. The main difference in the rate of shrinkage is observable between 4 and 14 hours after mixing; Cement H-6 reaches a maximum rate of shrinkage of 0.29 percent/hr after 9 hours, again an effect of its coarseness. Cement C-6 shows a maximum shrinkage rate of 0.12 percent at 4 hours and C-7 shows 0.13 percent at 5 hours, while both class C cements go through a minimum just when Class H is reaching a maximum rate of shrinkage. The three cements reach a stable period at 14 hours, after which their rates of shrinkage fluctuate between 0.03 and 0.01 with a tendency to decrease with time.

Other comparisons were made, varying the w/c ratios of Class H cement mixes. Similar volume change behavior was observed in 0.30 and 0.375 w/c Class H mixes up to 14 hours, but after this time the mixes with the higher w/c ratios continued to change volume significantly, indicating the importance of controlling the w/c ratio.

THERMAL PROPERTIES

Two main types of thermal property studies are currently being made. The first is the determination of the heat evolution characteristics of cement hydration behavior, to ensure reproducibility of properties and to enable prediction of the heat evolved during emplacement and the early postemplacement period. The second study is on thermal expansion of hardened materials, the properties which may be used to predict thermomechanical compatibility of plug/seal material with host rock.

Heat Evolution During Hardening: Calorimetry

Effects of Components. Since the major mineral components of portland cements are the silicates, heat evolution characteristics of tricalcium silicate (Ca_3Si) and dicalcium silicate (Ca_2Si)

and their mixtures were investigated. The hydration of the more reactive Ca_3Si is characterized by a small first peak of heat evolution, followed by an induction period of relative inactivity which is, in turn, followed by the acceleration period to give rise to a second peak, whereas the hydration of β-Ca_2Si has only a small first peak, followed by an inactive period which does not give rise to a second peak within the period measured. Additions of Ca_2Si to Ca_3Si did not significantly affect the hydration of Ca_3Si, but proportionately depressed the total heat evolved within the early hours.

Effects of Storage. Since effects of storage (aging) of cement can control its performance during hydration, these were investigated using some simulated aging techniques. While experiments were carried out for long periods, it was found that simulated aging at 95 percent relative humidity for even 1 day caused a significant retardation in heat evolution as characterized by decrease in amplitude and shift (delay) in peak positions by as much as 1 day.

Temperature Dependence. Since temperature is known to accelerate hydration reactions, a series of experiments examined this temperature dependence. Expected plug emplacement temperatures will of course be higher than room temperature. Furthermore, accelerated tests are used to predict longer term performance of plug materials, and the effects of elevated temperature curing on potential properties must be known. Three types of cement (I, III, and V) were studied (25, 35, 45, and 55 C). Figure 1 shows the relation between the rate of heat evolved (dQ/dt), represented by the maximum of the second peak of the heat evolution curve. The relationship appears to be linear when plotted on a log scale versus 1/T, as expected. Activation energies for hydration may be determined from plots of time of maximum reaction versus temperature and the relationships used in some instances to make comparisons between normal and accelerated reactions, and to determine the limits of performance extrapolation.

Thermal Expansion

A series of experiments is in progress to determine the thermal expansion characteristics of cement pastes and composites containing various additives and to determine the magnitude that might be expected from various materials. Four series of samples were prepared and run to measure thermal expansion. Those samples are: H-3, H-3 + 30 μm quartz, H-3 + fly ash, and H-3 + NaCl. In all the samples, API mixing procedures were followed. The w/c ratio was 0.375 and the cement/additive ratio was 4. The heating rate was ~3 C/min.

Figure 2 shows the typical thermal expansion for all the cement mixes in which there is expansion up to about 100 C, followed by a volume contraction due to the loss of both evaporable and nonevaporable water. If the heat was cycled in the higher temperature range, the sample continued to contract on the cooling cycle; this was followed by expansion on the heating cycle, due to true thermal expansion of the solid.

Comparisons in the region below 100 C showed that cement paste thermal expansion generally decreased with curing time, that cement composites with solid additives (such as quartz) showed a lower thermal expansion than the paste, and that with additives such as fly ash there was a negative thermal expansion up to about 6 weeks of curing time, apparently due to the lower degree of reaction than in neat cement paste. With longer curing time and a

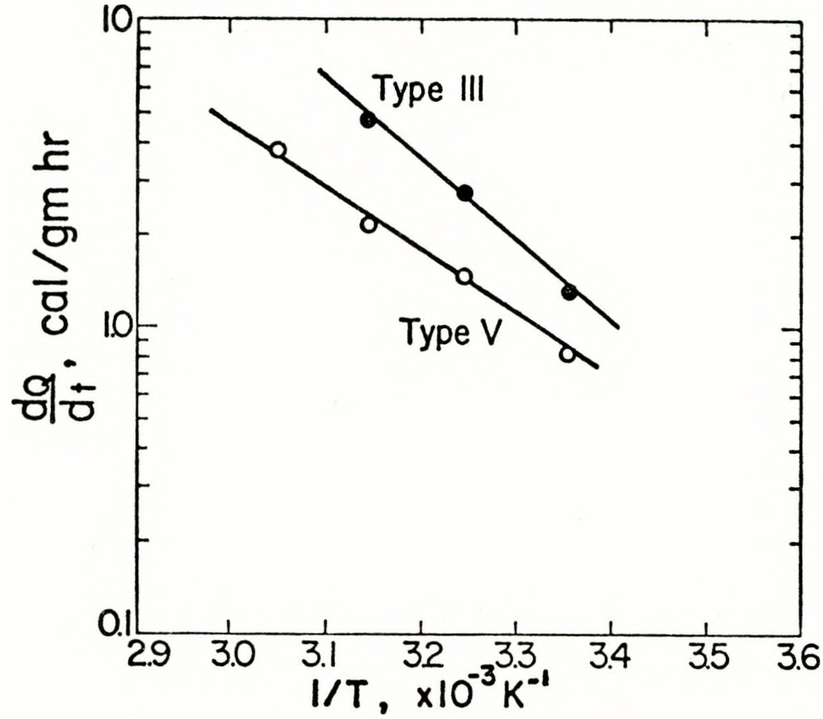


FIGURE 1. AMPLITUDE OF SECOND PEAK AS A FUNCTION OF TEMPERATURE

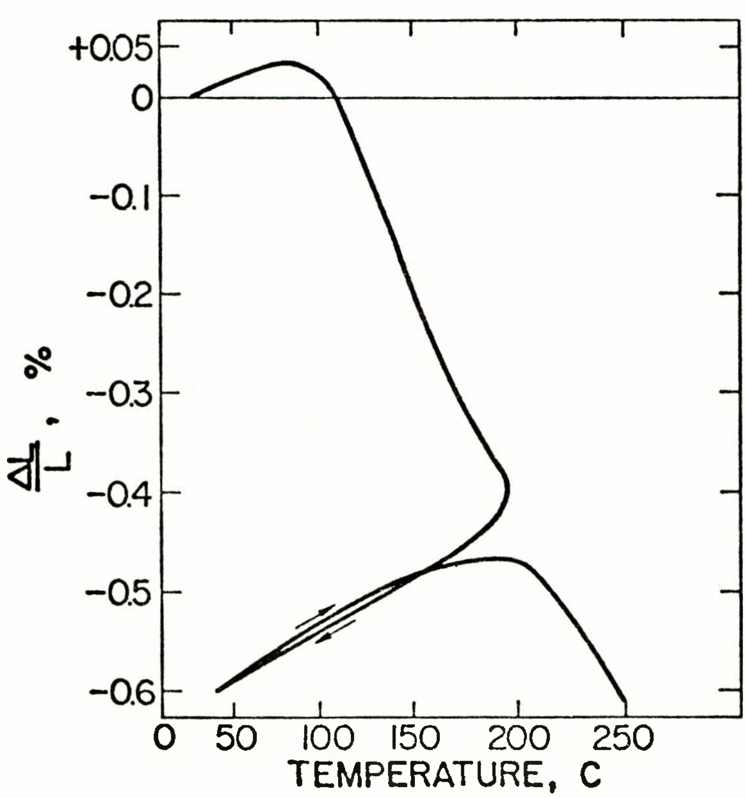


FIGURE 2. TYPICAL THERMAL EXPANSION OF CEMENT MIXES

larger percentage of additive (aggregate), the thermal expansion characteristics will apparently take on more characteristics of a dense rock.

MECHANICAL PROPERTIES

Investigation of a range of mechanical properties is important for diagnosis of new materials. Among the measurements made are compressive strength, microhardness, and elastic moduli.

Compressive Strength and Microhardness

Because microhardness measurements are easily made on small samples and in interfacial zones with rock, such measurements are used for characterization of a number of materials. The relationship between microhardness and compressive strength has been further investigated, during this period, on a new slag-containing mix formulation. This series of experiments was also designed to permit comparison of the results utilizing cylindrical sample molds (1 inch in diameter) and the results of curing at two different temperatures. Many experimenters have found it difficult to cure samples at 90 C, and it was desired to test the effectiveness of the method used.

The data are summarized in Table 2, which shows the compressive strengths (normal destructive testing) and microhardnesses of the mix, cured at either 27 C or 90 C immersed in saturated $Ca(OH)_2$ solution for 14 days. The standard deviations obtained were satisfactory for both cylindrical and cube mold specimens at both temperatures, and as usual the strengths measured were higher for the 2-inch cubes than for the cylinders. The microhardnesses measured were independent of the sample geometry, which reflects a difference in the characteristics of the property measured. However, the averages of both compressive strength and microhardness were found to increase at increased curing temperature, by about 35 percent for the former and 28 percent for the latter.

Elastic Properties

A series of studies is under way to determine elastic moduli by sonic resonance frequency measurements. Young's modulus obtained by static destructive tests will be compared with the values obtained by sonic measurement. Some low w/c pastes have been prepared which have very high compressive strengths as measured destructively. Measurements of Young's modulus, modulus of rigidity, and Poisson's ratio are under way using bars cast from the same mixes and torsional, transverse, and longitudinal resonance frequencies. Also, standard Lavite samples are being measured for reference.

PERMEABILITY: THE EFFECT OF W/C RATIO AND CURING TEMPERATURE

Permeabilities are, of course, one of the major concerns regarding the performance of seal/plug materials. Experiments are in progress to determine factors that control permeability in a given series of cementitious mixes. Porosities for a series of Type I cement pastes with

TABLE 2. COMPARISON OF COMPRESSIVE STRENGTHS AND MICROHARDNESSES OF CUBE AND CYLINDRICAL SPECIMENS OF A CLASS C + SLAG + QUARTZ ADJUSTED PORTLAND CEMENT (C/S = 0.83, w/s = 0.45) $Ca(OH)_2$-SATURATED SOLUTION CURED 14 DAYS

Sample No.	Sample Geometry	Curing Temp, C	Compressive Strength, MPa[a]		n/na	Microhardness, MPa[a]		n/na
800389	Cylinder	27	45.93	(2.35)	3/5	213.78	(10.59)	10/10
800390	Cube	27	57.64	(0.90)	3/5	207.30	(8.24)	9/10
800391	Cylinder	90	64.88	(2.14)	6/6	264.42	(9.60)	9/10
800392	Cube	90	76.85	(4.15)	4/4	273.94	(11.28)	10/10

(a) Values in parentheses are $\pm \delta$.

w/c = 0.35, 0.40, and 0.45 cured for 4 weeks at 27 and 60 C were determined from both saturated and dry weights. As expected, the porosities increased with increasing w/c ratio. The porosities of the 27 C series were higher than those of comparable members of the 60 C series, presumably due to a lower extent of reaction. However, for each member the 60 C series had a higher permeability. Thus, not only the total porosity but also the pore size distribution is important in controlling permeabilities. More complete results will be reported subsequently.

REFERENCES

Roy, D. M. 1980. "Geochemical Factors in Borehole and Shaft Plugging Materials Stability", paper presented at International Borehole Plugging Conference (ONWI-DOE/OECD), Columbus, Ohio, May.

WBS 1.2.3

Project: Repository Sealing Project

Principal Investigator: D'Appolonia Consulting Engineers (E. E. Stephenson)

ONWI Project Manager: F. L Burns

Objective

The objectives of this program include: (1) review and coordination of ongoing WIPP site studies and field testing for borehole plugging, (2) development of initial but generic design criteria for both borehole plugging and shaft sealing, (3) evaluation of differences and similarities between shaft sealing and borehole plugging, (4) evaluation of other sites as they influence generic aspects of design criteria, (5) development of a Quality Assurance Manual applicable to generic repository sealing studies, (6) participation in the development, review, and evaluation of the ONWI program of geochemical studies for repository sealing, (7) participation in defining and developing the overall objectives of the NWTS repository sealing program and in the review of the current activities, and (8) participation in the organization of a workshop in repository sealing.

Progress Reported Previously

This project was initiated on November 6, 1978. Liaison with the field activities at the WIPP site continued. The geochemical needs of the repository sealing program were reviewed and a preliminary outline of the requirements formulated.

Activities During the Reporting Period

Objectives

Work conducted this quarter consisted of refining the preliminary engineering designs for repository sealing, continuation of the review and evaluation function for the geochemical program, and liaison with other groups performing repository sealing studies for ONWI. Development of program plans continued for the repository sealing field test in bedded and domal salt to be conducted during FY 81.

Procedures

Contact was maintained with the experimental group at Sandia. Visits were made to the field site to observe the final gas releases from the instrument package and review monitoring of the performance of the plug itself.

Conceptual designs for repository seals were studied through sensitivity analysis of shapes and fluid flow. Continued refinement of these design concepts is being conducted using numerical modeling techniques to perform sensitivity analysis on the designs.

Geochemical requirements were determined to assist in the defining of a study program to help answer questions concerning the longevity of sealing materials. A review of all efforts directed toward repository sealing was conducted. The list of the requirements of ONWI's geochemical program was completed and transmitted to ONWI as a preprint for review.

Results

Seal designs are being analyzed by the finite-element technique. Two shapes have been studied to determine their effect on fluid flow. Results to date indicate that:

- Shapes that remove the disturbed zone around a penetration and provide complete bonding to the rock will reduce the fluid flow.
- If the contrast in the permeability of the seal and host rock is not very large, the total flow potential is not appreciably changed from that in the undisturbed rock.
- As seal length is increased, flow is decreased.

A report was completed on the differences in borehole and shaft and tunnel seal requirements and a recommended program of investigation was developed. The main differences were:

- The size of shafts and tunnels allows better access (than boreholes) and subsequent construction and quality control for seal installation.
- Large seal volumes for shaft and tunnel seals require further research in installation and behavior of bulk seal material.
- Tunnels, due to their orientation, present a special condition of unsymmetrical stresses as well as difficult sealing at the crest (top) of the tunnel.

The objectives of the NWTS Repository Sealing Program were reviewed and updated in cooperation with ONWI and new milestones were established.

Conclusions

The repository sealing program has been progressing as scheduled. A uniform and comprehensive goal for designing seals has been developed and designs are being evaluated to determine how well they meet the goal. The plan for the ONWI and NWTS Repository Sealing Program was reviewed and is being updated and modified to reflect the progress and development of the past three quarters.

WBS 1.2.3

Project: Borehole Plugging Program

Principal Investigator: Sandia Laboratories (C. L. Christensen)

ONWI Project Manager: F. L. Burns

Objectives

The objectives of this program are:

(1) To develop, test, and evaluate candidate cementitious grouts and other materials for use in and support of the laboratory and field testing program; to assist in development and implementation of a geochemical program to ascertain and verify the long-term stability and suitability of cementitious and other materials as well bore plugging materials

(2) To assess, develop, and modify appropriate instrumentation techniques to obtain the data required to verify plug performance

(3) To provide an in situ environment for emplacing and evaluating potential plug designs.

Progress Reported Previously

The current Borehole Plugging Program (BHP) was initiated in September 1978 with full-scale operation under way by February 1979. The program has evolved into four major tasks: management, materials, instrumentation, and field test. The management function has defined a series of laboratory and field-test concepts directed at achieving the program objectives. The remaining tasks have undertaken the implementation of these concepts. Materials development centers around cementitious plugging materials with both fresh water and brine mixes, along with fly ash and other additives to improve permeability and emplacement characteristics; instrumentation development assesses program needs and provides resources as required; and the field test implements the in situ plug emplacement, testing, and verification as required. The current field test is the Bell Canyon Test (BCT).

The prognosis from previous work indicates that cementitious materials could provide adequate plugs; their attractiveness stems from the availability of existing technology coupled with their favorable economics of materials and emplacement. One of the useful results obtained to date shows that push-out strength tests, frequently employed in concrete testing procedures, are inadequate to assess the permeability of the interfaces between the grout and the rock. Heretofore bond strength was considered to be an indicator of plug adequacy; it has been demonstrated that a strong bond does not necessarily result in a low interface permeability. Additionally, when grouts are tested as plug material in a candidate rock sample, the type of mix water is important. Initial testing of grouts used a brine mix water on the assumption that these plugs, when emplaced in a salt formation in a brine-filled wellbore, would result in a better bond to the formation. However, when these mixes were cast in the anhydrite rock samples of the BCT plug zone, higher-than-expected permeabilities occurred at the interface due to a salt residue resulting from the cement hydration. A change to a fresh-water mix alleviated this effect and is utilized in the plug mix currently in place in the BCT. While results are still being evaluated, indications are that in nonsalt emplacement, the impact of brine mix water must be carefully assessed.Testing of this hypothesis is under way at the U.S. Army Corps of Engineers Waterways Experiment Station, Vicksburg, MS. This testing is directed at determining the acceptable salinity which should be permitted in a given plugging application.

Progress reported last quarter included a program review and update including an approval to proceed with the Potash Core Test (PCT). Work was initiated to develop a calculational model to assist in field-test plug design.

Activities During the Reporting Period

MANAGEMENT AND DESIGN

Objective

The objective is to provide tested designs for repository plug systems.

Results

Consequence assessment models, which include borehole plug efficiencies, were drafted and provided to Sandia. An internal review has been made and it was recommended that plug formation permeabilities be incorporated in the revised version. The plug design model will incorporate field test results and the effects of in situ stress relief at the plug zone.

The draft of the BCT results report has been submitted for review.

MATERIALS

Objective

The objective is the laboratory development of candidate cementitious mixes for repository plugs.

Procedures

Work has been initiated at Waterways Experiment Station to evaluate the effect of capillary action in a porous plug when an interface between brine and gas exists. Ibrahim, Tek, and Katz (1970) showed that a threshold pressure exists for gas flow between a brine and gas phase in a porous plug; permeability testing generally uses a liquid source on a saturated sample or a gas source on a dry sample to determine permeability. In the threshold pressure test a gas source is used on a saturated sample. Results suggest that in this case pressures of several hundred psi may be required to force the gas through the sample in the low permeability regime of the grout and rock. The impact of such an effect must be included in plug design.

Conclusions

Test results to date support the acceptability of grouts as plug materials in the short term.

REFERENCE

Ibrahim, M. A., M. R. Tek, and D. L. Katz, 1970. "Threshold Pressure in Gas Storage", American Gas Association, Inc., 1515 Wilson Blvd., Arlington (Rosslyn), Virginia, 22209.

WBS 1.2.3

Project: Geochemistry of Cementitious Materials

Principal Investigator: Corps of Engineers, Waterways Experiment Station (K. Mather)

ONWI Project Manager: F. L. Burns

Objective

The Structures Laboratory will optimize proportions for grouts to be used in tests at AEC-7 and similar geologic settings. Cements, pozzolans, and admixtures with fresh water or water containing salts appropriate to render the grout compatible with appropriate physical, mechanical, chemical, and thermal properties of the wall rock will be considered. This will require characterization of wall rock, grouts, and ultimate hydration products. Also investigated will be other grout mixtures for different geological settings using different materials and expansive systems. Precision and accuracy data on methods for characterization and testing will be developed.

Progress Reported Previously

This is the second quarterly report for this project. Work began on 2 January, 1980. Technical progress consisted largely of obtaining and testing materials for specification compliance through applicable ASTM methods and crystalline phase characterization through petrographic methods.

Activities During the Reporting Period

Objectives

The objectives have been:

(a) To summarize previous work that had been conducted in cooperation with the Grouting Subgroup, and to extract from that work items that had suggested concepts further developed in FY 79 under a small planning task with ONWI

(b) To identify the sources and complete the analyses, testing, and characterization of cement, pozzolan, expansive additives, and water-reducing admixtures that have been used in the Bell Canyon Tests and that are to be used in improving the proportions of grout to achieve the best possible formulations in terms of ultimate properties

(c) To continue obtaining and characterizing different materials that will be used in optimizing grout mixtures, to combine different amounts of these materials into grout mixtures, and to test these mixtures to find the optimum mixture or mixtures for different environments.

(d) To consider and demonstrate the mechanisms of formation and the sources of materials that do contribute to the expansion of systems consisting of cement without tricalcium aluminate, fly ash, plaster of paris, and water

(e) To improve the characterization of fly ashes by developing a method for progressive solution and analysis combined with repeated X-ray examination of the samples, with the aim of determining the proportions and composition of glass and crystalline materials that are present in samples from the same source or from different sources

(f) To conclude planning of the work by the Structures Laboratory (SL) and by the Materials Research Laboratory of the Pennsylvania State University to establish mutual credibility, precision, and accuracy.

Procedures

The Cement and Pozzolan Group completed physical and chemical testing of two fly ash samples (AD-592(4) and AD-615(2)) and of a silica fume (AD-536(3)) in accordance with Federal Specification Sheet SS-C-1960/5A, "Pozzolan, for use in Portland Cement Concrete". This is much like American National Standard ANSI/ASTM C 618, "Standard Specification for Fly Ash and Raw or Calcined Natural Pozzolan for use as Mineral Admixture in Portland Cement Concrete", except that the Federal Specification calls for doing the lime-pozzolan test with cubes instead of cylinders. Our Group has found the use of cubes to be preferable. AD-592(4) is the latest shipment of the fly ash that was used in the two WIPP-site tests; AD-615(2) is an unusual fly ash obtained from the Nevada Test Site; AD-536(3) is a new shipment of silica fume used in ongoing research work at the SL. The Materials and Concrete Analysis Group (M/CA) completed testing of expansive cement (RC-855) for restrained expansion by ASTM Designation C 806, "Standard Method for Restrained Expansion of Expansive Cement Mortar". The petrography and X-ray portion of the M/CA Group did X-ray diffraction work on these pozzolans and on other samples. The SL Concrete and Grout Group made concrete specimens with and without AD-627. This is a chemical water reducer that may be a high-range water reducer. The specimens were made for testing in accordance with American National Standard ANSI/ASTM C 494, "Standard Specification for Chemical Admixtures for Concrete". The SL Evaluation and Monitoring Group is testing these concrete specimens in accordance with American National Standard ANSI/ASTM C 666, "Standard Test Method for Resistance of Concrete to Rapid Freezing and Thawing", Procedure A.

Results

In general, the characterization of materials has shown the expected results. Some specific items are mentioned below.

- Maleic acid treatment, followed by X-ray diffraction examination, of the Class H Portland cement (RC-853) from the Lone Star Maryneal plant at Sweetwater, Texas, showed it to contain a small amount of noncubic tricalcium aluminate (C_3A).

- X-ray diffraction examination of the no-C_3A Incor cement (RC-854) from the same plant verified that no detectable crystalline C_3A was present.

- Intensive study of the Dowell fly ash (AD-594 and subsequent shipments) by X-ray diffraction indicated that the glass interfaced with satisfactory identification of all phases. This problem was the basis of a task to determine whether selective dissolution by chemical treatments followed by X-ray diffraction examination can result in more satisfactory identification of all the crystalline phases that may be present in such a complex material. This is the fly ash that was used in the grout during the September 1979 and February 1980 Bell Canyon field tests at AEC-7.

- The fly ash from the Moapa Power Co., Moapa, Nevada, (AD-615(2)) which was received from the Nevada Test Site was unusual in that it probably came from an older, less efficient collection system. It had a high loss on ignition (11.5 percent), was coarse, and was high in quartz content; the first two items are probably due to a high carbon content.

- The new sample of the silica fume (AD-536(3)) proved to be similar to earlier samples, which is what was desired.

- The restrained expansion test of expansive cement RC-855 showed average expansion of 0.03 percent at 7 and 28 days. This is slightly less than the minimum 0.04 percent at 7 days specified by ASTM designation C845, "Tentative Specification for Expansive Hydraulic Cement". However, review of previous data for this material from this source shows that this is in line with the usual results. As a result of this, another source of expansive cement is being considered in addition to this one.

- Evaluation of the water reducing admixture (AD-627) is still under way.

Conclusions

The complexity of the crystalline phases in modern lignite and subbituminous fly ashes is such that phase identification procedures need modification and improvement if identification is to be complete.

WBS 1.2.4

Project: Data Transmission Alternatives

Principal Investigator: TRW (P. Alexander)

ONWI Project Manager: N. C. Henderson

Objective

The objective of the Data Transmission Alternatives project is to develop and analyze techniques to transmit, to the surface, sensor data collected within, or adjacent to, a subsurface nuclear waste repository. The transmission system should be compatible with a wide variety of undefined measurement techniques, and adaptable to the geologic media encountered in all candidate repositories. Specifically, critical performance criteria which relate to data transmission systems connecting subsurface sensors with the ground surface will be defined. Moreover, methods for transmitting data from the waste repository to the surface which have the least potential impact on the geologic integrity of the repository, while not compromising data transmission requirements, will be identified.

Activities During the Reporting Period

During this period a tentative schedule was developed for performing the tasks required to accomplish the program objectives. A program plan governing implementation of the tasks is also being prepared. This plan contains a detailed description of program objectives and scope, the technical approach, program interfaces, a milestone schedule, and a cost schedule.

One of the first problems facing the project team is to prioritize the large number of variables involved in this data transmission problem. An evaluation matrix has been developed to aid in this process. A three-dimensional representation of this matrix is presented in Figure 1. Each transmission concept considered (leftmost axis) must be evaluated in terms of the behavior of the component subsystems (rightmost axis) as measured against the expected performance criteria (vertical axis).

The example illustrates that each of the axis entries has a number of associated subentries which are not shown. It is anticipated that a ranking scheme will be developed so that the matrix can be used as a screening tool to select the more promising transmission concepts for detailed evaluation. Dealing with the evaluation matrix can be greatly simplified by taking a two-dimensional slice through any one of the axes. For instance, for a particular transmission concept it is only necessary to construct a table relating subsystems to performance. Alternatively it might be more desirable to look at transmission link advantages of various concepts by tabulating expected link performance for the various transmission concepts. Another possibility would be to evaluate the impact of various transmission concepts on geologic integrity by evaluating the impact of the subsystems. These various approaches will be considered during the next quarter.

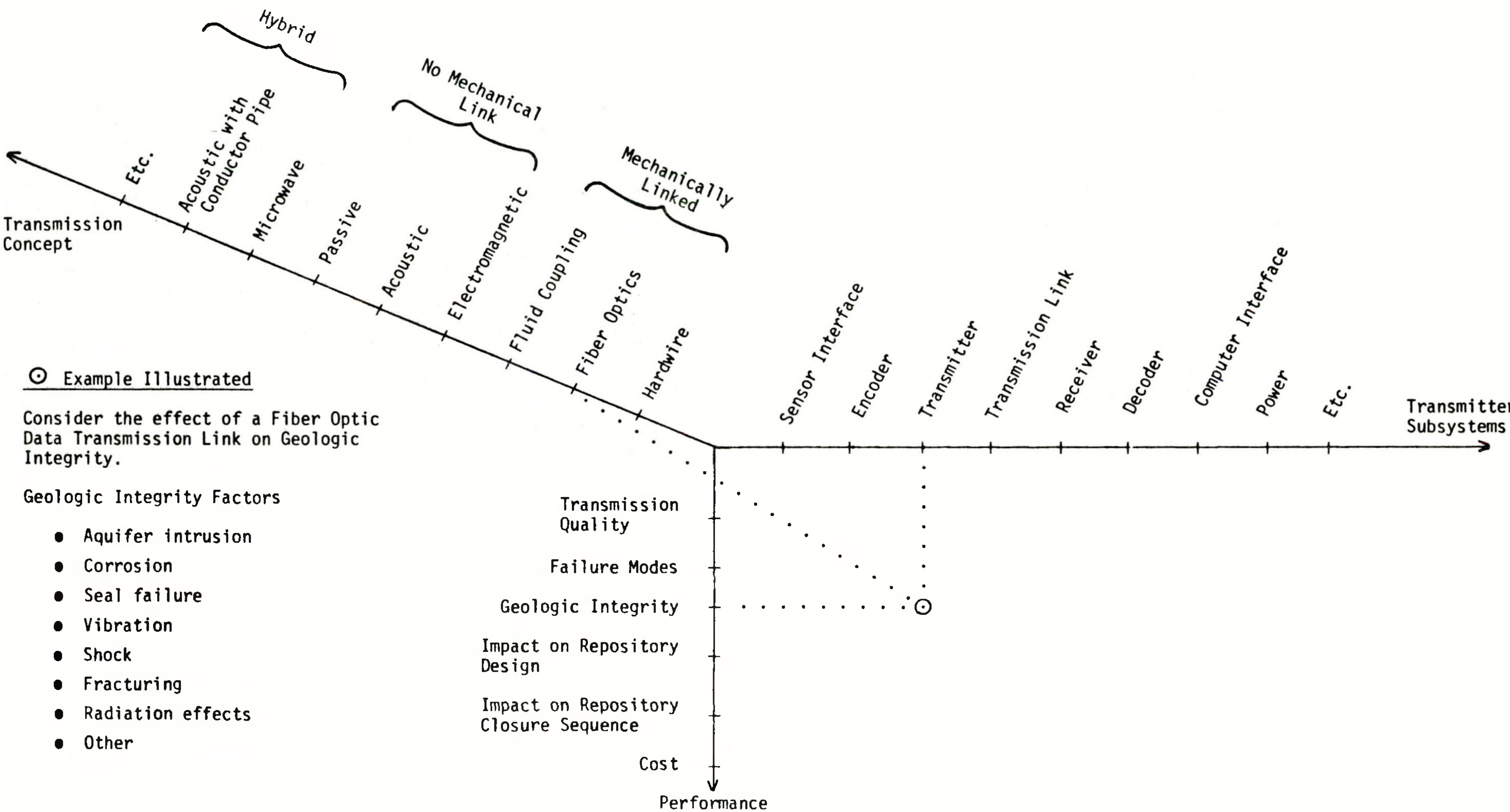


FIGURE 1. THREE DIMENSIONAL EVALUATION MATRIX

WBS 1.2.4

Project: Definition of R&D Needs for Repository and Field-Test Instrumentation

Principal Investigator: Envirosphere Co. (L. T. Skoblar)

ONWI Project Manager: N. C. Henderson

Objective

The overall objective of this study is to ensure that all required instrumentation for both field testing and geologic repository testing/monitoring is available when required to support ONWI's master NWTS development plan. To accomplish this objective, original work and literature searches are conducted to determine the gaps, if any, that exist between "what needs to be monitored" and "currently available commercial instruments". One result of such a comparison is the identification of explicit research and development and/or further study needs to support the NWTS program.

Progress Reported Previously

This study was initiated 1 March 1980. Progress reported previously noted the development of a format, outline, and overall structure through which the technical work would be conducted.

Activities During the Reporting Period

OBJECTIVE

The ONWI Program Plan was reviewed to identify all previous suggestions for instrumentation R&D. In the process, the task force was to establish functional requirements and define anticipated operating environment and interface requirements for all necessary instrumentation. Based on this data and the task force's own expertise, areas for R&D were defined where necessary to meet all relevant performance requirements. The final objective of this effort was to develop a Program Plan, i.e., a strategy for accomplishing the requisite R&D.

In addition to Program Plan development, a report is being prepared which provides many of the details not appropriate for a Program Plan. This backup report will serve to document and provide references for pertinent information.

Finally, the activities this quarter included efforts to present the latest planning information, including task descriptions and schedules, regarding studies and R&D necessary to support instrumentation technology development for a mined geologic repository.

PROCEDURES

A comprehensive assessment was conducted of all existing repository design reports, instrumentation needs for the field testing program, and other instrumentation program plan documentation. Functional requirements were identified where possible, and the capability of currently available instrumentation was evaluated against these requirements. From this process, the technical scope of instrumentation R&D needs (including the need for further study) were identified. Once identified, specific work elements necessary to carry out the studies and/or R&D were structured.

RESULTS

Although a more complete identification of instrumentation development needs is not expected before year's end, it is possible at this time to identify a partial list of such needs and provide a brief description of the work effort anticipated. In the following listing, potential development efforts are identified by the nature of the effort, i.e., "further study" implies that sufficient information is not yet available to determine whether or not R&D is required; conversely, "R&D" indicates that a scope of work and technical objective can be identified at this time.

Test and Verification Instrumentation

Geologic

In Situ Stress Monitoring. (R&D)—To develop accurate and reliable in situ stress measuring instrumentation for use in the repository operations and postclosure monitoring time phases; (Study)—To define required sensitivity, durability, and environmental requirements (initiated during field-testing time phase)

Surface Displacement. (Study)—To determine feasibility of upgrading present piezometers to meet life-span and reliability requirements (initiated during field-testing time phase)

Subsurface Displacement. (Study)—To evaluate the accuracy and sensitivity of available instrumentation, including the possible use of laser interferometers (initiated during field-testing time phase); (R&D)—To develop present extensometers to extend their accuracy for use in the repository operations and postclosure time phases

Thermal. (R&D)—To develop in situ testing techniques for measuring emissivity, thermal heat transfer coefficient, thermoelastic constants, thermochemical and thermomechanical properties for use in all three time phases

Tectonic

Passive Seismic Monitoring. (Study)—To evaluate and refine current technology with emphasis on acoustic emission instrumentation, define sensitivities required for microseismicity monitoring systems, and perform modeling studies to reduce the subsurface acceleration associated with both distant and near-field seismic events (initiated during the field-testing time phase)

Active Seismic Monitoring. (Study)—To establish a seismic data base which includes travel time from near-surface sources to sensors located in, and adjacent to, the repository; repeated high resolution reflection surveys; and repeated surveys of frequency attenuation associated with changes in in situ repository conditions. To develop modeling to determine the required instrumentation sensitivities (initiated early in the repository operations time phase)

Hydrologic

(R&D)—To refine existing porosity measuring instruments and to relate porosity to permeability in host rock types of interest; (R&D)—To refine surface resistivity equipment and techniques; (R&D)—To develop and refine crosshole tracer techniques suitable for various host rock types; (R&D)—To refine borehole TV loggers; (R&D)—To refine and increase the capabilities of macropermeability testing.

The above development activities will be used in all three time phases.

Ground-Water Geochemistry

(R&D)—To improve the sensitivity of borehole resistivity logging instruments; (R&D)—To improve the accuracy and reliability of borehole Eh sensors; (R&D)—To develop better analytical techniques for dissolved aluminum

Related Generic Activities

Boreholes. (R&D)—To develop drilling technology which will minimize contamination; (Study)—To determine whether existing technology can provide useable boreholes with acceptable life spans

Radiological Monitoring Instrumentation

Facility Monitoring

(R&D)—To develop a continuous Iodine-129 monitoring system which will operate in dust or salt airborne leadings up to 10/mg/m^3 (required for the repository operating time phase)

Environmental Monitoring

(R&D)—To develop a standardized method for routinely detecting ^{124}I in milk at a level of sensitivity of 1 pci/liter (required prior to repository operations); (R&D)—To develop a standardized method for the detection of ^{99}Tc in ground water (useful to all three time phases)

Environmental Monitoring Instrumentation (Nonradiological)

No study or R&D needs have been identified within this category to date.

Facility Monitoring Instrumentation (Nonradiological)

No study or R&D needs have been identified within this category to date.

Data Acquisition and Analysis

Data Transmission

(R&D)—Data telemetry techniques have been under investigation to provide a system for transmission of subsurface test information to surface data gathering stations (should be continued and expanded to address the longer operation time spans required for the repository operations and postclosure time phases)

Power Supplies

(R&D)—To develop reliable long-term power supplies for subsurface instrumentation and related electronics (required for the repository operations and postclosure monitoring time phases)

Generic Repository

(Study and R&D)—To develop a plan and hardware for ensuring reliable long-term operation of electrical interfacing components (i.e., connectors) in a hostile (corrosive) environment; (Study)—To develop three-dimensional conceptual arrangements of repository instrumentation in order to develop trade-off studies which include:

- Cluster-sensor packaging
- Electromagnetic interference problems
- Power supply grouping
- Data transmission techniques
- Data acquisition/signal conditioning
- Data display/storage configuration
- Instrumentation reliability/maintainability

These trade-offs need to be completed prior to repository operation.

One study which cuts across all instrumentation classification lines is a generic study to determine viable methods for environmental qualification testing of underground instrumentation. All repository monitoring and test instrumentation that will be emplaced within or immediately adjacent to the subsurface operations/storage area and intended for use in the repository operations and/or postclosure monitoring time phases will require qualification for both the hostile environment and long time periods of unattended operation. A generic study aimed at identifying the viable options to meet these requirements should prove to be a cost-effective approach before specific instrumentation development activities are initiated.

CONCLUSIONS

Some of the more significant preliminary findings resulting from instrumentation planning activities conducted thus far are:

- Not all R&D necessary to support repository operations can be identified at this time. Additional study activities must be initiated to refine these requirements.
- Location of instrumentation packages within the repository, e.g., clustering, depends to a great extent on details of repository designs not yet available. Some R&D could be eliminated/initiated based on this information.
- Many of the development needs identified relate to the longevity of instrumentation in the anticipated hostile environments.
- Developments to support the field-testing phase deserve top priority.

WBS 1.2.4

Project: Monitor for Detecting Nuclear Waste Leakage in a Subsurface Repository

Principal Investigator: Lawrence Berkeley Laboratory (S. Klainer)

ONWI Project Manager: N. C. Henderson

Objective

The purpose of this research is to develop an ultrasensitive specific monitor for actinides and tracer materials. The analytical approach selected by Lawrence Berkeley Laboratory (LBL) is resonance fluorescence spectroscopy. The end result of this research will be to provide an "early warning system" and a long-term monitoring capability for incipient waste-package failure. Such instrumentation will also assist in the conduct of certain field experiments such as brine migration and nuclide migration.

Introduction

A new ultrasensitive analytical technique based on the laser-induced fluorescence fluorimetry (LIFF) technique allows quantitative measurements of actinide, lanthanide, and tracer abundances in water samples with sensitivities many orders of magnitude higher than those presently achieved with current analytical methods. The principal focus of the present program is to develop monitoring instrumentation for those elements in ground waters associated with nuclear waste repositories.

The monitoring system provides for two modes of analysis: (a) an in situ system that provides direct chemical measurements in natural water systems over long distances (>1 km) using fiber optics and (b) the field laboratory system which is far more sensitive and involves (on-site) LIFF measurements on these materials after they have been coprecipitated (from ground-water samples) with an inorganic material such as calcium fluoride.

Proof of principle for the remote fluorescence measurements has been made at 0.2 km using an organic fluorescent tracer and communication-grade fiber optics coupled to a laboratory fluorimeter. Sensitivities in the parts per billion range and quantitative measurements with ~1 percent linearity have been realized.

Initial results, using coprecipitation, have demonstrated lanthanide sensitivities of 10^{-9} ppm and uranium sensitivities below 10^{-7} ppm. It is expected that uranium will be detectable below 10^{-9} ppm when the approach is fully developed. The projected plutonium sensitivity is of the same order of magnitude.

Activities During the Reporting Period

DESCRIPTION OF MEASUREMENT SYSTEM

A versatile laboratory fluorimeter (fluorescence spectrometer) has been assembled which is capable of making measurements utilizing both the fiber optic (remote) technique and the coprecipitation (high-sensitivity) method. The spectrometer has the following lasers:

- A Spectra Physics Model 171 multiline krypton laser which covers from 360 to 640 nm with a total of 8 watts of power.

- A Chromatix dye laser pumped by a high-repetition frequency pulsed neodymium laser for continuous scanning of excitation spectra over much of the visible spectrum.

- A Spectra Physics 165 argon laser with a total output of 4 watts to provide an alternative set of laser lines.

The procedures are as follows:

(1) The three lasers are coupled, with a set of beam redirector mirrors and a Claissen filter for isolating the desired excitation wavelength, to a specially made Spex right-angle optical bench containing an f/1.4 illumination lens and a f/1.2 collection lens. The lenses are in alignment mounts that permit a common focus ~100 μ in diameter to be obtained in a sample holder inclined at 45 degrees.

(2) The collected light is fed at f/8 into a Spex No. 14018 0.75-mm-focal-length double monochromator equipped with holographic gratings blazed at 5000 A.

(3) The monochromatized light is reimaged at f/2 onto a cooled RCA C31034A GaAs photocathode photomultiplier (PMT) in a Products for Research RF-TSA cooled housing. The PMT is operated at $<$ 2000 volts using a Power Design adjustable filtered HV source.

(4) The photoelectron pulses are conditioned, windowed, and counted by an Ortec photon counting system consisting of an Ortec 9301 pulse discriminator, an Ortec 9302 pulse amplifier/conditioner, and an Ortec 9349 ratemeter.

(5) The output of the ratemeter is fed to an HP 3455A electrometer having an HPIB interface and controlled by a Tektronix 184 Time Mark Generator.

(6) The electrometer is, in turn, coupled to a Tektronix 4051 graphics processor having a flexible disk attachment, a Tektronix 4631 hardcopy generator, and a Tektronix 4662 plotter.

Auxiliary equipment such as laser power monitors, beam attenuators, and polarizers are also included in the system.

The performance of the system is best checked by measuring a Raman (rather than a fluorescence) spectrum. Figure 1 shows the Raman spectrum of naphthalene generated as a systems calibration check. The far lower sensitivity of the Raman phenomenon, compared with that of fluorescence, permits the system's efficiency to be demonstrated.

IN SITU MONITOR

The in situ monitoring of an underground waste repository is accomplished by utilizing a network of buried sensors (fiber optic devices) in and around the burial site. Specifically, a laser fluorimeter (which can be placed in an environmentally controlled room) is connected to a network of communications-grade, radiation-resistant, fiber optics which have sensing

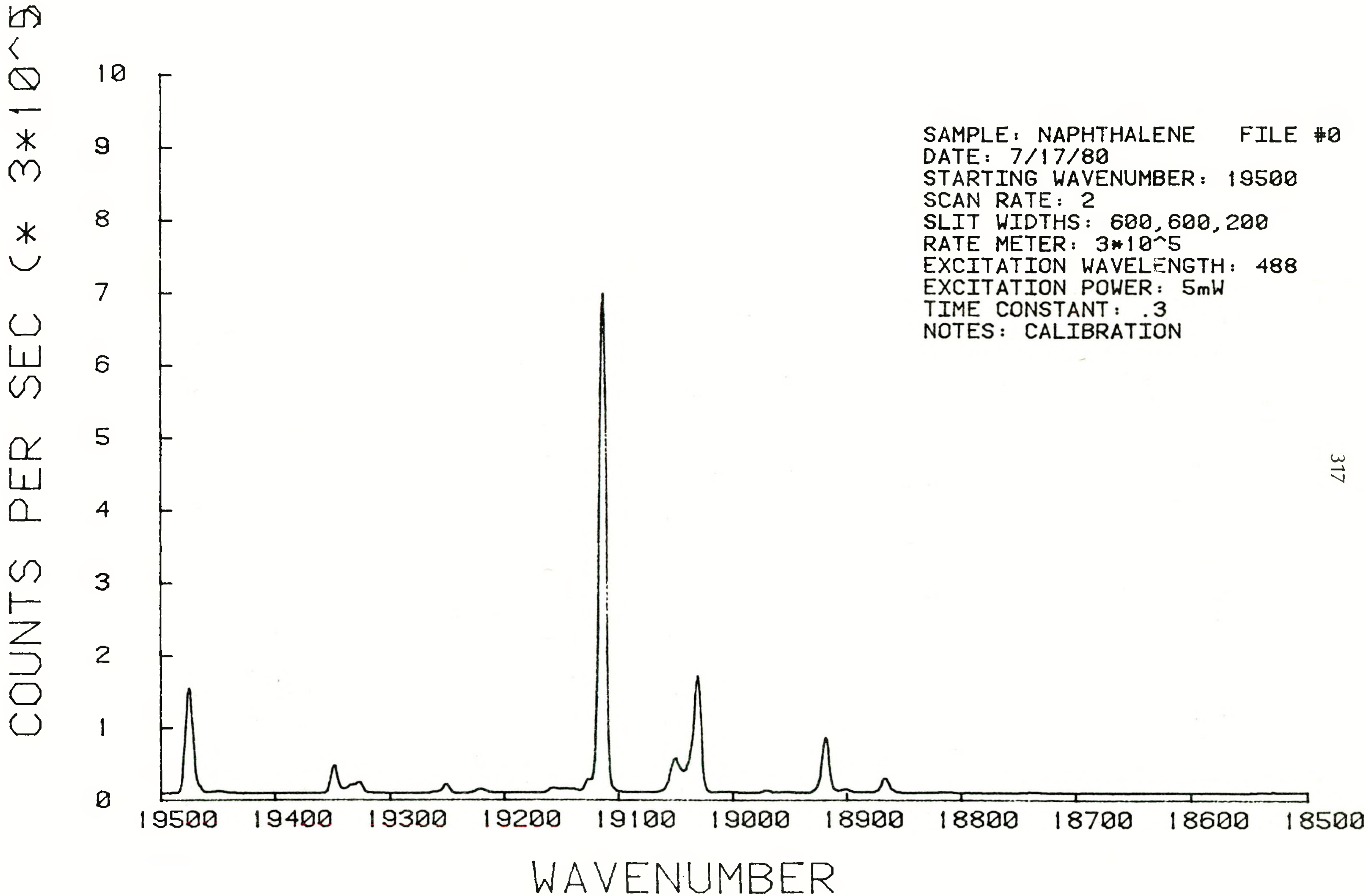


FIGURE 1. RAMAN SPECTRUM OF NAPHTHALENE

terminations and which are buried in the repository. Here the sharp focussing abilities of the laser are used to get the light into the fiber, which carries it with remarkably little loss for more than 1 km to the sample. A fraction of any fluorescence from the sample will be directed backwards toward the fiber. This will then propagate back through the fiber to the sensor. Here the returning beam is separated by a dichroic or geometrical beamsplitter and measured. The concentration of naturally fluorescent compounds can be determined from the signal intensity. Nonfluorescent compounds can be determined by coating the fiber termination with appropriate extracting reagents. The sensitivity of this type of device will be below the parts per billion level. This would be more than adequate to detect significant container leakage, as the effluent would contain strongly fluorescent ions such as actinides or, perhaps, lanthanide tracers in a fairly high concentration. Alternatively, the outside of the containers can be coated with fluorescent tracer ions to detect material influx (mass motion) in the immediate environment of the containers prior to the occurrences of any leakage. Different compounds can be distinguished by using different excitation and observation wavelengths and by different coatings on the fiber. Several hundred locations can be interrogated with one instrument by means of electrooptic switchable couplers.

HIGH-SENSITIVITY MONITOR

The high-sensitivity approach is to be used to detect microleaks, for monitoring in the far field, or for detecting minute contaminant levels in the ground water. The requisite parts per trillion or less sensitivity is not available in remote detection, and it becomes necessary to recover samples for measurements within the instrument. The possible inconvenience is more than offset by an increased sensitivity of 10^2 to 10^5 orders of magnitude over extant methods. Before selecting any one approach, a very large number of techniques were evaluated and only the coprecipitation-selective laser excitation fluorescence approach seemed sensitive enough to work at the required concentration levels.

In this technique the sample is mixed with reagents that precipitate each other to form a host crystal lattice into which the actinide ions will coprecipitate as fluorescent species. This concentrates the actinides and separates them from background impurities and fluorescence. In this new environment, the absorption cross section of the actinide ion is enhanced and its fluorescent quantum efficiency increased. Because of the ordered nature of the crystal lattice, all the bands narrow with large increases in their peak intensity. This can be further enhanced by cooling the sample.

During this quarter the following were accomplished:

(1) A laboratory system was constructed for routine collection and computer processing of high-sensitivity, high-resolution fluorescence data at ambient temperature.

(2) A fiber optic system was coupled to the laboratory spectrofluorimeter, and several fiber terminations were designed.

(3) Remote detection of trace concentrations of fluorescent compounds was demonstrated, and the linearity of the signal with concentration was established.

(4) Additional optimized parts were ordered for the fiber optics system and special mounting interfaces were designed.

(5) A mathematical analysis of the effective pathlength and signal levels in the fiber optic system was completed.

(6) A literature search covering fluorescence properties of uranium and plutonium compounds, and their analytical use, unearthed a large number of references which were studied in detail.

(7) The fluorescence behavior of uranyl-doped CaF_2 lattices at low temperature was studied using a tunable pulsed laser and time-resolving electronics with the aim of better understanding the coprecipitation process.

(8) An initial version of a sample preparation protocol was prepared and tested by optimizing reagent concentration and temperature.

(9) Approximately 50 sample runs were undertaken to establish optimal instrument settings and to determine the spectrum of UO_2^{++} under a variety of operational conditions.

(10) Reagent blanks for a variety of compounds were determined and sample preparation precautions were delineated to assure that background contributions are minimized.

(11) The linearity of the signal with sample concentration over 3 orders of magnitude was established.

(12) Research into the method's quantitative reproducibility was begun.

WBS 1.2.5

Project: NWTS Repository Equipment Development Plan

Principal Investigator: Battelle Columbus Division (T. M. Trainer)

ONWI Project Manager: N. C. Henderson

Objective

The objective of this effort is to develop and expand the *Preliminary Development Plan for Repository Equipment* to include all National Waste Terminal Storage (NWTS) repository processes/equipment requiring R&D.

Progress Reported Previously

This project was initiated in May 1979 to provide temporary assistance to the Engineering Development Department (EDD) of ONWI in planning for the procurement of repository equipment. The emphasis of this work was on a geologic repository in salt. The effort resulted in a report which identified nuclear waste repository processes/equipment requiring ONWI-stimulated R&D, outlined recommended R&D approaches in an ONWI Work Breakdown Structure format, and outlined preliminary major milestone schedules for accomplishing the recommended R&D.

The scope of the preliminary plan is to be expanded to include all NWTS processes/ equipment requiring R&D. Development plans for NWTS repository equipment are to be developed which have rationale consistent with ONWI organization and technical structures.

During the first quarter of the program, a revised plan was prepared.

During the second quarter, many comments were received in regard to the contents and the format of the plan. It was apparent that significant changes were needed for the plan to be integrated with other NWTS plans and activities.

Activities During the Reporting Period

The objectives of the work during the quarter were to obtain the remaining NWTS comments and to prepare the second draft of the plan. In addition, work was to be started on the draft of a description of the plan suitable for publication as a technical paper.

The second plan draft, reflecting the NWTS comments, was prepared.

WBS 1.2.5

Project: Engineering Design Criteria Methodology Development

Principal Investigator: Los Alamos Technical Associates, Inc. (LATA) (R. J. Kingsbury)

ONWI Project Manager: N. C. Henderson

Objective

The objective of this study is to develop a methodology and format which will be used by ONWI and ONWI's subcontractors to aid in preparing engineering design criteria and specifications for equipment used at a nuclear waste disposal facility.

Progress Reported Previously

The review, analyses, and characterization of the repository conceptual design criteria for NWTS-R1 and NWTS-R2 was completed, and a structured functional flow diagram was developed. This diagram is the foundation for the criteria development methodology. The resulting design criteria will be organized by function and referenced to the functional flow diagram. In addition to serving as the basis for the functional flow diagram, the output from the conceptual design study review provides significant input to the methodology in terms of significant design parameters, performance requirements, and interface requirements.

Activities During the Reporting Period

Objective

The objective of the work performed during this quarter was the development of a methodology, based on the generic repository functional flow diagram, to aid in preparing process and equipment design criteria for any given nuclear waste repository. Input to the methodology will include programmatic objectives and constraints, applicable codes and standards, and the facility conceptual design. The methodology output will be design criteria for the repository processes and equipment. The methodology will be sufficiently flexible to accept changes in input as the repository design effort progresses.

Procedures

The initial effort consisted of structuring the methodology output. A standard output format was established and will be used for each function on the functional flow diagram. Following establishment of the standard output format, efforts were directed toward determining the user interface with the methodology and the sequence of events to be followed by the user.

For each category on the standard output format, a checklist of potential requirements was developed. The checklist was based on input from a multidisciplinary team of LATA personnel and data extracted from the conceptual design review. Input requirements were established for items on these checklists and organized into a standard format.

Data base management systems were evaluated for handling and manipulating the data required for this methodology. COBOL was selected for the task.

Results

A standard output format for the methodology has been developed. Major headings are as follows:

- Function
- Interfaces
- Performance
- Safety
- Environmental Protection
- Codes, Standards, and Regulations
- Quality Assurance
- Safeguards.

Checklists of potential requirements in each output category have been developed.

Conclusions

The basic elements of the methodology are well developed, and sufficient effort has been devoted to user interaction procedures to predict that the methodology will meet program objectives and provide a useful tool for development of process and equipment design criteria.

WBS 1.2.5

Project: Equipment Reliability and Maintainability (RAM) Methodology

Principal Investigator: General Atomic Company (D. D. Orvis)

ONWI Project Manager: N. C. Henderson

Objective

The objective is to synthesize a methodology for RAM analysis that can be used to establish criteria for equipment in an NWTS facility to ensure that a repository operates with high availability. This project involves study of the RAM requirements of reference facility designs and the available analysis methodologies, and then adapts those judged to be most appropriate for applicability to a waste repository. The methodology will be developed into a guidebook that can be used by ONWI, repository contractors, design personnel, and RAM specialists. The selected methodologies are being demonstrated through evaluation of selected portions of the Conceptual Reference Repository Design.

Progress Reported Previously

Progress in the previous quarter involved initiation of the study of RAM requirements of the Conceptual Reference Repository Design and preparation of the Project Plan.

Activities During the Reporting Period

The purpose of work performed during the quarter was to initiate the program and to develop an approach for applying RAM methodology to availability considerations of a mined geologic nuclear waste repository. The program plan, review designs, and approach were scheduled and completed during the quarter.

The principal technical effort scheduled for the quarter was the development of an approach for the RAM Guidebook that is customized to the needs of the NWTS program. The procedure for accomplishing this included review of conceptual repository designs to become familiar with the processes, types of operations, and types of equipment expected to be employed in a repository. This review relied primarily on the descriptions, drawings, and criteria documents of the Conceptual Reference Repository Description (CRRD) prepared by Bechtel National, Inc. Additional reviews included information on repository characteristics contained in conceptual design reports for NWTS Repository No. 1 (Stearns-Roger Engineering Company) and NWTS Repository No. 2 (Kaiser Engineers).

Since the number of mined geologic repositories is expected to be small, it is imperative that the few repositories remain operational (or "up") a large fraction of the time during their intended lifetime (i.e., they must exhibit high "availability") in order to avoid potential constrictions on the use of power reactors because of interruptions in the disposal of radioactive wastes. Although there are several refinements to the concepts of availability and capacity factor that can be applied to an NWTS repository, the following general definition of availability provides a framework for discussing the activities of the RAM program:

$$\text{Availability} = \frac{\text{Uptime}}{\text{Total Period Time}} = \frac{\text{Uptime}}{\text{Uptime} + \text{Downtime}} .$$

Long uptime (time between failures) is a measure of high system reliability, while short downtime (time to repair or restore) is a measure of high system maintainability. Hence, high availability is achieved through high reliability and high maintainability.

The most important requirement for a given repository is that it (safely) emplaces its proportionate share of the national production of nuclear waste. It is therefore necessary to ensure that the facility has the throughput capacity to process its scheduled waste load in spite of periods of full or partial unavailability. The methodology being developed in the RAM program will help realize this goal.

The principal activity during the quarter was preparation of a working draft of the Guidebook for ONWI review. The Guidebook begins with an overview that emphasizes the need to apply a structured RAM program to assure that high availability is realized in an operating repository. The principal methodology is presented in sections on availability, reliability, and maintainability which define the activities and analyses which are to be performed during each phase of design evolution from conceptual to final.

Additional accomplishments during the quarter included trial applications of qualitative RAM methodology to gain insight into potential availability concerns of a repository. These activities are summarized below.

Availability Block Diagram and Fault Tree

"First-cut" availability block diagrams of the overall repository (CRRD), the high-level waste handling process, and the weld and test cells were developed. In addition, a preliminary fault tree was developed for the weld and test cells. These models helped to (1) communicate the CRRD makeup to other program personnel and (2) gain initial experience with the degree of difficulty or utility in applying alternative modeling techniques to this type of facility. The top-level models illustrate that the CRRD may be considered to contain three district material flow streams which may be analyzed separately. However, they are linked to each other by common hardware [such as the waste shaft hoist and the underground transport systems for the high-level waste (HLW) and low-level waste (LLW)] or by time sequencing (as between the emplacement and mining operations). The dependencies represented by these links must be considered in the evaluation of availability for the respective process streams.

Failure Mode and Effects Analysis

To aid in understanding the system interfaces, a failure mode and effects analysis (FMEA) was performed for the CRRD spent fuel handling process from the rail and truck yard to emplacement in the mine. The analysis was limited to major subsystem or major equipment level. The results of this exercise will aid in making decisions on methodological applications and, with refinement, can serve as an example of this technique in the Guidebook.

Maintainability Considerations

To provide a basis for maintainability methodology, the CRRD equipment types were listed and categorized with respect to function, and whether they are unique to repository needs or more generic. The initial survey was confined to elements of the HLW and LLW handling. The results of this review indicate that radiation does not pose overwhelming constraints on most maintenance activities. However, some items of special concern were identified, such as the recovery from possible dropped bare spent fuel elements at the drying station ahead of the weld and test cells, possible high-level contamination in selected areas of the weld and test cells, and recovery from possible canister drops in the upper corridor between the special handling and the weld and test cells. Determination of the quantitative impact of these and other accessibility problems and radiation constraints has not been attempted to date.

Analytic Availability Analysis

The application of analytical approaches to availability assessment has been investigated for the type of systems used in radioactive waste management. Markov models and direct integration techniques were used to develop formulas for radioactive waste system availability. These models included the effects of lag storage between process stations, as well as the effect of common-mode failures in redundant equipment. Sensitivity studies using preliminary data indicate the importance of surge storage as an availability improvement technique. The models developed seem to provide reasonable results so long as the exponential failure and repair models are not extrapolated out into the "tails" of the distribution.

Simulation Modeling

A simplified simulation model of the CRRD as a network of flow streams and surge storage was developed using the GASP IV program to investigate the applicability and utility of this methodology to repository availability prediction. Initial computer runs showed the content of the surge storage increasing and decreasing as failures occurred downstream and upstream of the surge storage. The failure rates and repair times used in the trial runs of the simulation model were arbitrarily selected as representative of systems in general, not for specific NWTS systems. Therefore, the results are not significant as a quantitative prediction of repository availability. However, this exercise provides a preliminary demonstration of simulation capability.

Further applications will be considered and compared with other analytical methods before finalizing the recommendations for the Guidebook.

SUMMARY

1.3 SYSTEMS ANALYSIS

The scope of Systems Analysis investigations covers Issue Analysis, Transportation Systems, Security and Safeguards, Criteria/Standards, Alternative Concepts, Systems Assessment, and Socioeconomic Analysis. The prime objective of this task is to identify the options available to resolve the problem of waste isolation and to make a choice among the alternatives by broad-ranging, multidisciplinary analyses.

Participants at two workshops held in support of the Naturally Sealed Rock Systems project concluded that laboratory and numerical studies could begin relatively soon, but that basic field data are first required. An extensive literature survey on conditions at great depths and a series of discussion papers were the basis for workshop discussions from which an assessment of key research needs was developed. Areas of study include geophysics, borehole stability, hydraulic fracture, hydrology, baseline characterization, and post-emplacement geochemistry.

Researchers on the Social-Institutional Aspects of Nuclear Waste Management have developed, by means of topical papers, a set of tentative recommendations for impact assessment. The application of these recommendations, which are based on a division of potential impacts into three categories, must be preceded by an extensive, broadly based, and public exercise in impact scoping. The categories and recommendations to ONWI for impact analysis studies are:

- Radiological Impacts. A greater degree of confidence must be gained in convening a genuinely public forum to discuss what is and is not known, what the experimental and data bases are, and what uncertainties remain.

- Conventional Nonradiological Impacts. A series of public workshops to explore perceptions and beliefs and to discuss what can and cannot be done, and what should and should not be done, would greatly help in establishing a credible and legitimate basis for professional impact scoping.

- Mixed Impacts (nonradiological impacts and activities whose dimensions are most profoundly altered by the fact that the materials involved are radioactive). There should be a series of professional workshops and meetings involving the widest possible range of disciplines and expertise to scope out what kinds of analysis can be performed, by whom, over what time, and at what level of effort.

To meet the objective of laying out the decision methodology of a pilot model for use in managing the very deep hole research program, three tasks were undertaken: (1) define the decision problem; (2) establish outcome measures; and (3) prepare an illustrative example. Although the decision problems are numerous, as are the possible outcome measures, the choices for a limited pilot project were established. The decision problem to be defined is that of which aspects of the VDH system to investigate. The outcome measures established are health effects, economic cost, and public acceptance. The strictly hypothetical illustrative example shows how research impacts on the ability to discriminate between the ultimate effectiveness of a mined geologic repository and a very deep hole.

WBS 1.3.1

Project: Performance Measures Development

Principal Investigator: Arthur D. Little, Inc.

ONWI Project Manager: J. Waddell

Objective

The objectives of this program are (1) to provide a complete set of performance measures in six categories (environmental impact, societal impact, safeguards, safety, economics, and resource consumption) for use in analyzing NWTS program options, and (2) to provide assistance to ONWI in implementing the measures in the NWTS System Evaluation Model.

Progress Reported Previously

This is the first quarterly report for the project.

Activities During the Reporting Period

During the reporting period the following steps were taken:

- Performance measure worksheets were developed.
- Performance category worksheets were developed.
- Tentative lists of performance measures for each category were completed.
- Performance measure worksheets were completed (in draft form) for each measure on the lists.
- Performance category worksheets were completed.
- The above material was reviewed.

WBS 1.3.3

Project: Safeguards and Security

Principal Investigator: Allied-General Nuclear Services (AGNS) (J. H. Ellis)

ONWI Project Manager: M. Pobereskin

Objectives

Objectives are to establish the level of safeguards/security measures required in the waste isolation system and to develop performance/design criteria required to support design and operation of the sytem.

Progress Reported Previously

The Waste Isolation System (WIS) Safeguards Development Program, which was started on May 5, 1979, consists of three major tasks. These tasks include preparation of a Scoping Study, a Program Plan, and an Annotated Safeguards Bibliography.

The purpose of the Scoping Study is to define the basic safeguards concepts to be applied to the WIS system. Since specific safeguards requirements for wastes do not exist, these concepts are to be based on interpretation of existing and foreseeable regulations and requirements (NRC, DOE, and IAEA) for other fuel cycle facilities.

Drafts of the various sections of the Scoping Study were completed and reviewed internally, including the WIS system description, threat definition, assessment of regulations and future trends, and WIS safeguards criteria. The Scoping Study was then submitted to ONWI for review.

The draft contains major sections covering waste and source facility definitions, threat definitions, analysis of existing and proposed regulations, bases for WIS safeguards requirements, and finally, a listing of the proposed primary design and performance criteria.

The basic conclusions of the Scoping Study were:

(1) A safeguards system will be needed due to the hazardous nature of the materials, the potential attractiveness of the material as a sabotage target, and because of the potential that the wastes could contain significant quantities of SNM.

(2) The safeguards system should consist of a comprehensive physical protection system and an item control type of material accounting system.

A draft of the on-going Program Plan was also submitted to ONWI with the Scoping Study. The Program Plan lists eight basic tasks, including:

(1) Specific design and performance criteria development
(2) New technology development
(3) System description
(4) System assessment
(5) Review of PIR/CRRD
(6) Title II design input
(7) Licensing input
(8) Computerization of the bibliography.

In preparing the Scoping Study, an extensive safeguards literature search was conducted, and AGNS personnel obtained and reviewed as many of the documents identified in this literature search as possible. This review was intended to provide the basis and references for definition of existing safeguards requirements, assessment of the trends for future requirements, and ultimately, the development of specific safeguards criteria for the Waste Isolation System. The review of available documents was completed as scheduled.

A safeguards bibliography containing over 1,700 entries was compiled from these documents. The entries were sorted by subject category and a determination of applicability to the WIS was made for each entry. Annotations (short abstracts) of each report were added.

Another phase of the contract work, review and evaluation of ONWI-related documents, has continued. Documents reviewed included portions of Chapters 3 and 8 of the Bechtel *PIR*, the draft *Environmental Impact Statement* on "Management of Commercially Generated Radioactive Waste" (DOE/EIS-0046-D), the LASL *Repository Safeguards Report*, the INFCE report on *Safeguards for Repositories*, and the *Design Criteria Report* for "A Nuclear Waste Repository in Basalt".

Activities During the Reporting Period

A meeting was held with ONWI staff members to discuss the completion of the Scoping Study and to discuss AGNS' preparation of a *Waste Safeguards Position* paper. ONWI comments on the Scoping Study have been reviewed and incorporated into the final draft of the Scoping Study.

Work is progressing on the *Waste Safeguards Position* paper. This document will identify the major issues related to safeguarding the Waste Isolation System and will describe the current position on each issue.

WBS 1.3.4

Project: Criteria Support Studies

Principal Investigators: Battelle-Columbus Laboratories (S. Rogers, K. Wurm, N. Miller)

ONWI Project Manager: A. Bauer

Objectives

The objectives of this study are to (1) identify the sources of policy and regulations which could affect the conduct of the NWTS Program, (2) postulate possible changes in policies or regulations, (3) evaluate the impact of these changes on the NWTS Program criteria, and (4) prepare a report on interim guidance for waste package design.

Progress Reported Previously

This study began in December, 1979. Information was collected on federal policy, federal regulations in effect and proposed, and federal and state legislation which relates to the ONWI criteria. These papers and documents were evaluated, annotated, and assembled into a review document.

Information on interim waste package performance and acceptance criteria was organized to conform to the organization of the draft of the ONWI waste package criteria document, and was revised and updated to comply with the present ONWI policy. A draft of the Package Design Guidance Report was also prepared.

Activities During the Reporting Period

Activities were begun to select potential changes in regulations and policies to analyze for a regulatory/policy impact report.

WBS 1.3.5

Project: Naturally Sealed Rock Systems

Principal Investigator: Lawrence Berkeley Laboratory (LBL) (W. Thur)

ONWI Project Manager: R. E. Best

Objectives

The objective is to develop information on deep and hydrologically isolated geologic systems in support of continuing assessment of the Very Deep Hole waste disposal alternative.

This project is aimed at further review and assessment of geological, hydrological, and geochemical uncertainties to improve the state of knowledge and provide bases for a program to define and develop the Very Deep Hole (VDH) waste disposal alternative.

Progress Reported Previously

Previous work involved followup activities to work done at LBL as input to the draft Department of Energy Generic Environmental Impact Statement (GEIS).

Activities During the Reporting Period

In approaching this task, a multi-disciplinary team of investigators was assembled from the staff at LBL's Earth Sciences Division and Terra Tek of Salt Lake City. This team prepared an extensive survey of existing literature on conditions at great depths, and a series of discussion papers for use at two workshops held during April in Berkeley. These sessions were attended by the project staff and an additional 22 outside consultants chosen as leading authorities in their respective fields.

A rock mechanics/hydrology workshop was conducted, consisting of four working subgroups—borehole stability, hydraulic fracture, hydrology, and geophysics. Contributions were made on various topics of discussion, and each participant was asked for his assessment of key research needs. Research on the following areas was recommended:

Geophysics

- High-resistivity crystal blocks
- Geophysical properties of meta sediments
- Low-velocity zones in crystalline rock
- Origins of intracontinental seismicity
- Development of MG radar logging systems
- A program of basic continental basement studies

Borehole Stability

- Laboratory simulation of very deep hole
- The damage zone around the hole
- Laboratory and numerical studies on self-healing (plastic) rock
- Instrumentation development for monitoring a VDH
- Stress measurement alternatives to hydraulic fracture

Hydraulic Fracture

- Fracture propagation mapping
- Thermo-hydraulic fracture studies
- Propagation from inclined holes
- Fracture propagation in plastic materials

Hydrology

- Fracture propagation mapping
- Dispersion in fracture systems
- Instrumentation development for well tests in deep holes.

In relation to siting potential, there was general agreement that a national crystal basement program such as that developed by the National Academy would provide direct information that would hasten assessment of the deep hole, though VDH could not be a sole funding source. The hydrologists felt that crystalline rock overlain by sediments would be ideal—the crystalline rock providing hole stability and the sediments being more predictable than fractured hard rock for ground-water transport.

Research should begin on rock mechanics laboratory simulations, but ultimate demonstration of VDH feasibility will require a dedicated facility in possibly several rock types.

The geochemistry/hydrology workshop had two subgroups—baseline characterization, concerned with the geochemical environment prior to emplacement in the hole; and geochemistry of the area around the hole after emplacement of waste. Recommendations involved the following.

Baseline Characterization

- Close look at ultra-basic igneous rocks
- Evaluation of U-decay dating techniques
- Development of water sampling techniques
- Study of natural analogs such as uranium deposits
- Assessment of geologic record for long-term permeability indicators
- Geochemical studies of waters in abnormally pressured zones
- Survey of oil company records

Post-Emplacement Geochemistry

- Improvement of coupled geochemical/rock mechanics/hydrology models
- Setup of a DOE-oil company connection similar to that of the geothermal programs
- Study of dehydration reactions
- Dating of time of natural fracture formation
- Participation in the scientific program for deep drilling of basic rocks in Cyprus
- Definition of the depth where diffusion dominates chemical transport
- Surface chemical interactions studies (e.g., Mossbauer techniques) and mineral surface studies by state-of-the-art technique

As with the rock mechanics group, there was considerable discussion over the relative advantages of crystalline basement and sedimentary basins. Like the rock mechanics group, this group felt that laboratory and numerical studies could begin relatively quickly, but basic field data are required. Dedicated facilities in a variety of rock types will eventually be necessary to demonstrate feasibility of the VDH concept.

Since the workshop sessions, a reduced level of effort has been directed at revision of the selected data base on geologic conditions at greatest depths.

WBS 1.3.5

Project: Very Deep Hole (VDH) Systems Decision Studies

Principal Investigator: SRI International (F. L. Offensend)

ONWI Project Manager: (R. E. Best)

Objective

The objective of this project is to develop a pilot decision model for use in managing the Very Deep Hole research program. The model is to be demonstrated with a preliminary evaluation of selected research strategies, including a preliminary comparison of the Very Deep Hole concept with the Mined Geologic Repository (MGR).

Progress Reported Previously

The project was initiated 7 April, 1980 and this is the first technical progress report.

Activities During the Reporting Period

The overall objective of the quarter's work was to lay out the decision methodology. Three separate efforts were undertaken: (1) define the decision problem, (2) establish outcome measures, and (3) prepare an illustrative example. The work is most easily presented by describing the three efforts separately.

Define the Decision Problem

A wide variety of decisions must be considered in setting a research strategy for the Very Deep Hole program. The most basic decision is whether to fund a VDH research effort, and, if so at what level. Concurrent with the funding decision is the timing decision (i.e., whether the research should be started now or postponed until later). Given that VDH research is to be done, decisions must be made on which aspects of the VDH system should be investigated (e.g., drilling technology, plug design, transport phenomena, etc.). Decisions must also be made on the type of research to be conducted (e.g., whether to conduct theoretical, computer simulation, laboratory, or in situ studies). Finally, specific decisions must be made on the exact experiment to be performed and the investigator to do the project.

Potentially, the decision methodology will be applied to each of these decisions. However, to limit the pilot effort, the methodology will be focused on a narrower set of decisions. The most important decision is whether or not to fund the VDH research program, and, if so, at what level. However, to analyze this decision, one needs to understand the value that might be derived from doing VDH research. This value is best understood by analyzing the separate components of the VDH concept. Thus, initial work will focus on the decision of which aspects of the VDH system to investigate (e.g., whether to fund migration studies, plugging studies, etc.).

Establish Outcome Measures

Outcome measures are required to characterize the performance of the different alternatives so that they can be compared on a consistent basis. Considerable work has been spent by other groups in identifying the different factors that must be considered in assessing the overrall effectiveness of a nuclear waste concept. Attempts to add to this literature were not made, but attempts were made to distill it into the basic components of performance that are often cited in assessing the effectiveness of a disposal concept.

The technical outcome measures tend to fall into five categories:

- Radiological impacts
- Environmental impacts
- Economic cost
- Level of security
- Time of availability.

Other outcome measures relating to public acceptance are often cited. Two such measures include:

- Public confidence in the decision-making process
- Equity.

The fully developed decision methodology must be capable of addressing all seven categories of outcome measures. However, to limit the pilot effort only two or three of the categories will be considered. Because of the overriding concern for health effects and economic cost, measures of those two effects will be included in the pilot model. Also included will be an outcome measure relating to public acceptance.

The decision methodology must also address the question of how to combine the various outcome measures into an overall measure of effectiveness. Several approaches are possible, each of which implies placing value on the different categories of outcome measures. One approach is to assume thresholds for each outcome measure and to consider the outcome measures separately. If any one threshold is not met, then the overall disposal system is deemed unacceptable. While this may seem like an appealing method for deciding if a disposal method is acceptable, it does not provide a means for deciding which of several acceptable methods is best. Furthermore, it does not allow for trade-offs among the different outcome measures if one measure fails to meet its threshold by just a small amount.

A second approach is to introduce explicit value assignments so that all of the outcome measures can be compared on a common scale. This method requires the explicit consideration of each value category and ensures that the value trade-offs are handled consistently from one decision problem to another. Sensitivity studies can be performed to determine how the comparison of alternatives changes in the value assignments.

Both approaches should be tested in the pilot model. It is hoped that the selection of a research strategy is reasonably independent of the method for incorporating value assignments.

Prepare Illustrative Example

The basic approach of the research planning methodology is to assess how possible research strategies change the state of information on the relative effectiveness of MGR and VDH. The research strategy sought is that which allows one to most efficiently discriminate between the ultimate effectiveness of the two disposal methods.

The key to implementing the methodology is to develop a credible research impact model—a model that describes which research outcomes might occur given a particular research strategy, and how those outcomes change the state of information about the relative effectiveness of MGR and VDH. To build that model one needs to work closely with the managers and researchers involved in waste disposal research. These individuals will be of better help if they understand the basic approach. Therefore much of the quarter was spent preparing a simple example that shows how research impacts on the ability to discriminate between the ultimate effectiveness of MGR and VDH.

The example is strictly hypothetical. It does not purport to represent reality; it is merely a vehicle to demonstrate methodology. Nor is the example complete; it omits much of the detail that is necessary to fully characterize the VDH research problem. In spite of these limitations, the example does show how research aids in the discrimination between two disposal methods.

The example considers a point in time about 1 year before a DOE deadline to make a final decision on whether or not to undertake a major research program on VDH. In this simple example, one assumes that the DOE has made a tentative decision to proceed with the MGR and that it is now only concerned with whether or not to supplement MGR with VDH. No other disposal methods are being considered. Several short-term research projects have been proposed to provide more information for the ultimate program funding decision. One project to investigate if there are any isolated hydrologic regimes is particularly interesting.

Long-term radiological impacts and economic costs are the only outcome measures considered in this example. For simplicity one assumes that the impacts fall into one of three categories: high, medium, and low. High impacts are considered unacceptable, medium impacts are marginally acceptable (of the order associated with an ore deposit), and low impacts are negligible.

Figure 1 is a schematic of the decision problem. The immediate decision is whether to fund the hydrologic regime study. (In practice there would be other research projects to consider, but they are not included in this example.) If the hydrologic regime project is undertaken, one assumes that there will be one of two outcomes: either at least one isolated regime will be found or no regimes will be found. Regardless of the immediate research decision, the DOE must decide 1 year from now whether to supplement the MGR research program with a major research effort on VDH, as shown by the second series of square nodes in the diagram. Once the research is accomplished, the level of radiological impact will be learned, as indicated by the circular nodes at the end of the diagram. Finally, depending on the projected level of radiological impact associated with the two disposal methods, a decision will be made on whether or not to supplement MGR with VDH.

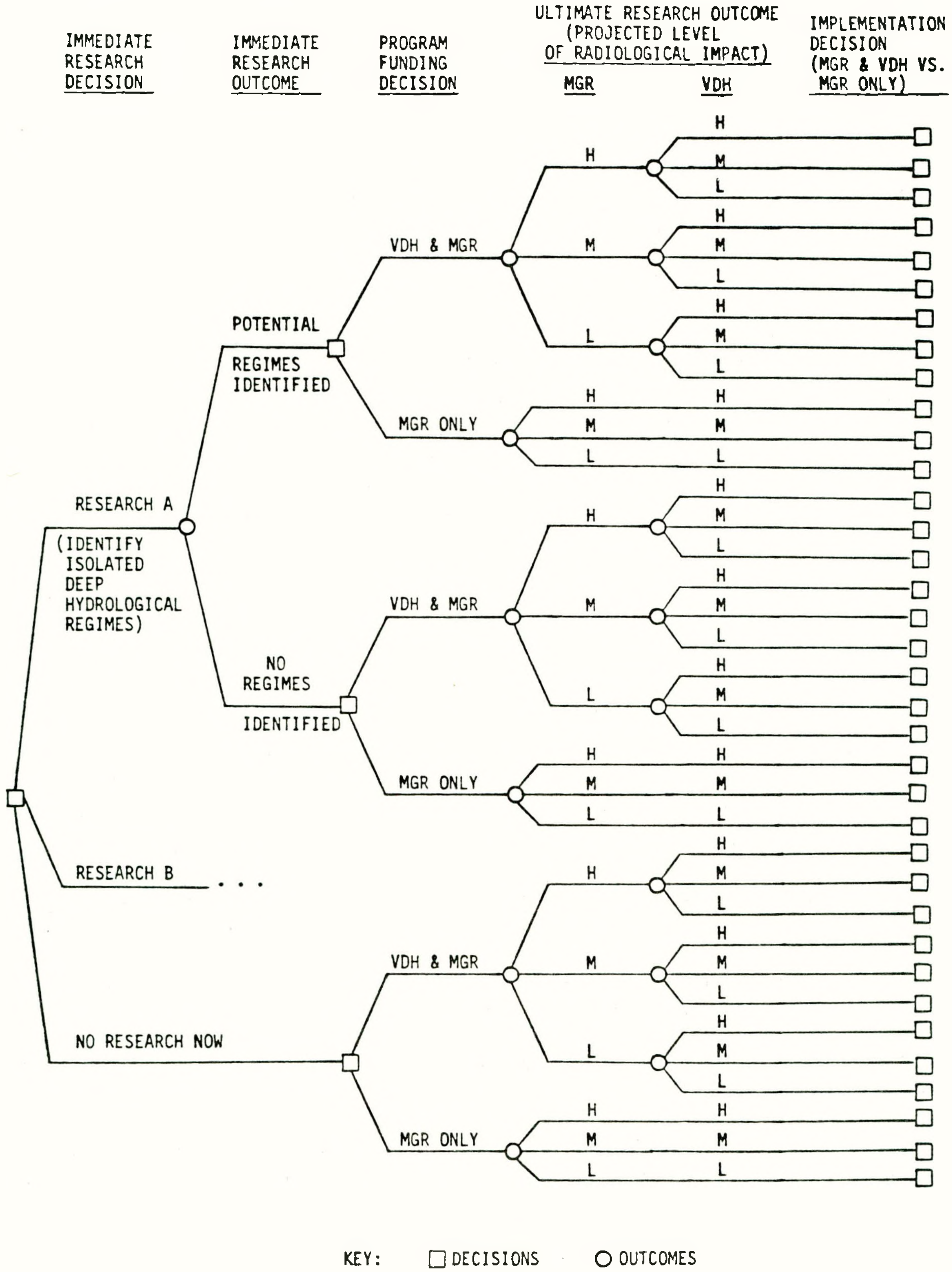


FIGURE 1. DECISION TREE FOR ILLUSTRATIVE PROBLEM

Even in its qualitative form, Figure 1 begins to show the value of research. Research does not guarantee that the radiological impacts will be low. What research does is to narrow the uncertainty on what those impacts will be. Doing research on VDH provides a hedging strategy. If research is performed on MGR and VDH, and if the radiological impacts of MGR are found to be high, then as shown in the diagram, there is still some chance of a successful disposal system because VDH may have low radiological impacts. Of course, budget constraints limit the extent to which hedging strategies can be followed. To assess the cost-effectiveness of the VDH research program, one needs to assess the cost of the program and the likelihood of VDH having lower radiological impacts than MGR.

Key inputs to the example included probabilistic assessments on the possible levels of radiological impact for VDH and MGR, given current information. The likelihoods of the possible hydrologic regime research outcomes were also assessed, as was the way in which the assessment of VDH effectiveness changed with each research outcome. The likelihood of VDH having a lower radiologic impact than MGR was calculated for each research outcome. The illustrative data and calculations showed a 5.2 percent change of VDH having a lower radiologic impact than MGR, given current information. If the hydrologic regime experiment was performed and no isolated regimes were found, then this probability decreased to 4.1 percent. If an isolated regime was found, then the possibility of VDH being more effective than MGR increased to 5.5 percent. These numbers are strictly hypothetical.

As previously indicated, the illustrative example is strictly hypothetical. No conclusions on the value of the VDH research program are to be drawn from the example. Firstly the input data were illustrative and developed with very little basis of fact. Secondly, the example only considers one category of benefit, and it may be that other benefits are valued so highly as to provide full justification for the VDH research program. Finally, the example was highly simplified and omitted several realities (such as the dependency of MGR effectiveness on VDH research outcomes). In spite of these simplifications, the example does show how research results impact on the comparison between VDH and MGR and how the cost of the research can be weighed against the discrimination potential provided by the research.

WBS 1.3.5

Project: Nuclear Waste Management Space Option

Principal Investigator: NASA Marshall Space Flight Center (MSFC) (C. C. Priest)

ONWI Project Manager: R. Best

Objective

The overall program objective is to assess the desirability of using a space option to dispose of certain high-level nuclear waste as an augmentation of the currently planned national nuclear waste management program. The overall technical objective of this year's activity is to obtain a realistic assessment of the space transport system status.

Progress Reported Previously

This project was initiated on June 1, 1979 under a NASA/DOE Interagency agreement. The activities associated with the original agreement were completed in March 1980. Final reports describing the results have been published.

The modification to the agreement became effective on 10 March, 1980 and study activities were initiated in May 1980. This is the first quarterly technical progress report for this activity under the modification to the agreement. Also included in this report are significant activities that have occurred since fulfillment of the original agreement.

Activities During the Reporting Period

The activities summarized include the following: (1) Draft Program Plan for the Space Disposal of Nuclear Wastes, (2) MSFC/Battelle/SAI 1979-1980 Conceptual Design Study, and (3) Boeing Aerospace Company Space Systems Study.

Draft Program Plan for the Space Disposal of Nuclear Waste

A draft document entitled *Concept Definition and Evaluation Program Plan for the Space Disposal of Nuclear Waste, 1980-1983* was completed on 28 January, 1980. The primary purpose of this document is to present an overall 4-year technical study program plan for the space disposal of some components of commercial and defense nuclear waste. This will lead to firm recommendations regarding the viability and incentives for the continued development of the space option. To this end, establishment of risk reduction and its associated cost would be the goal of the 4-calendar-year program. Four years would be required to conduct the study because of (1) the interaction required among the various studies of components of the system and their environmental and other implications, (2) the systematic nature of the proposed effort, and (3) the basis of the experience gained over the past few years in studying various facets of the concept. The first year of activity would deal with identifying and assessing all major options available, and the identification of major areas of uncertainty. The second year would involve the selection of preferred options. The third year would entail the more detailed study of the preferred concepts, leading to the selection of a baseline concept. The fourth year of effort would be to prepare detailed baseline systems designs and to develop a program plan for the development phase. The primary study areas would include: nuclear waste systems; space systems; domestic and international affairs; impact assessments; and program management, assessment and integration. The program plan is currently under review.

MSFC/Battelle/SAI 1979-1980 Conceptual Design Study

The 1979-1980 Conceptual Design Study involved Marshall Space Flight Center studies and a study in selected supportive areas with Battelle's Columbus Laboratories, and Science Applications, Incorporated. The system, program definition, and integration activities were accomplished by MSFC. The Battelle/SAI activities included characterization of commercial and defense waste, safety assessment, environmental impact analysis, and program planning support analysis. The study activity was initiated in June 1979 and completed in March 1980.

Boeing Aerospace Company Space System Study

The Boeing Aerospace Company is conducting a study on the analysis of space systems for the space disposal of nuclear waste. Work to date has been on the Waste Payload System task, Flight Support System task, Space Disposal Destinations task, and Launch Vehicle Systems task.

Principal accomplishments in the Waste Payload Systems task include a review of past studies and definition of ground rules and assumptions, and waste payload system requirements. Characterization of source terms for the reference PW-4b waste mix is under way. Work in the Flight Support System task has commenced with a review of concepts and requirements from previous studies. Fourteen potential space disposal destinations have been identified in work on the Space Disposal Destination task. Characterization of these destinations in terms of 14 evaluation criteria is in progress. The Launch Vehicle System task has begun with establishment of a data base to be used in characterization of four candidate launch vehicles.

WBS 1.3.7

Project: Social-Institutional Aspects of Nuclear Waste Management

Principal Investigator: University of California at Berkeley (G. I. Rochlin)

ONWI Project Manager: J. Finley

Objective

The objective is to examine, identify, and characterize social-institutional aspects of high-level commercial radioactive waste management and disposal. These include: how organizational design and institutional relationships could be structured to maintain program efficiency and credibility as well as responsiveness and safety; what types and degree of socio-economic and socio-political impact analysis may be required and for what purposes; and what are likely to be the political and institutional relationships to which the program might have to respond.

Activities During the Reporting Period

As a result of work under this project, a number of topical papers are being generated. The subjects of these papers include:

- A survey of the current state of the art and applicability of a range of impact assessment techniques and methodologies, primarily for those with a social-science orientation

- A comparative study of approaches to siting and socio-economic analysis that have been proposed for this particular issue, with some analysis of applicability and scope

- A two-part study of the role of state and local governments in this area where strong and sometimes preemptive federal legislation and authority exists, with a special examination of the proposed process of consultation and concurrence

- A survey of the relevant social science literature on organizations and institutions to determine if the degree of responsibility and responsiveness that public and local governments are demanding of the organization can be met by any particular set of formal design criteria, or if other conditions and criteria need to be specified

- A discussion of the state of existing data and projections to determine the adequacy of data and ways of organizing them to fit the needs of a more extensive social science program assessment.

Impact Assessment

The paper surveying impact assessment is an attempt to categorize the various sources and types of impacts that a radioactive waste management and disposal program will engender, and to identify just what level of prior assessment is necessary, sufficient, desirable, or possible for each category.

Separation into the four aforementioned criteria is most important. There is considerable demand from public spokespersons, public interest groups, and a variety of state and local government officials and agencies for some degree of prior impact assessment before various program activities are allowed to proceed. Moreover, given that the program is relatively far from full-scale "commercial-level" implementation, there are entire categories of activities that have not as yet been introduced. Thus, one can anticipate that the present range of demands for assessment and analysis will be expanded further.

At this point, the program is simply not well enough specified in industrial and technical detail to allow for comprehensive site-specific analysis. A thorough examination of a broad range of impacts for all possible or potential sites, and for all variation in probable technical, industrial, managerial, regulatory, and political options would consume more analytic resources that are presently available even if refined, textbook methodologies and adequate data bases were already available. Prior impact analysis is therefore governed by a series of ad-hoc discriminatory scoping decisions. Initially, one must determine which of the various activities entail mutual overlap.

To determine what set of activities might result in a bounding, if not a mapping, of that area of overlap, it is most useful to divide potential impacts into three categories:

- Radiological
- Conventional nonradiological
- Mixed nonradiological.

Radiological is the most obvious category. This category should include all those activities, such as the requirement for radiological monitoring, health and safety supervision, and working condition regulations, which are directly related to the possibility of routine exposure, and such other important social and political activities as planning for accidents and emergencies.

Conventional nonradiological impacts are those arising from activities not involving radiation. The most important entry in this category is the conventional socio-economic impact regarding roads, schools, crime, population shift, taxation, and so on. To be comprehensive, this category should also include indirect and deferred impacts, for example, distributional equity considerations, permanent land withdrawals, costs of compensation, and impact mitigation.

Neither of these categories presents any profound epistomological difficulty for research design. Many aspects of impact assessment in these categories, most particularly for those impacts that are direct and immediate, may be nearly ready for analysis. However, neither of these categories really describes what makes radioactive waste management different from other, similar activities in U.S. society. To begin addressing the central questions, one must include those impacts described as "mixed"—nonradiological impacts or activities whose social, economic, and political dimensions are most profoundly altered by the fact that the materials being transported and handled are radioactive, and that radiological risks are perceived to be "different" from others. The re-evaluation of otherwise nonradiological activities in light of public and governmental concerns over the safe handling of materials (whose hazard is perceived as unique) shapes the impact and its assessment.

The mixed impacts can be divided into those that are direct and relatively immediate, and those that are deferred, or delayed, or both. In either case, perceptions of, and responses to, mixed impacts tend to be fundamentally sociological and political.

The direct impacts include perceptions of quality-of-life changes (fears, anxiety, stress, and their effects); regulatory activities and responses to them; security activities and responses to them; changes in perception of social role; and changes in the distribution of power, authority, and responsibility among various levels of government. In retrospect, it is precisely this class of mixed impacts that most governs the issues addressed in the topical papers. Design of an appropriate managing organization and its roles in relation to other regulatory, operational, and government bodies, for example, must be quite different from other activities to accommodate not only specific operational differences, but radically different public and governmental perceptions on how reliable and responsive the organization must be.

General implications of taking these mixed impacts into account were briefly studied. These studies were undertaken to explore the possible range of required assessments, and not to set up the enormous agenda for exploring all ramifications of impact analysis scoping. What is most immediately needed is a comprehensive and multidisciplinary effort to scope: first, the required impact analysis; second, the current state-of-the-art in the various disciplines whose expertise needs to be brought to bear; and third, the criteria by which a set of analyses can be determined to satisfy the joint conditions of what *can* and *should* be done over the next few years.

There is also a question regarding the amount of data that can be used as technical-industrial input for impact scoping activities. Some data are in a form unusable for social science analysis. Moreover, the definition of the actual industrial, technical, social, and political specifications under which radioactive waste will be managed, handled, regulated, stored, transported, and emplaced may be determined in the process of deployment itself and shaped by ongoing estimation of the nature and scope of "mixed" impacts. Thus, the impacts may be self-determining; they may be determined not by technical or geological data, but *by the conditions imposed upon program activities* as a result of informed perceptions of the differences between the handling of radioactive versus conventional, nonradiological activities.

A tentative set of recommendations for impact assessment has been developed. First, an extensive, broadly based, and public exercise in impact scoping must be performed before any work can be done on specific impact analysis studies. These are separated according to the class of impact because the state of the art is so different from one class to another. The recommendations are:

(1) *Radiological Impacts.* A greater degree of confidence must be gained in convening a genuinely public forum to discuss what is and is not known, what the experimental and data bases are, and what uncertainties remain. Not all salient issues will be resolved; however, public ventilation can only help in the long run.

(2) *Conventional Nonradiological Impacts.* A series of public workshops to explore perceptions and beliefs and discuss in depth what can and cannot be done, and what should and should not be done would greatly help in establishing a credible and legitimate basis for professional impact scoping.

(3) *Mixed Impacts.* There should be a series of professional workshops and meetings involving the widest possible range of disciplines and expertise to scope out what kinds of analysis can be performed, by whom, over what time, and at what level of effort. Social and physical scientists must have an opportunity in advance to indicate what research they will not engage in, and what types of exercise they consider futile. With this information, agencies and professional groups can better proceed with public scoping workshops for conventional impact analysis.

Comparative Approaches to Siting

The paper on comparative approaches to siting examines modalities for conflict resolution within the framework of socio-economic impact analysis under a variety of alternative planning and decision-making processes for site selection and implementation. Four different proposed siting processes are being compared, both with each other and to see how well, taken together, they span the range of possibilities.

Resolution of siting controversies is a difficult problem. There is an expressed desire at many levels of government to foster the maximum possible public participation, but the responsibility for safe management of high-level radioactive wastes belongs, both by philosophy and law, to the federal government. Thus, there is some question as to whether the federal government can delegate real authority to state or local agencies, since a division of responsibility from authority is often illegal. Simple pro-forma involvement of the public, public interest groups, and state and local governments without giving them any real voice or influence in the process is likely to engender difficulties for the program.

Accordingly, the role of each involved group—public, public interest groups, state and local governments, and various federal agencies—in the siting procedures needs to be examined carefully.

These same considerations enter into the paper on the role of state and local governments in other formal and informal decision-making and planning processes, particularly consultation and concurrence.

The Role of State and Local Governments

The two forthcoming topical papers on state-federal relations will attempt to provide a political and social overview that aids in evaluation of what is being attempted, and provides guidance on pending outcomes. The first paper, which is on consultation and concurrence as a general issue, will systematically order both the "players" and the "stakes", and then outline a view of the politics in terms of historical state-federal roles and the special nature of the issue.

The second paper, addressing the matter of the State Planning Council*, will attempt to fit this proposal, and the rapidly evolving definition of its own role that is emerging as the Council begins its activities, into the more generalized analytic framework.

*A proposal in which a state body would share a certain amount of federal authority regarding the issue of a nuclear waste repository.

Criteria Design and Specification

The fourth topical paper will involve the design and specification of the entity (or perhaps entities) who will be in charge of actual operations once the program grows out of its exploratory phase.

The question is whether any particular choice of organizational design (e.g., federal agency, government-chartered public or private corporation, etc.), or any particular formal specification of how the organization should be internally arranged will guarantee in advance the degree of responsibility and responsiveness that is necessary if the program is to proceed on schedule and succeed.

The thrust of this paper will be first to separate those details of organization and management for which the literature proposes clear recommendations, and second, to identify those areas where the literature clearly does not suggest any hard-and-fast answers. The third point will be to discuss the extent to which any prior formal specification of the organization in formal terms is either necessary or sufficient to ensure the level of actual performance and perceived reliability and responsiveness that is desired.

Adequacy of Existing Data for Social Science Program Assessment

The fifth topic involves the problem that interferes most greatly with the ability to perform meaningful impact assessments in the short term, even for the less confusing aspects of social impact.

The operating system, when deployed, will consist of organizations; decision-making procedures and mechanisms; those who regulate, coordinate, and schedule; unions, managers, governmental actors from every level of government, and a variety of workers; as well as machines, manufacturers, reactor operators, casks, pools, mines, and so forth. It will operate in an environment that has been very critical, and contains many whose reaction must be taken into account at each step. For the system to operate well, these social and technical systems must interact smoothly and reliably, and interfaces between and among operators and organizations must be well coordinated and understood. But the technical and geological data, however refined, can address only a limited range of these issues. Moreover, the unit facility assumption almost completely neglects those costs and impacts that are entirely systemic. Certainly, management and decision making will have certain direct impacts and costs associated with them. Perhaps more importantly, there needs to be an assessment of just what the increased complexity does to reliability, responsiveness, and other parameters which to some extent govern the direct and indirect social and political impacts of the operations themselves. This is, and has always been, somewhat of a challenge for new industries and new technologies.

Growth of the nuclear industry must also be considered. Since there must necessarily remain variables, such as the future size of the nuclear industry or the number of sites that will be required, which cannot be determined at this time, it is necessary to treat the matter of growth parametrically.

The purpose of this last, but central, paper is to focus attention on the classes and types of data that are needed for appropriate estimates to be improved. This set of concerns may seem quite long-range and removed from immediate programmatic problems and goals. But an artificial separation of near-term objectives from the long-term structure of the waste management system has been one of the major underlying sources of public anxiety and political concern. The general public, as well as governmental representatives, tend to make a clear distinction between scientific/research and engineering/implementation activities. In general, there has been far more trust of the former perhaps due to the perception that engineering/implementation will directly affect persons lives and those of their families, friends, neighbors, and children. What is implied is that whatever successes the present program may have, these may not be easily translatable into general consent for actual commercial-scale activities to proceed. For that to happen, there will have to be a greater public understanding of how the waste management system *as a system* will look, and what its systemic impacts might be.

SUMMARY

1.4 SITE IDENTIFICATION

Technical work continued in the site exploration area. The final *Gulf Coast Salt Dome Regional Summary and Area Recommendation* report and the draft *Permian Area Environmental Characterization* report were transmitted to DOE. No environmental field activities were conducted during this quarter. Environmental studies in all regions are being held in abeyance, pending completion of corresponding geologic studies or state consultation and concurrence.

Two documents were prepared on the generic environmental effects of geologic and geophysical activities and deep drilling. Work began on preparing annotated outlines of characterization documents and NEPA documents required during the NWTS site selection process.

Field work in the Gulf Coast Salt Dome Region was conducted in Louisiana, Mississippi, and Texas. Water supply wells at five sites have been installed, and nine deep wells at four sites have been completed. Pump tests have been conducted at two deep-well sites, and site restoration has been completed at two of the sites. Data analysis of 30 additional shallow borings at Cypress Creek and 10 shallow borings at Richton Dome was initiated. A third high-resolution reflection seismic line was completed at Cypress Creek, and three lines were completed at Richton Dome. Deep-well site restoration is complete in Texas. Contacts with landowners were initiated to obtain rights of entry for high-resolution seismic lines for the Keechi Dome laboratory studies, and analysis was conducted on caprock and salt core in Texas, Louisiana, and Mississippi. Hydrologic data collection and water sampling continued in Louisiana, and hydrological analysis continued in Texas, Louisiana, and Mississippi.

The report, *Results of Hydraulic Tests of Wells DOE-1, -2, and -3 Salt Valley, Utah,* was printed and distributed (USGS Open File Report 80-205). Analysis of data from the hole-to-surface resistivity, cross-hole seismic, and surface electromagnetic surveys at Salt Valley continued. Coring and open-hole hydrologic testing of the Gibson Dome No. 1 borehole (GD-1) was completed to a depth of about 2700 feet. Hole-to-surface resistivity measurements at GD-1 out to radial distances of approximately 6300 feet from the hole were completed.

Characterization of the stratigraphy and facies of salt-bearing sedimentary-rock units continued to be a primary task in the Permian Basin. Facies studies of the lower Clear Fork Formation were completed. A depositional model was developed for coastal sabkha salt-pan environments. Isopachous maps were completed of the alternating coarse-grained fan-delta clastics and algae-foram wackestones and packstones of the granite wash producing zone in the Mobeetie Field. Approximately 340×10^3 metric tons/year of sediment are discharged from the Little Red River Basin, and approximately 1.3×10^6 metric tons/year are discharged through the gaged portion of the Prairie Dog Town fork of the Red River. Lineament analysis of Landsat photos of the Texas Panhandle is complete. The extent of salt dissolution and contiguous ground collapse has been determined for the northern margin of the Palo Duro Basin and adjacent margins of the Dalhart and Anadarko Basins. The Ogallala and Permian hydrological systems are chemically distinguishable as a result of water-rock interaction in spite of the fact that the ground waters are hydraulically connected.

The National Screening for Geologic Repositories is continuing on schedule. The project plan is under review, and preliminary screening specifications are being evaluated. Literature review is in progress. However, much of the literature necessary for the study resides in state agencies and institutions. Consequently, access to that data is limited in light of DOE policies regarding consultation and concurrence.

Geologic assessment of the Devonian-Mississippian shale sequence in the Appalachian, Illinois, and Michigan Basins is being finalized. Within the Appalachian Basin, there are sizable areas in which thick deposits of undeformed shales occur at reasonable depths. Within these areas, there are shales, low in hydrocarbon potential, that have not been extensively affected by boreholes. Although more detailed studies are needed, there is regional potential toward the shale sequence in certain areas of the Appalachian Basin. Large parts of the Illinois Basin have favorable geologic conditions and are underlain by shale units that could be suitable host rocks for subsurface disposal of radioactive waste. Additional study is needed to characterize freshwater resources and to evaluate deeper, brackish water formations. Oil and natural gas occur in various intervals of thick shale in different parts of the Michigan Basin. Major groundwater resources occur in the glacial drift that covers most of the basin and in Paleozoic sediments in the southern portion. Although considerable work remains to definitize the potential for waste isolation in the Appalachian, Illinois, and Michigan Basins, there are many reasonably thick deposits of relatively undeformed shale present at suitable depths.

Work in the Salina Basin has been suspended pending resolution of consultation and concurrence issues.

Well-log digitization is continuing in central New York. As of June 1980, 130 logs have been digitized and checked for accuracy. The process is working well, and displays of reproduced logs are accurate and realistic.

WBS 1.4.2

Project: Survey of Argillaceous Rocks

Principal Investigator: Oak Ridge National Laboratory (G. D. Brunton, T. F. Lomenick)

ONWI Project Manager: R. Nicks

Objective

The objective of this work is to conduct a regional evaluation of the Devonian shales in the northeastern states to identify, determine, and describe the geological, hydrological, physical, and chemical properties of these shales that relate to their utility for the storage/disposal of radioactive wastes. This work is part of a larger national screening effort involving an expanded investigation of various nonsalt geologies.

Progress Reported Previously

This work was started during the last quarter of FY 79. Data on the Appalachian Basin have been reported previously.

Activities During the Reporting Period

This quarter's work finalized the regional geologic assessment of the Devonian-Mississippian shale sequence in the Appalachian, Illinois, and Michigan Basins.

On the basis of this preliminary assessment, much of the Appalachian Basin appears to exhibit a suitable geologic framework, while the Middle to Upper Devonian and Mississippian shale (clastic) sequence within that region also appears to display favorable characteristics. The basin has been tectonically stable since the end of the Paleozoic when its eastern margin was involved in various deformational events which produced the Appalachian Mountains. With the exception of numerous folds and thrust faults, also along its eastern margin, the strata within the basin proper show evidence of only gentle warping, and regional dips are less than a degree throughout. There is one principal cross-basin zone of faulting but it is primarily narrow and tends to be localized when compared to the large regional expanse of the entire basin. There are large sections of the basin which lack (on the basis of readily discernible geologic data) any major folds, faults, or extensive fractures. Joints are developed in many of the strata at the surface but in most such areas it remains to be demonstrated that these smaller scale structures affect rock units in the deeper subsurface.

Seismic activity within the basin has likewise been minimal, with many large areas never having experienced an event of an intensity greater than V on the Modified Mercalli (MM) Scale, and many areas never having experienced any events. Seismic-hazard rating for most of the basin is similarly low; only a small area in northeastern Ohio and western New York shows values above the generally low figures for the basin as a whole, and even here the difference is slight. Some external effect to the southeastern and south-central parts of the basin might be anticipated from the historically significant Charleston, South Carolina, seismic center and the possibly related northwest-trending belt that reaches western North Carolina. Slightly higher seismic hazard values in this part of the basin reflect the proximity of these seismic areas which lie well to the east of the basin.

The shale or clastic sequence reaches several thousand meters in thickness, and individual, more promising intervals within the sequence generally range from 80 to 300 or more meters in thickness. These same intervals, where they attain acceptable thicknesses, occur within depth ranges generally of 600 to 900 meters, although some are shallower or deeper depending upon exact location within the basin.

There are numerous black and dark brown shales which are rich in organic matter, exhibit higher natural radioactivity, and commonly yield gaseous hydrocarbons. Such zones have already proven to be productive for many years in portions of Ohio, Pennsylvania, West Virginia, Kentucky, Virginia, and New York. The most sizable gas fields are located in southwest Virginia and easternmost Kentucky. There are conversely several shale zones that are either interspersed with the black to dark brown intervals or laterally equivalent to them where lesser amounts of organic matter are present, and where the hydrocarbon potential is decidedly lowered, especially if the thermal maturation has not been appreciably greater. Porosity and permeability in all the shale intervals are low unless natural fractures have been effective. Fractures in some areas are related to more deeply buried structures and to thrust faults in other areas, and may be stratigraphically controlled in yet others. There is little evidence which ties surface joints to deeper fracture porosity; similarly, there is no agreement on how to detect subsurface fractures outside those areas where established gas production has already proven their existence.

Several other mineral resources are produced within the basin; those with the greatest potential for conflict with the shale sequence are oil, gas, and coal because the extent of development of each is large and overlaps with areas where sufficiently thick shales occur at moderate depth. Where reservoirs deeper than the shales have been actively sought, penetrating boreholes also become a factor. Although coal, either that undergoing mining now or that planned for future production, lies shallower than the shales, it poses conflicts regarding surface acreage.

Ground water does not appear to present the same potential conflicts as petroleum and coal. Relatively little ground water is used within the basin, and that which is comes mainly from very shallow, nonbedrock aquifers. Ground water deeper than the shale sequence is saline and not developed. More geohydrologic information specifically about the shale sequence which is not pursued as an aquifer is needed for a full characterization; the same holds for any smaller study areas.

Within the Appalachian Basin there exist sizable areas in which thick deposits of undeformed shales occur at reasonable depths. Within these areas there are shales which are lower in their hydrocarbon potential, have not been extensively affected by boreholes, and lie outside areas with competing resource applications. Although much more detailed study is needed, there clearly is a regional potential toward the shale sequence within certain areas within the Appalachian Basin.

The Michigan Basin appears to have a geologic framework and a series of thick shale deposits that may be locally unsuitable for the underground disposal of radioactive wastes. The basin has been tectonically stable since Precambrian time, and the sedimentary rocks contained within it are nearly flat-lying and lack significant deformation. Earthquake activity in the region has been relatively low inasmuch as only four events of MM V or greater have ever been recorded in the Southern Peninsula, and all parts of the basin are assigned to Seismic-Risk Zone 1.

The thickness of the shale sequence ranges from about 150 meters in the southeast part of the basin to as much as 500 meters in much of the west. The Antrim-Ellsworth part of the sequence underlies the entire basin and is typically from 150 to 300 meters thick, whereas the overlying predominantly argillaceous Coldwater Formation ranges from 150 to 300 meters thick in the western half of the basin. The area of greatest shale thickness, namely the central and western parts of the basin, is also where the stratigraphic units consist almost entirely of lighter colored shales that are low in organic matter. Depth to the top of the shale sequence is less than 300 meters only around the perimeter of the basin, while elsewhere in the basin the depth ranges up to a maximum of about 850 meters.

Black, brown, and dark-gray shales with high organic content predominate in the eastern half of the basin and extend as a westward-thinning wedge across the remainder of the basin within the lower part of the shale sequence. Thus, the greater proportion of the shales in the west are light gray and greenish to bluish gray, and generally lack significant amounts of organic matter. Porosity of the shales is typically low; permeability is extremely low, except where the rock is naturally fractured, whereupon both these physical properties become highly variable.

Oil and natural gas occur in various intervals of the thick shale sequence in different parts of the basin. Major production comes from the Berea Sandstone in the east, but commercial production has also been found in the Ellsworth Shale in the west and in the Antrim and Coldwater Shales at widely scattered locations throughout the basin. Dark shales that are rich in organic matter contain moderate amounts of natural gas in fractured zones in various areas. Special attention therefore needs to be paid to the possible occurrence of these hydrocarbons as they would invoke special mining and safety procedures in the event of a subsurface excavation.

Petroleum production in the Michigan Basin comes mainly from rock units that underlie the Devonian-Mississippian shales; consequently, there are local areas where numerous boreholes penetrate the shale sequence. Most of this drilling, however, is concentrated in specific areas or along specific trends. There are therefore large segments of the basin where boreholes drilled into the shales are few or widely spaced. Other penetrations of the shales include the salt mines and brine wells that currently recover resources from Silurian and Devonian strata.

Major ground-water resources occur in the glacial drift that covers most of the basin, and also in several Mississippian and Pennsylvanian sandstones in the southern portion. Other sources of ground water are scattered throughout the basin.

Portions of the Illinois Basin have a favorable geologic framework and are underlain by fairly thick shales that could be suitable host rocks for the subsurface disposal of radioactive wastes. Most of the region has been tectonically stable since Precambrian time, and the sedimentary strata in the basin have not been subjected to mountain-building processes. Although few faults are present in the northern half of the basin, the southern area contains the regionally extensive Shawneetown-Rough Creek and Wabash Valley fault zones, as well as a number of smaller faults throughout the mineralized zone of southern Illinois and western Kentucky. Recorded seismic activity follows this trend; namely, the northern and eastern parts of the basin have had few earthquakes of MM V or greater and lie within Seismic-Risk Zone 1, whereas the southern area is adjacent to the New Madrid seismic zone, the site of major earthquake activity nearly 170 years ago, and falls within Risk Zones 2 and 3. Because of the pronounced seismic activity and known structural complexities in the southern part of the basin, this area is considered to have a very low regional potential.

Thickness of the New Albany Shale ranges from 30 to 120 meters in most parts of the basin, while depths typically range from 150 to 1,200 meters. The shale is thickest in the southern part of the basin, where it also is deepest. In most of this area the shale is up to 120 meters thick and up to 1,200 meters deep. On the east side of the basin as much as 60 meters of shale is present locally at moderate depths as shallow as 750 meters, but over much of this eastern area the unit is thinner and shallower than that. A well-developed sequence of shales low in organic matter is present to the northwest in the so-called Petersburg Basin area. Much of this area is underlain by more than 60 meters of shale at depths between 300 and 450 meters.

In much of the basin the shale is predominantly brownish black to black and rich in organic matter. There are, however, some large areas where one or several of the units is light gray to greenish gray and contains little organic matter. Porosity of the shale is low and permeability is extremely low, except in areas where the rock has been fractured and there porosity and permeability values are highly variable. Useful data on fractures within the shales are now being collected under the Eastern Gas Shales Project (EGSP) and will prove valuable to this program as well as in any future assessment of potential fluid flow into or through the shales.

EGSP studies have shown that modest to moderate amounts of natural gas are present in the shale from some parts of the Illinois Basin, and that there are a few areas such as southern Indiana where commercial amounts of gas occur in fractured shale. Because of the need for special mining and safety techniques for excavating rock containing natural gas, considerable attention must be paid to the distribution, character, and quantity of such gases that might be present in any such study area.

Oil and some natural gas are produced from many fields, chiefly in the southeast half of the basin. Most of the production comes from rock units above the New Albany Shale, although some petroleum is produced from older or deeper formations. There are large parts of the basin, particularly in the northwest, where few boreholes penetrate the shale unit. Ground-water resources are found in the glacial drift that mantles much of the basin, as well as in both sandstone and carbonate aquifers. Additional study will be needed to more fully identify fresh water resources and to evaluate deeper brackish water formations that may lie close to the New Albany Shale.

The operational success of several underground storage caverns which have been mined in shale and limestone formations in the basin is also noteworthy. Almost all of these caverns have operated for many years without evidence of water inflow or structural fracture, and the slight water inflow observed in two caverns has not presented any problems.

In summary, there are areas in the Illinois Basin where reasonably thick deposits of undeformed New Albany Shale are present at moderate depths.

WBS 1.4.2

Project: National Screening for Geologic Repositories

Principal Investigator: Woodward-Clyde Consultants (A. S. Patwardhan)

ONWI Project Manager: R. Nicks

Objective

The objective is to systematically screen the contiguous 48 states to identify those portions that may be suitable for further investigation for the location of radioactive waste repositories, and to establish a nationwide data base that may be used in further studies by the DOE in support of the evaluations required by the National Environmental Policy Act (NEPA).

Progress Reported Previously

This is the first Quarterly Report for this project.

Activities During the Reporting Period

Procedures

Six technical tasks have been developed to meet the objective. They are described below.

Task 1 — Project Plan. Project plan development, detailing what will be done in the various tasks of the study, including the identification of major milestones, specification of government agency interfaces, and an outline of the project quality assurance program.

Task 2 — Screening Specifications. Numerical specifications development which will guide the screening and ranking processes.

Task 3 — Literature Review. Collection, review, evaluation and cataloging of the published and unpublished data that will be utilized in the various tasks of the study; development of the data management system to handle the needs of Task 3 and its interrelationships to the other tasks.

Task 4 — Data Compilation and Screening. Compilation of the data, application of the screening specifications, and implementation of the screening process to identify portions of the U.S. that may be suitable for further investigation for the location of radioactive waste repositories.

Task 5 — Analysis and Ranking of Regions Identified. Ranking of the regions in order of the preferability for additional investigation.

Task 6 — Final Technical Report. Summarizing the results of the study, identifying extent and limitation of data base, methodology of the study, and those portions of the U.S. which appear to be suitable for further investigation for repository siting.

Results

Only the first three tasks were initiated during the reporting period. The significant results of each task are described below.

Task 1 — Project Plan. The objective of the Project Plan is to describe in detail the approach and methodology that will be applied in each task of the National Screening for Geologic Repositories. Major technical milestones are identified in the Project Plan. Government interfaces are discussed regarding their type and importance to the project. The project quality assurance program is also introduced in the Project Plan. The Project Plan incorporating the items stated above was submitted for review.

Task 2 — Screening Specifications. The objective of this task is to identify and establish screening specifications which define a level of achievement (for screening) in terms of the overall objective of the study (i.e., identify portions of the U.S. suitable for further study in siting nuclear waste repositories), and which provide a mechanism for successively reducing the study area. The approach or procedure tht is applied to develop the specifications will:

(1) Define the major issues that must be considered in identifying areas for repository siting

(2) Determine the specific considerations that make up each issue

(3) Identify possible evaluation measures and screening specifications for each consideration

(4) Determine how these measures and specifications could be applied in each major type of geologic medium

(5) Identify data requirements and availability for each measure and specification

(6) Identify the set of specifications for use in screening.

During the reporting period the effort toward developing specifications proceeded through Step 2. In general terms, the issues of concern for siting a nuclear waste repository have been defined as dealing with:

- Public health and safety (including natural and man-made conditions)
- Environmental impacts (including socioeconomic and institutional factors)
- System cost and reliability.

Potential specific considerations identified for each issue are listed in Table 1. It is important to note that not all the considerations will ultimately have measures and specifications developed for them. The actual development and application of measures and specifications will be closely tied to their practical and reasonable use in a national screening process such as the one being conducted.

Task 3 — Literature Review. The primary objective of Task 3 is to collect, review, and catalog the data to be utilized in the national screening for geologic repositories.

In particular, the data are collected for use in Task 2, Screening Specifications; Task 4, Data Compilation and Screening; and Task 5, Analysis and Ranking. The approach or procedure to accomplish Task 3 is to:

(1) Identify the basis for the literature review

(2) Identify the data sources

(3) Obtain the data

(4) Process the data through review and evaluation, followed by cataloging in a storage and retrieval system.

The work accomplished in Task 3 to date has involved all four steps listed above. These efforts have been directed primarily at supplying the data supporting the development of screening specifications and the data that will be utilized in Phase I of screening.

Three basic assumptions have been identified which provide a basis for the literature review:

- The data to be collected, reviewed, and cataloged will consist of readily available published and unpublished literature generated to date.
- The compilation and cataloging of the data will be primarily from the standpoint of their probable utilization in the siting process with the application of present-day technology.
- The coverage and detail of the data may vary depending upon the size of the area under study. The data utilized for a national-level assessment may not be the same as those used for assessing smaller areas such as candidate areas. Thus, the scale of the data collection effort will depend upon the screening phase for which use is intended.

Data screening and entry forms have been developed which provide a mechanism for screening the acquired data (both in text and map form) and which compile the information needed for the data cataloging and retrieval system.

TABLE 1. POTENTIAL CONSIDERATIONS

Issue: Public Health and Safety

A. Potentially Adverse Natural Conditions

a. Fault rupture
b. Generation of new faults
c. Earthquake ground motion
d. Tectonic movement
e. Ground water contamination
f. Flooding
g. Volcanic hazards
h. Geothermal condition
i. Ground failure (landslides, karst, dissolution)
j. Erosion/denudation
k. Stratigraphic condition
l. Geomorphic changes
m. Major climatic changes
n. Geochemical rock properties

B. Potentially Adverse Human Activities

a. Aircraft impact
b. Hazardous facilities
c. Transportation
d. Induced seismicity
e. Subsurface mineral exploration and extraction (including water)
f. National defense and security
g. Man-made hydrologic changes (flooding, impoundment)
h. Operational radiation release

Issue: Environmental Impacts

a. Areas of ecological value (protected species)
b. Important agricultural land (prime and unique land)
c. Special management areas (national parks, wildlife refuges)
d. Air quality

Issue: System Cost and Reliability

a. Surface site preparation
b. Subsurface site preparation

The library capabilities of the computerized Geographic Information System (GIS) will accommodate the cataloging and retrieval of the data sources. This will provide for quick and easy entry into the cataloging system, and will expand the capabilities of retrieval through geographic location by providing a geographic system which is linked to the maps used in the screening and ranking tasks.

GIS library capabilities have been applied to the needs of the literature review task. Four cross-referenced categories appear to be the most useful in cataloging and retrieving the data utilized on the project:

- Author
- Geographic location (probably by state and/or county)
- Discipline and/or key word
- Phase of screening and ranking.

The primary data sources for use in the projects have been identified and may be summarized generally in the following manner for each applicable task:

Task 2:	Primarily federal agencies and NWTS contractor reports
Task 4, Phase I:	Primarily federal agencies (e.g., USGS, USNRC, US Department of Interior, etc.).
Task 4, Phase II:	Primarily state agencies; secondarily, federal agencies.
Task 4, Phase III:	Primarily state, federal and local agencies.
Task 5:	Primarily state, federal and local agencies.

As can be seen in this breakdown, substantial contact with state agencies (e.g., geological surveys, environmental agencies, natural resources departments, water resources boards, etc.) will be necessary to obtain adequate and appropriate data.

To date, data have been obtained from only federal agencies or institutions. The data collected are to support Task 2 and Phase I of Task 4. These data have been processed using the data screening and entry forms developed in Step 1 and will be introduced into the GIS library.

WBS 1.4.2

Project: Shale Screening Factors Study

Principal Investigator: Sandia National Laboratories (L. D. Tyler)

ONWI Project Manager: G. E. Raines

Objective

Because of the lithologic variability of argillaceous rocks, there is real uncertainty regarding the specific rock type and geologic setting that might prove the most favorable for emplacement of waste. This study considers the content of expandable clays and their position with respect to the water table as variables in an attempt to develop a set of relative screening factors that might limit the allowable emplacement densities in argillaceous rocks. As such, it combines limited calculations and material-property data collection in an effort to assess limitations to existing data, to determine data that might be required in the future, and to assess modeling approaches and limitations.

Progress Reported Previously

This project was initiated in March of 1980. This is the first progress report on the project.

Activities During the Reporting Period

Properties, Data Needs, and Limitations

Reliable thermal properties are required for reliable thermal calculations. Such properties exist, in part, for shales poor in expandable clays, i.e., "high-illite" shales, but not for those that contain abundant expandables (smectites). Conductivity data contained in the Generic Environmental Impact Statement (GEIS) are in excellent agreement with conductivities calculated from the average mineral composition of Paleozoic shales, except that the factors of pore water content and volatilization are not included in the GEIS. Extension of the same formalism to a shale high in expandable clays, such as the Pierre shale, indicates that the natural-state, fully hydrated thermal conductivity of this rock should be about 1.52 W/m/C parallel to layering, as opposed to 2.19 W/m/C in the case of generic high-illite shale. The attempt to validate the thermal conductivity model experimentally has been hampered by lack of material from representative portions of the Pierre. Conductivity measurements on material from the Mobridge Member of the Pierre, which is generally quite calcareous in contrast to the formation as a whole, average about 2.0 W/m/C parallel to layering. The material will be analyzed mineralogically to provide a check with the interpretation that calcite is responsible for the high conductivity.

Thermal expansion data are sparse for high-illite shales and almost totally absent for high-expandable rocks. Results to date indicate that expansion of high-illite shales is dominated by the expansion of quartz. Due to their high porosity, expansion of high-expandable shales under high pore pressures is dominated by the expansion of contained pore water. Expansion/contraction of these rocks under low pore pressures appears to be dominated by a combination of pore collapse due to water release and changes in basal spacing of expandable clays. The apparent complexity of thermal expansion in argillaceous rocks, involving at least partial coupling of mineralogy, water content, porosity, permeability, and fluid pressures, is noteworthy.

Modeling

Thermal calculations have almost been completed for the cases involving high-illite shales. Initial calculations, using the thermal properties specified in the GEIS, were in excellent agreement with similar calculations made by SAI as part of the Shale ERE report. The model being used was then changed to include variable rock thermal conductivity and pore-water boil-off, in addition to the presence of crushed formation material and the canister/sleeve assembly. These modifications had only about a 10 percent effect on peak rock temperatures (decreased from 187 to 165 C for emplacement of 10-year-old HLW at 60 kW/acre, 1.2 kW/can). However, calculated waste temperatures were increased from 218 to 305 C, an increase of almost 50 percent. It thus appears that uncertainties in the thermal properties of engineered backfill materials could have a greater effect on waste temperatures than uncertainties in thermal properties of the emplacement medium.

Generation of the detailed model to be used in stress calculations is almost complete. The model is nonlinear and three-dimensional, and is compatible with the general-purpose finite-element code SANDIA-ADINA. The definition of the correct mesh, proper boundary conditions, and suitable pre- and post-processing has required considerable effort. However, except for the change in mechanical properties, the model will be applicable to both high-illite and high-expandable shales. Most calculations should be complete within a month.

It has generally been assumed that the major mechanism of water loss from rock in and near a waste repository would be by boiling of pore water. Both theoretical and experimental investigations indicate, however, that significant dehydration can occur as a result of simple evaporation. Thus, for a repository emplaced below the water table, there are two competing effects: (1) seepage into the underground workings as a result of Darcy flow driven by the hydraulic head, and (2) the evaporative loss process itself. At present, the best model of the evaporative process appears to be diffusion or forced flow of water vapor through the rock, away from a well-defined evaporation front. A model has been developed based on this phenomenon. One-dimensional calculations involving both Darcy flow and the evaporative process will be performed in order to estimate the position of the evaporative front. Consideration will also be given to possible changes in permeability of different types of shale as a result of variations in relative humidity.

Some preliminary calculations have been completed to examine both potential water inflow rates and fluid pressurization in a repository emplaced in argillaceous rocks. Assuming rock-mass dehydration to be negligible, calculated inflow rates range from approximately 10^{-3} to 1 gallon H_2O/per meter of drift per year for rock permeabilities of between 10^{-17} and 10^{-21} square meters. Preliminary fluid pressure calculations indicate that fluid pressures resulting from in situ heating could possibly exceed the lithostatic load, depending upon the in situ permeability and heating rates. In most cases, however, fluid pressures remain quite low. These calculations will be extended to include the variable porosities and permeability-temperature relationships resulting from variable contents of expandable clays.

WBS 1.4.3

Project: Gulf Coast Salt Domes

Principal Investigator: Law Engineering Testing Company (D. E. Pauls)

ONWI Project Manager: O. E. Swanson

Objective

The overall objective of the Geologic Project Manager (GPM) project is to identify, evaluate, and rank potential candidate sites for a nuclear waste repository. Other scientific investigations have been established by ONWI to evaluate the geologic and hydrologic framework in the study areas of northwest Texas, Louisiana, and Mississippi. The GPM will utilize results of these investigations to arrive at conclusions for dome priorities.

Progress Reported Previously

The Geologic Project Manager began activities on 29 August, 1977. The original program required:

(1) Review of previous project activities, overall assessment of project status, establishment of a project schedule, and allocation of budgets

(2) Evaluation of the geologic and hydrologic framework in the area of two or three salt domes in each state (Texas, Louisiana, and Mississippi), and provision of a uniform data base for each of six to eight potential domes within these areas

(3) Evaluation of suitable domes in the states of Texas, Louisiana, and Mississippi.

Eight salt domes were identified for further consideration during an Area Characterization study phase now in progress. These salt domes were:

Texas:	Keechi Oakwood Palestine
Louisiana:	Rayburn's Vacherie
Mississippi:	Cypress Creek Lampton Richton

Data collection for evaluation of the domes under study during Area Characterization includes the following activities:

- Deep borings to explore the sediments enveloping the domes to determine the existence or nonexistence of pathways for leakage of waste to the biosphere

- Core borings into the salt stock to obtain preliminary information on the character of the salt itself
- Shallow borings for surface geologic mapping, with emphasis on stream terrace deposits
- Geophysical and drilling mud logging for lithologic grain-size analysis and correlation of transmissivity and permeability of the aquifers
- Pump tests to determine transmissivity, permeability, and other aquifer properties
- Gravity field work and modeling to determine the geometry of the domes
- Terrace mapping to gather evidence of Quaternary faulting which might represent a threat to domal containment integrity
- Thermal imagery to aid in the identification of lineaments and other anomalies with surface expression
- High-resolution seismic reflection field work and purchase of seismic data to aid in the interpretation of the geologic structure and stratigraphy of the study areas.

Data acquisition and evaluation continued in support of Area Characterization. Deep drilling operations for the Area Characterization phase were completed in Texas and Mississippi. These operations consisted of drilling 6 deep wells and 1 water well in Texas and completing the wells in Mississippi. Pump tests to determine aquifer properties were completed in Texas and Mississippi. Site restoration was completed in Mississippi and nearing completion in Texas.

Twenty shallow borings were made in Texas, and 107 shallow borings were made in Louisiana in support of surface mapping programs of Texas Bureau of Economic Geology (TBEG) and Louisiana State University (LSU), respectively.

Gravity field work has been completed and models of the salt stock have been prepared for six domes based on purchased and measured gravity data and supplemented by seismic data and well control data where available.

Evaluations from high-resolution seismic lines were completed from data taken from the Cypress Creek Dome.

In Louisiana, water wells were completed at three of five deep-well sites, and drilling and geophysical logging of three of eleven planned deep wells were completed.

Activities During the Reporting Period

Field Operations and Data Acquisition

The objectives of the reporting period were to complete acquisition of land access for planned activities, complete the land restoration in Mississippi, conduct high-resolution reflection seismic surveys in Louisiana, and complete site restoration in Texas. New activities include obtaining high-resolution reflection seismic data at the Keechi Dome and conducting a shallow boring program at the Vacherie Dome in support of the LSU Quaternary studies.

Texas. Restoration of the deep well sites in Texas has been completed. Contacts with landowners were initiated to obtain rights-of-entry for high-resolution reflection seismic surveys at Keechi Dome.

Louisiana. Water supply wells at five sites have been installed, and nine deep wells at four sites have been completed. This completes nine of eleven planned deep wells in Louisiana. Pump tests have been conducted at two deep well sites, and site restoration has been completed at two sites. High-resolution reflection seismic surveys are being planned for Rayburn's and Vacherie Domes.

Mississippi. Data reduction from shallow borings at Cypress Creek and Richton Dome was completed. Data analysis from high resolution seismic lines was completed at Richton and Cypress Creek.

A model of the salt stock at the Richton Dome was prepared based on gravity data and well control.

Analysis and Technical Reporting

The objectives of the reporting period were to complete the interpretations, evaluations, and analyses necessary to characterize the geologic and hydrologic conditions in the study areas.

Included in the analysis were:

(1) Historic review of the Gulf Coast Salt Domes Project

(2) Regional geologic characterization summary including generic reports on:

- Salt Dome Growth
- Internal Structure of Salt Domes
- Descriptions of Mines in Gulf Interior Region (GIR) Salt Domes
- Seismicity of the GIR
- Erosion and Sedimentation Potential
- Mineral Resources.

(3) Selection of salt domes for Area Characterization studies.

East Texas Study Area. Detailed interpretation of regional reflection seismic data to assist in delineating the regional structural geology has continued. Interpretation of five new lines and revision of three previously interpreted lines were completed for the East Texas Study Area.

In Texas all aquifer tests on shallow borings drilled during the field investigations were completed. Aquifer tests on ten shallow borings were analyzed and transmissivity, storage, and hydraulic conductivity values of these aquifers were computed.

Louisiana Study Area. Drilling and aquifer testing is still ongoing in Louisiana; to date, only one aquifer test has been completed and analyzed at Site LH-2. Transmissivity and hydraulic conductivity values for three wells at that site have been calculated. Cation/anion ratio contour maps and total dissolved solids contour maps of the Sparta and Wilcox aquifers have been completed.

Vertical travel times of water around domes to the biosphere in all salt dome basins have been calculated.

Three structural contour maps of the study area—the top of the Midway Group, base of the Ferry Lake Formation, and top of the Sligo Formation—were completed. Deep subsurface faults were interpreted (most of the previously interpreted faults were confirmed) from missing well log sections. Three geologic cross sections were constructed for the study area using well log data.

Five structural contour and four isopach maps of the Vacherie Dome and Rayburn's Dome areas were completed. Analysis of the maps (based on sparse data, especially at Rayburn's) confirmed previous dome growth interpretations.

The computer gravity model of Vacherie Dome was rerun to incorporate additional well control. The size, shape, and location of the dome at depth remain virtually unchanged.

Interpretation and analyses of existing well data and of purchased seismic data continued.

Mississippi Study Area. Analysis of remote sensing data, including lineament drainage and topographic analyses, was completed. Known faults were projected to the surface to assess correlation with lineaments, and poor to very poor correlations were found. Drainage patterns in the three candidate dome areas were interpreted by contouring of drainage-link frequency and drainage ratios. These analyses do not indicate any clear evidence of any recent domal movement influencing drainage patterns.

Eight structure contour maps, ranging from the top of the Lower Cretaceous-Lower Tuscaloosa Formation to the Oligocene Vicksburg Formation, were completed. Analyses of the structural trends as well as well log correlation defined ten fault zones within the study area. Three of these fault zones exist on the flanks of Cypress Creek, Lampton, and Richton domes. Glazier, Tatum, and Sunrise Domes also have fault zones on their flanks.

Analysis of the structural trends indicates that a change in attitude of the strata occurred between Cretaceous and Late Tertiary time. Regional strike, locally influenced by apparent large salt-withdrawal basins such as the Perry Basin, has a northwesterly trend in Cretaceous strata and trends nearly east-west in Late Tertiary strata. The shift apparently reflects a change in depocenters from the Mississippi Embayment to the present-day Gulf Basin.

Four deep, common depth point seismic lines were interpreted. These lines cover the eastern one-third of the study area and generally confirm the structure contoured. A large, normal, fault-cutting strata from the Louann Salt, perhaps cutting strata in the presalt basement, to Cretaceous beds was identified on one of the seismic lines. Displacement along the fault is approximately 1700 to 2600 feet. The fault is located within the Perry Basin and lies near the southeast flank of Cypress Creek Dome.

All three high-resolution seismic lines at Cypress Creek Dome were interpreted. They do not indicate any significant faulting near or over the dome. However, the southernmost line indicates that the dome extends about 1/2 mile farther south than the current gravity model indicates. This is believed due in large part to the presence of anhydrite, up to 600 feet thick, below the salt overhang. The existence of the anhydrite, unknown when the model was made, was discovered during interpretation of the recently obtained Shell Oil Company well logs.

All aquifer test data for Mississippi have been analyzed. A water-table map for the study area was completed by utilizing ground-water levels from LETCo wells and wells in the study area that have been inventoried by USGS. Water-chemistry analysis of ground- and surface-water samples has been characterized, to the extent possible, in order to determine the relationship of surface water to ground water. Cation/anion ratios for all aquifers of interest in Mississippi were statistically analyzed to chemically characterize these water-bearing units and determine the amount of flushing by meteoric waters.

WBS 1.4.3

Project: An Investigation of the Utility of Gulf Coast Salt Domes for the Storage or Disposal of Radioactive Wastes

Principal Investigator: Louisiana State University (J. Martinez)

ONWI Project Manager: O. E. Swanson

Objective

The objective is to evaluate salt dome suitability for use as a repository, through geologic and hydrologic studies on Louisiana salt domes, including geomechanics, geohydrology, regional geology, and Quaternary geology studies.

Progress Reported Previously

Geomechanics Studies

Geomechanics studies have included monitoring of any current ongoing movement over the dome with a complementary system of field instrumentation and numerical modeling. These studies include: (1) tiltmeters, (2) precise releveling, (3) corehole closure monitoring, (4) seismicity monitoring, (5) microseismic monitoring, (6) numerical modeling, and (7) planning of laser ranging systems.

Geohydrology Studies

Geohydrology studies have included the drilling of seven exploratory-observation wells. A possible saline plume was detected to the east and southeast of Vacherie dome (no such plume was observed in the vicinity of Rayburn's dome). Numerical modeling activities have been initiated to simulate domal saline plumes. Several existing salt mines in the Gulf Coast were studied in regard to leaks. The chemical and isotopic analyses of the water from leaks at Belle Isle, Weeks Island, and Jefferson Island salt mines strongly indicate that the mine brines are formation waters. A technique was developed to conduct routine measurements of $\pm$ 0.002 wt percent water in salt. Preparations were begun for isotopic analyses of trace water extracted from salt.

Regional Geology

Regional geology studies, covering structure and stratigraphy of the north Louisiana salt dome basin, were completed in previous years, as were several seismic studies of Vacherie salt dome. Chemical analyses on a reconnaissance basis of salt core samples taken at 20-foot intervals have been completed. Mathematical approaches to the inverse density interpretation of gravity data over salt domes have been developed. Work last quarter included studies of anhydrite content and minute fluid inclusions in halite and revisions in chemical analytical techniques for use in high-precision analyses.

Quaternary Geology

Quaternary geology studies have focused on tectonic stability, hydrologic stability, and the possible effects of erosion during the next 250,000 years. Studies at Vacherie dome to date indicate that the dome is tectonically stable. Studies at Rayburn's dome are not sufficiently advanced to make a determination concerning tectonic stability there. As regards hydrologic stability, there is evidence of minor dissolution at Vacherie dome and of considerable dissolution (as much as 100 feet) at Rayburn's dome during Quaternary time. Quaternary studies of the effects of erosion indicate that a maximum of 120 feet of erosion can be expected during the next 250,000 years at both sites. This would have no effect at Vacherie, but would expose caprock. The deleterious effects of such exposure at Rayburn's dome is debatable.

Activities During the Reporting Period

GEOMECHANICS

The overall objective of the geomechanics study is to monitor and analyze any possible ongoing movement that can be associated with salt domes. Field work and relevant analyses currently are focused on the two north Louisiana study domes, i.e., Vacherie and Rayburn's.

Monitoring and analyzing possible movement over the two study domes involve close interaction between field work and data analyses. The latter will be assisted by numerical modeling of possible modes of dome movement. Initially, the geomechanics effort concentrated on monitoring possible upward long-term movements of the study domes to assess their current tectonic stability. However, it soon became evident that the instrumentation, numerical modeling (via the finite-element method), and general methodology of the geomechanics study were also potentially useful for analyzing other possible current movements over the domes, e.g., subsidence associated with salt dissolution from either man-made or naturally occurring hydrologic effects. In addition, the study furnishes baseline data on minute "undisturbed" movements over the study domes prior to any significant man-made activities there. Should one of the study domes be selected for more intensive study, then these data would become highly significant.

The geomechanics study currently includes the following seven substudies, which involve both field studies (with instrumentation) and analyses (with numerical modeling where appropriate): (1) two systems of tiltmeters over Vacherie and Rayburn's domes, respectively; (2) periodic precise releveling of monument networks over Vacherie and Rayburn's domes [the networks were established by the National Geologic Survey (NGS) in the early summer of 1977, and tied into the national NGS network]; (3) monitoring of the coreholes in the study domes for closure rates versus depth by periodic caliper surveys; (4) monitoring of seismicity in wells and coreholes over the domes; (5) monitoring of microseisms near the caprock over the Rayburn's dome; (6) numerical modeling of possible dome movement and any effects related to interpreting field instrumentation data; and (7) planning relative to possible laser ranging of horizontal movements coupled with any vertical dome movement.

Following is a description of the status of each of these substudies.

Tiltmeter Systems—Field Operations

Four tiltmeters currently are emplaced around the periphery of Vacherie dome as depicted in Figure 1. A tiltmeter site previously denoted as T4 was abandoned at Vacherie because of repeated flooding associated with an exceptionally high and fluctuating local water table.

Three tiltmeters currently are emplaced around the Rayburn's dome as indicated in Figure 2. Again, because of repeated flooding, a tiltmeter site previously labelled T4 was abandoned. Because Rayburn's dome is relatively small, it was decided that three tiltmeter sites were adequate to detect any tilt motion (rotation) associated with possible dome movement.

The tiltmeters have been generally performing satisfactorily. Data are being collected, and plans have been essentially completed to assess and analyze these data relative to possible dome movement. It is now tentatively planned to return all tiltmeters to the LSU laboratories for recalibration late in the summer of 1980.

Tiltmeter Data Processing and Analysis

The data acquired from the tiltmeter installations were recorded initially on strip chart recorders. More recently, the data have been recorded on digital cassette tapes. A major part of the data-processing work load has been related to the digitizing of the earlier strip chart recordings and transferring data to IBM compatible tapes. This task should be completed during the summer of 1980.

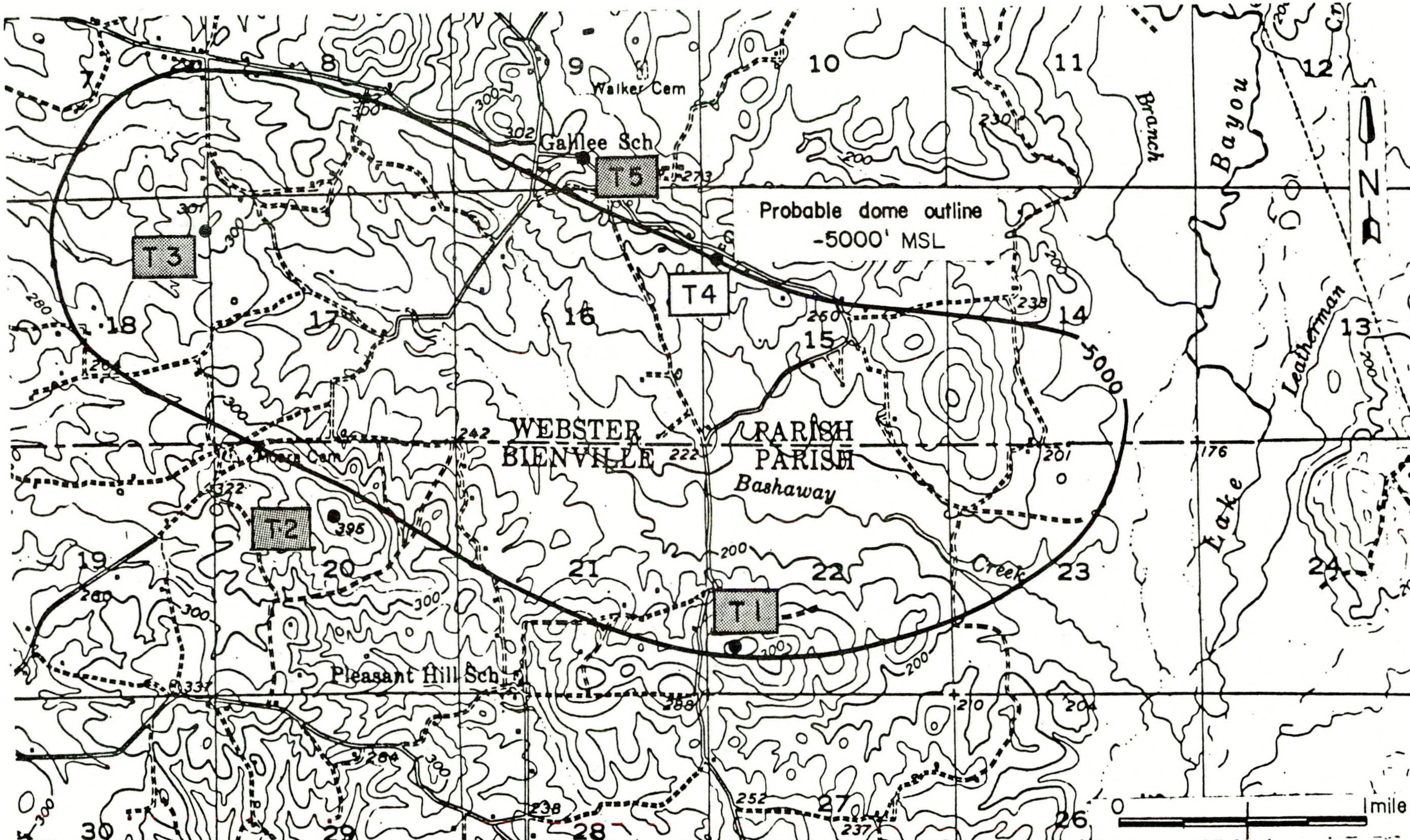
Precise Releveling of Monument Networks

Plans now include precise releveling of the monuments network over the Vacherie dome in the summer of 1981. Whether the Rayburn's dome network will be releveled will depend upon the future level of interest in that dome as a possible repository.

Generally, precise releveling has been previously accepted as a reliable and viable method for assessing trends in surface earth movement over the relatively long term. It is undoubtedly the premier method for assessing possible vertical ground movements in accessible locations scattered over a fairly large area. Further, the method is well documented and the associated techniques are clearly understood, thus lending a high degree of confidence in associated data and their interpretation. Quality assurance requirements consequently are readily satisfied by competent professional subcontractors performing precise releveling surveys.

Monitoring Corehole Closure

The coreholes in the Vacherie and Rayburn's domes were extended to a total depth of 5000 feet (1524 meters) largely to provide an opportunity to monitor hole closure at depth in salt.



= ACTIVE TILTMETERS

FIGURE 1. LOCATIONS OF TILTMETER SITES, VACHERIE DOME

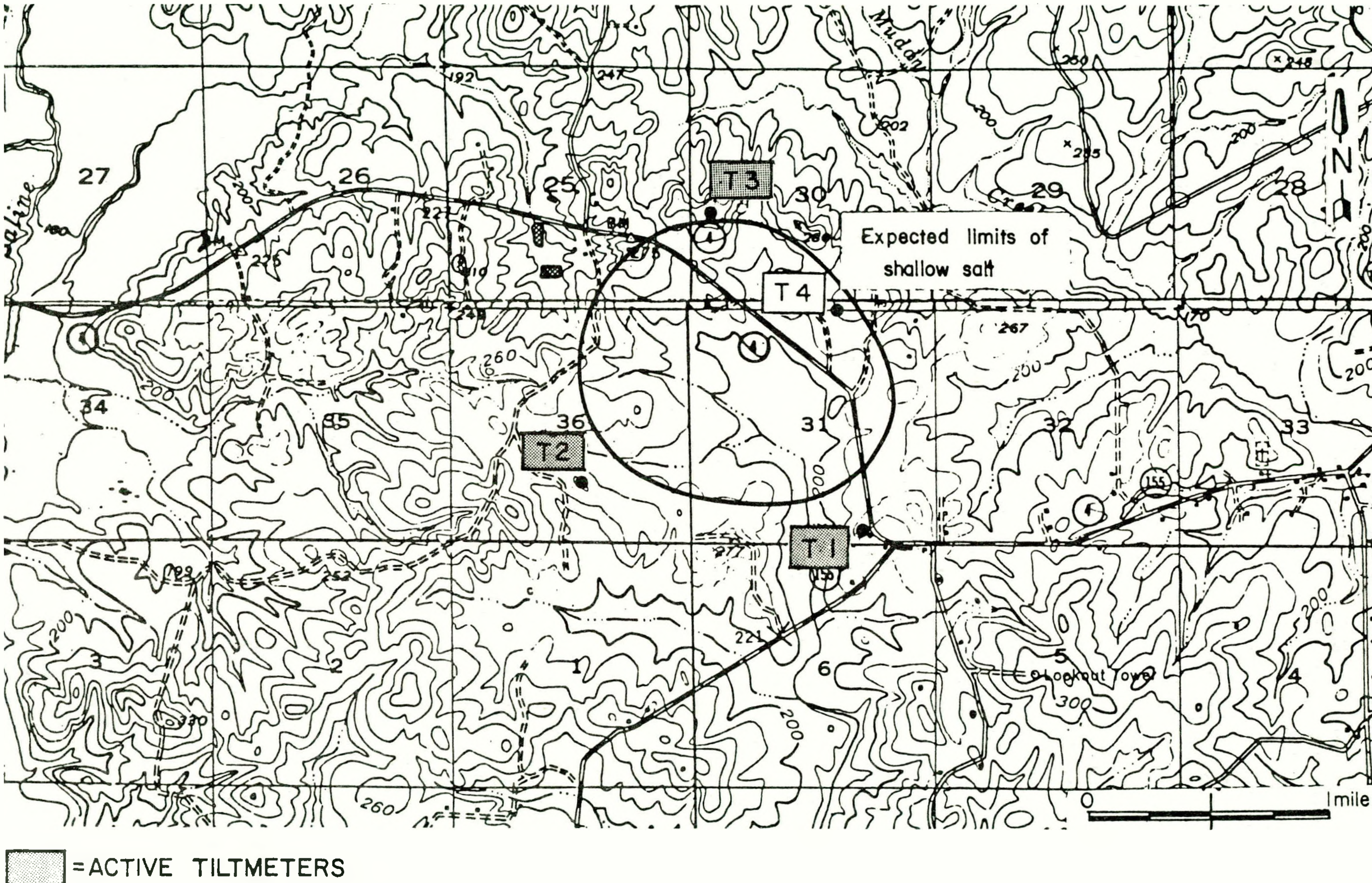


FIGURE 2. LOCATIONS OF TILTMETER SITES, RAYBURN'S DOME

Work is continuing on this substudy, with caliper relogging of the coreholes planned for mid-summer of 1980. In addition, precise monitoring of the fluid level in the Rayburn's corehole should begin about that time. As noted in previous reports, the fluid level in the Rayburn's corehole has been observed to be essentially static since the completion of that well in May, 1978.

Monitoring Seismicity Over Vacherie Dome

A borehole seismometer has been obtained to monitor possible seismicity in a water observation well at the Vacherie dome. A similar instrument had been tried in the well over a year ago; however, brine apparently penetrated the insulation over the wire conductors and "shorted-out" (and destroyed) the instrument. Current plans include installing the seismometer at a depth near the top of salt in the Vacherie well and monitoring possible seismicity.

Monitoring Microseisms Over Rayburn's Dome

Monitoring of microseisms over the Rayburn's dome is in progress at the present time (June, 1980). Geophones have been dropped in boreholes which penetrate to depths near the top of the caprock. The portable monitoring equipment is set up during field trips in an instrumentation shack which has had 110 ac power installed in it. Microseismic data currently are being collected and analyzed in a preliminary manner. Following collection of additional data and learning more about the site-specific characteristics of the Rayburn's dome, the data analyses associated with microseismic monitoring will move to a more advanced phase.

Numerical Modeling

The numerical modeling of the domes as 3-D geologic structures has been relatively dormant. However, the models currently are being reactivated with the objective of obtaining useful numerical aids for interpretation of field data.

Planning of Laser Ranging

Approximately 4 years ago, the concept of high-precision laser ranging was introduced as a potential technique for monitoring possible vertical movements of salt domes. Vertical movements of domes will result in coupled lateral stretching (with upward motion) or compression (with downward motion) of the overburden material.

The countryside over the north Louisiana study domes is generally covered with either trees or thick brush, and furthermore does not exhibit much relief. Laser ranging requires line-of-sight vision between monitoring stations, which ideally would be situated at the tiltmeter locations surrounding the domes. This would entail the erection of relatively tall, approximately 30 to 60-foot (10 to 20-meter), portable towers at these sites for periods of several weeks. The technology is available to carry out the laser ranging study if an intense monitoring effort is to be mounted for a particular dome.

Additional Substudies

In addition to the ongoing substudies described briefly in the preceding sections, the status of two other substudies is outlined here.

In Situ Soil Properties Over the Vacherie Dome. In 1977, a series of soil exploration in situ studies and samplings were carried out over the Vacherie dome. Cone penetrometer results were detailed from those studies. Subsequently, complete findings which incorporate laboratory test results and analyses for the soil samples taken were reached. Two findings are that soil type is the most important factor influencing consolidation, and the average modulus of elasticity, E_s, and Poisson's ratio, μ, to be used in the finite-element analysis conducted to model the dome movement are 862 kg/cm^2 (84.5 mPa) and 0.43, respectively. Table 1 indicates typical values obtained for the Vacherie soils engineering properties.

Two items should be noted relative to the soils data presented here, i.e., (1) the soil samples were taken at the tiltmeter sites on "high" points around the periphery of the dome (see Figure 1 of this section) and (2) the samples were taken at depths of interest for engineering analyses. In particular, the listed properties should be useful for relatively near-surface analyses; however, they should not be regarded as typical of properties of the geologic media near the upper or lateral surfaces of the dome. These media can be anticipated to be much stiffer (larger magnitudes of E_s) than the near-surface soils discussed here.

Natural Temperature Distribution Around Salt Domes. In summary, the technical research associated with this project has been completed, and a report should be forthcoming.

TABLE 1. TRIAXIAL TEST RESULTS

Soil	UIT, kg/cm^2	E_s, kg/cm^2	E_{s_k}, kg/cm^2 (b)	μ	γ, gr/cm^3
A	9.00	800.00	1666.66	0.42	2.00
A(a)	7.57	727.27	454.00	0.48	2.01
B	9.17	888.88	1666.66	0.41	2.05
B(a)	7.75	615.38	660.00	0.42	2.04
C	7.47	615.38	1666.66	0.46	2.04
C(a)	5.72	448.48	476.00	0.37	2.03
D	7.90	1142.80	1176.47	0.44	2.02
D(a)	6.55	1142.80	1428.57	0.46	2.01

(a) Soil at high temperature (182 F, 83.33 C).
(b) E_{s_k}, modulus of elasticity by Kondner method.

GEOHYDROLOGY

The objective of the geohydrologic investigations is twofold: (1) to determine the hydrologic stability of the Vacherie and Rayburn's salt domes and (2) to evaluate the hydrologic integrity of mined openings developed for nuclear waste isolation. The first objective will be achieved by assessing the presence or absence of dissolution of the salt stocks now and in the future. If salt dissolution is an active process, rates and patterns of the natural process must be identified. The second objective will be achieved by assessing the effectiveness of a salt stock to block inflow of water into and outflow of water from a mine chamber in a dome through the study of subsurface leaks in some existing salt mines. A thorough understanding of the mine leaks will provide a basis for predicting the degree of hydrologic isolation that a repository will afford for the isolation of the nuclear waste.

Evidence of dissolution of the salt stock is provided by the presence of saline plumes. Such a plume was detected at Vacherie in the Wilcox (Eocene) aquifer on the basis of salinities derived from electric logs of petroleum wells in the area. It is located just east and southeast of the dome. Further studies suggested the presence of a similar plume in the deeper aquifers (Upper Cretaceous). The plume remains untested by drilling. However, some information on the geohydrologic conditions of the north and south flanks of the dome and the sediments/salt interface was obtained by drilling four exploration-observation wells in the dome area during 1977-78. During the same period, three exploration-observation wells provided data that confirmed the absence of a saline plume in the Wilcox aquifer west and southwest of Rayburn's dome. However, surface salines and salt springs reported in the area may be indicative of hydrologic instability. The origin of such salt springs remains unstudied. The wells drilled in the salt dome areas provided geological information, water samples, and water-level data important to the investigation of the local geohydrology of the domes. However, the total data available to date are inadequate for resolving the question of hydrologic stability.

As part of the study, numerical modeling activities have been under way to simulate saline plumes associated with salt domes. The three-dimensional model developed so far is essentially a transport model, based on a set of coupled, nonlinear, partial differential equations of continuity, momentum, and solute transport that describe the spatial and temporal distribution of NaCl concentration in the subsurface environment in the vicinity of a dome. During the quarter, efforts were made to model ground flow in an unconfined aquifer around a salt dome similar to Vacherie dome.

For an assessment of hydrologic isolation of mined openings in salt domes, a study of subsurface leaks in the existing mines of Louisiana and Texas was initiated in January 1976. A large number of water samples collected from the Belle Isle, Weeks Island, and Jefferson Island salt mines were chemically and isotopically analyzed. Most of them are Na-Ca-Cl brines bearing strong similarities to formation (connate) water. In order to develop a thorough understanding of mine leaks, access to additional operating mines was sought. During the quarter, an initial inspection visit was made to the 500-foot level of the Avery Island mine where small water pools with no active leaks located near the RE/SPEC sites were observed and sampled.

Related to the mine leak studies is the determination of the (trace) water content of solid salt. A technique for analysis for such trace water has been developed. Preliminary results have suggested that routine measurements of $\pm$ 0.002 wt percent water in salt are possible on 1-gram samples, with greater precision possible on larger samples. Preparatory to the isotopic analyses of the trace water extracted from salt, efforts to modify and improve the hydrogen-isotope ratio mass spectrometer were begun.

Mine Hydrology

Under the current program of mine leak studies, the Avery Island salt mine was visited and inspected at the 500- and 700-foot levels. Eight areas of active leaks (mostly on the ceilings) were visited, and 20 water samples were collected. Five water wells located on the surface above a major leak at the 500-foot level were later accessed. In order to compare the character of the mine leak water with that of the ground water in the overlying aquifer, water samples were obtained from those wells from a depth range of 20 to 50 feet. The chemical analyses of the mine leak and ground-water samples have just been completed. An evaluation of the resulting new analytical data will be initiated soon.

Isotopic Studies

The trace water analysis of solid salt was continued during the quarter with a variety of sample types. Previously reported measurements of the water content of salt samples were refined and revised. Measurements completed thus far show that water contents, in weight percent, of mine samples range from 0.01 to 0.09 for Weeks Island, 0.0024 to 0.52 for Belle Isle, 0.0007 to 0.0162 for Jefferson Island, and 0.0036 to 0.005 for Avery Island. Core samples from the Vacherie dome range from 0.005 to 0.023 wt percent. A halite crystal from the Rayburn's dome had only 0.0004 wt percent water. Further refinement of these measurements is planned.

Loose granular mine samples have 10 to 100 times the water of coherent hand samples, indicating that significant quantities of water can be absorbed by salt exposed to atmospheric moisture. In Weeks Island, salt associated with sandstone inclusions had a water content three times greater than that of the main salt stock, suggesting that the trace water content is greater near these anomalous zones.

During volatilization of the halite (a preliminary step of the water content determination procedure), it has been observed that gases in addition to water are released. The gases, not yet identified, are being collected and measured.

The hydrogen-isotope mass spectrometer has been made operational. A preliminary measurement of δD on the water of a salt core from the Avery Island mine has been completed and the resulting data are being reduced. Efforts are under way to assemble an oxygen-isotope mass spectrometer.

Numerical Modeling of Domal Saline Plumes

The salinity and velocity distribution for flow around the Vacherie salt dome with certain boundary conditions has been modeled using the continuity and momentum equations for flow through porous media. Output from the computer program is being obtained as Varian plots of velocity vectors and salinities parallel to the axes of the elliptical dome. For the modeling conditions, the domal dissolution rate has been calculated to be smaller than the surface solution rate predicted by correlations for solution mining. A separate report on the procedures, calculations, and results of modeling work accomplished so far is in preparation.

REGIONAL GEOLOGY

Studies by the Regional Geology Group during the third quarter of FY 80 have included (1) continuing investigations of the petrology and mineralogy of the salt cores from Vacherie and Rayburn's domes; (2) geochemical analyses of salt samples from these cores; (3) further development of the mathematical model for inverse gravity interpretation over salt domes; and (4) continued processing of Tertiary samples, obtained from Quaternary boreholes, for paleontology studies. Of 127 samples washed from Rayburn's borings, only 24 were found to have recoverable fossils. This small-scale paleontology program will continue until all such samples have been processed.

Work in the second quarter of FY 80 included studies of the anhydrite content of various types of halite, studies of and searches for minute fluid inclusions in halite, and additional attempts to obtain suitable thin sections of halite and anhydrite from the cores. Also, a method was established for the preparation of polished slabs and for grain mounts of salt in oil and epoxy.

Petrology

A program to study the chemical variations in the layering observed in the Vacherie core has been started. To date, approximately 70 samples have been prepared.

Geochemistry

Emphasis this quarter has been on sample preparation and dissolution methods. A series of grinding experiments was conducted using the Pitchford Pica Blender Mill to grind the rock salt samples to fine powders. Various operating conditions were investigated to determine the optimum method for reducing the bulk of the sample to less than 100-mesh grain size, which is necessary for effective dissolution of the sample prior to chemical analysis.

Geophysics

Progress this quarter has involved development of a gridded interpretation program for abstracting gravity data sets and interpolating them onto a rectangular grid. It is necessary that the data be gridded in order to apply the Fast Fourier Transform.

At present, the gravity interpretation program is written to accommodate no greater than a 64 x 64 grid of actual data values, and solve for 64 x 64 x 48 density contrast values. It is being written to accommodate much larger grids of data and solution variables, as well as to taper data values on the edge of the data set, to minimize "edge effects".

An additional version of the gravity interpretation program is being written and will include prior estimates of the density structure of a salt dome, upon which improvements will be made.

QUATERNARY STUDIES

The purpose of Quaternary studies is to determine whether Quaternary deposits have been (a) moved upward by tectonic movement of the salt dome or (b) displaced downward by dissolution and collapse of the underlying salt. Directly associated geomorphic inquiries include (a) the effects of erosion during the next 250,000 years, (b) the tectonic or hydrologic significance of the topographic lows above some domes, (c) the distortion of Quaternary beds above domes known to have moved upward during Quaternary time, and (d) in-depth assessment of the applicability of the Fiskian concept of Gulf Coast terrace formation and chronology to the study area.

In studying the tectonic or hydrologic significance of the topographic lows above Rayburn's and Vacherie domes, a Styrofoam, three-dimensional model of the Vacherie area was constructed to a scale of 1 inch = 500/100 feet horizontal/vertical.

In addition, a short paper on recent results of a preliminary study of stable carbon and oxygen isotope ratios is included. To date, it has not been possible to determine whether the boulders in the Rayburn's "boulder zone" are fragments of calcite caprock, or are marine, possibly algal reef limestone, of Cretaceous or Tertiary age. The paper concludes, on the basis of preliminary data, that the boulders are weathered calcite caprock.

Three-Dimensional Model of Vacherie Dome

During this quarter, a three-dimensional Styrofoam model of the Vacherie salt dome and surrounding areas was constructed to a scale of 1 inch = 500/100 feet horizontal and vertical. The model represents a surface area of approximately 18 square miles and extends to a depth of -3000 feet mean sea level (MSL). Surface topography is based on a 20-foot contour interval. The boundary between Quaternary and Tertiary deposits is indicated on the model surface, as is an outline of the salt dome at -1000 MSL (Figure 3). The model has been cut along two lines of selected borings, and subsurface cross sections developed from well logs have been attached to the interior vertical faces. The result is two easily visualized cross sections across the width and the length of the dome and surrounding areas.

The SW-NE cross section (Figure 4) incorporates information such as formation thickness and depth to salt derived from the logs of six oil wells, one Institute for Environmental Studies (IES) water well, the IES deep corehole, approximately 20 shallow Quaternary borings, and seismic surveys. The NW-SE section (Figure 5) roughly parallels Bashaway Creek along the long axis of the dome and incorporates information from additional borings.

Construction of the three-dimensional model at a 5:1 horizontal to vertical scale required preliminary construction of several two-dimensional sections at a 1:1 scale and the integration of these sections into the scale of the three-dimensional model. To keep the model as simple as possible, a minimum number of faults were postulated above the dome to account for known displacements. Positions and dips of these faults were generally based on previous IES and LETCo studies.

Lithologic and paleontologic evidence indicates that the Cane River Formation, a Tertiary marine unit containing diagnostic faunal assemblages, has been offset from 600 to 800 feet over Vacherie dome. Kolb (in Martinez, et al, 1978) postulated an essentially flat-lying Cane River deposited directly on caprock during Cane River time. It was speculated that in post-Cane

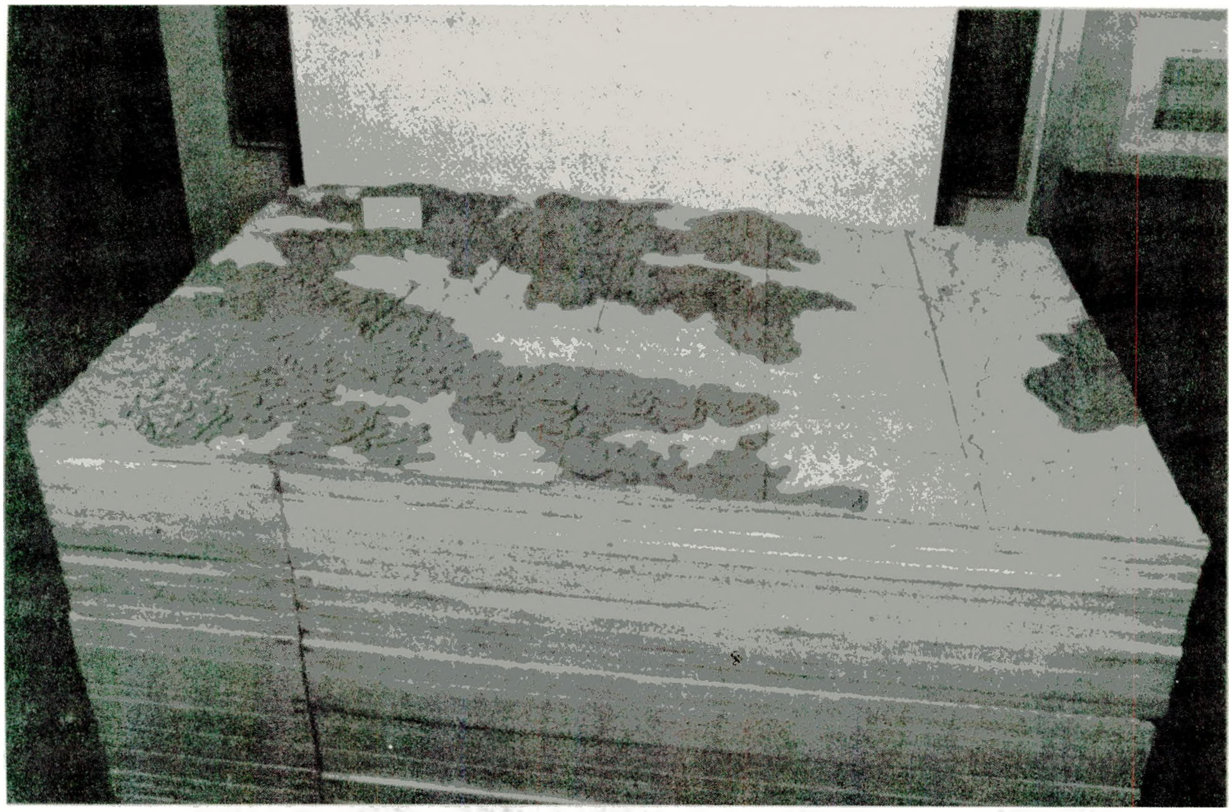


FIGURE 3. THREE DIMENSIONAL MODEL OF VACHERIE DOME

Surface area shown covers 18 square miles. Dark colored areas—deposits of Tertiary age—light colored areas—deposits of Quaternary age. Outline of dome at -1000 feet MSL faintly visible in left central portion of model.

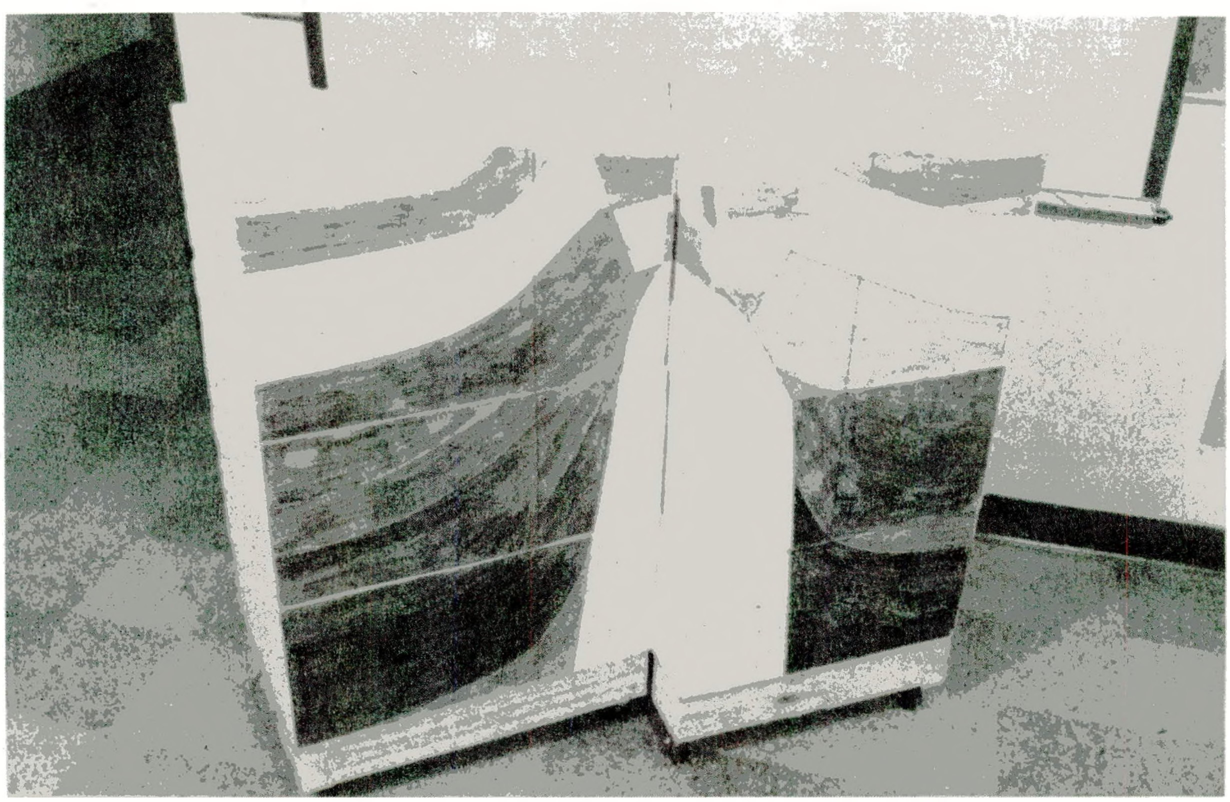


FIGURE 4. SW-NE CROSS SECTION OF MODEL

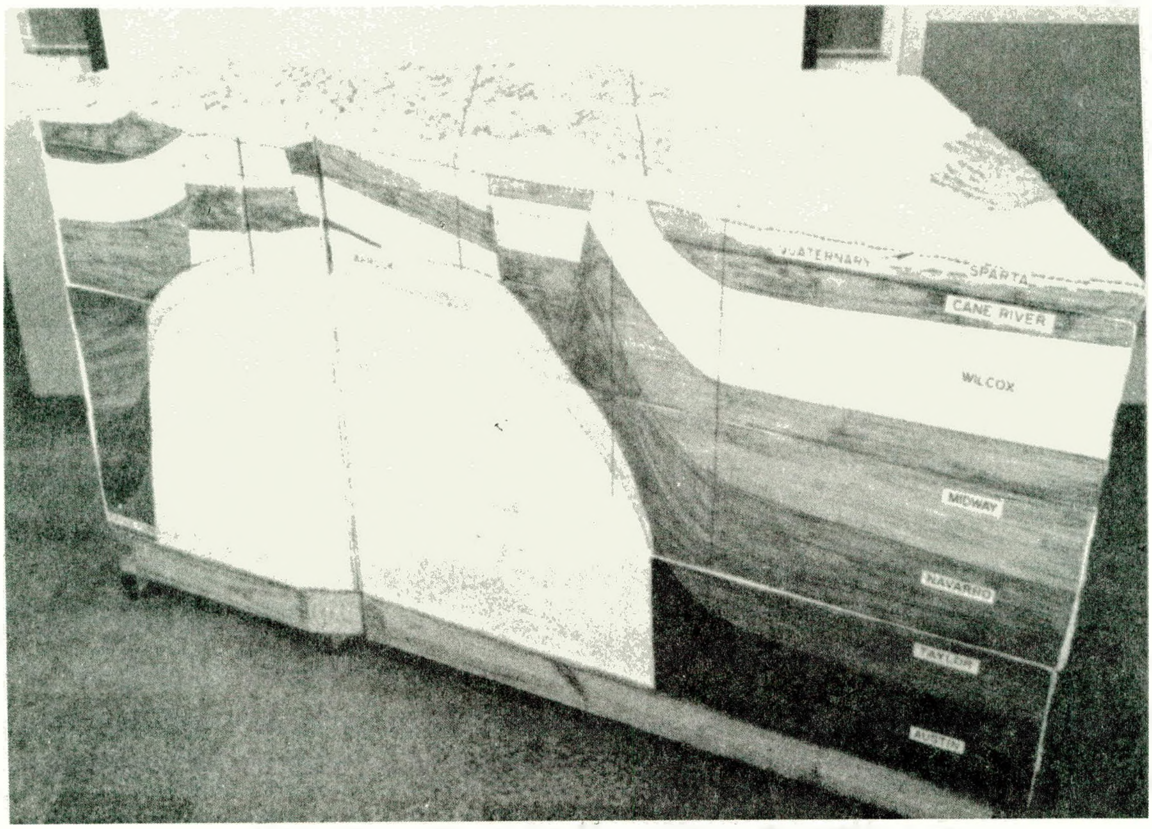


FIGURE 5. NW-SE CROSS SECTION OF MODEL

River time upward movement of the dome imparted moderate dips to the Cane River and the overlying Sparta Formations. Kolb concluded that displacement of the magnitude found at Vacherie could not be due solely to release of tensional stresses and the formation of grabens above the dome, but could be due only to dissolution and collapse of the underlying salt.

Work with the model strongly supports this conclusion. The Cane River and Sparta Formations along the flanks of the dome were continued as gently arched units above the dome on 1:1 scale diagrams. The amount of lengthening of the units caused by the uplift was carefully measured, and hypothetical voids caused by tensional stress release were filled by the downward movement of a wedge of sediment above the central part of the dome. The study indicates that displacement of individual strata as a result of downward movement of this wedge of sediment, given the conditions present at Vacherie dome, is no more than 100 feet.

It was also concluded that the wedge of soil displaced downward through upward movement of the salt must, indeed, be a wedge coming to a point at its base, and that the apex of the wedge cannot touch the rising caprock if the overlying sedimentary material acts as a competent rock. This is contrary to a number of known diagrams in the literature where grabens with broad bases are shown resting directly on caprock. Such a situation could, of course, occur if the overlying sediment acts incompetently and "settles" downward and laterally to fill the voids formed by tensional stresses. Calculation of the amount of such downward and lateral movement at a 1:1 scale also indicates that displacements of no more than 100 feet could occur at Vacherie.

Previously postulated was a flat-lying marine deposit overlying a rather evenly upwarped dome during Cane River time. Present work with the sectional diagrams and the model, in an effort to conceptualize about the shape of the dome during earlier periods of deposition, suggests a significantly different shape of the dome during Cane River time. For example, at the location of water well No. 7, the Cane River Formation rests on caprock, whereas at the corehole (some 2800 feet west), Cretaceous sediments are in a similar position. To explain this anomaly, it is hypothesized that a knoblike structure protruded some 300 feet above the remainder of the caprock surface at water well No. 7 which allowed deposition of the Cane River Formation directly on caprock. Dissolution and collapse of this knob would allow for the resulting juxtaposition of the Eocene and Cretaceous sediments as they are now observed.

Constructing the model required diagrams, at 1:1 and 1:5 (vertical to horizontal) scales, postulating conditions at the time of Cane River deposition, at the time of maximum uplift of the Sparta-Cane River, and at the present time (Figure 6). Several questions were raised.

For example, laboratory studies using colored sand strata and other substances, which were moved upward or displaced downward by movement of a hypothetical salt dome, support the hypothesis that normal faults are developed as a result of a rising salt dome, while reverse faults are produced if there is downward movement above the dome due to dissolution and collapse. The faults shown on Figures 4, 5, and 6 reflect this thinking up to a point. Those directly above the dome are shown as reverse faults, but those at the flanks are based on faults postulated on 1:1 diagrams that formed during uplift and are consequently shown as normal faults. They may, of course, be reverse faults, but it is almost impossible to account for the positioning of the various formational units as shown if the dips on the flanks of the dome are reversed. If one considers them to be normal faults formed during the rising phase of the dome, the amount of offset of the formational units is too great to be accounted

FIGURE 6. SW-NE SUBSURFACE CROSS SECTION

for. Is it possible—particularly along the flanks of the dome—that dissolution and collapse of the salt dome can reactivate a normal fault causing continued downward movement along the established fault plane? Although useful in itself, it is highly probable that the simplistic presentation of the model may not and probably may never take into account the complex system of both normal and reverse faults that exists above the dome.

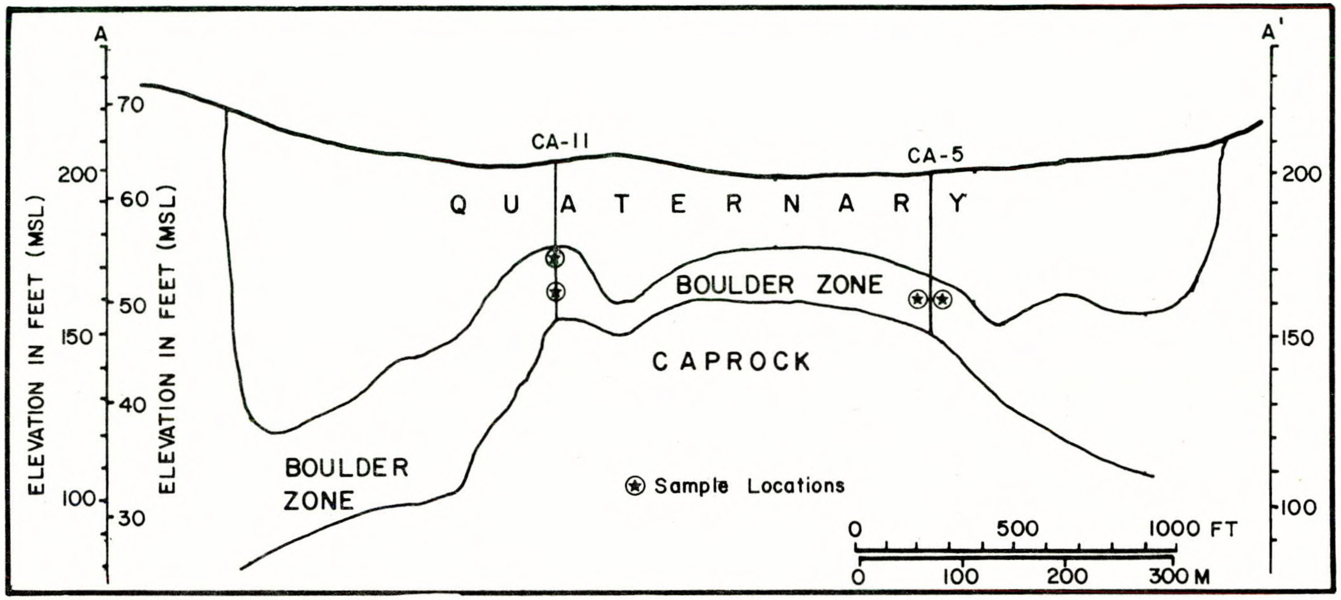
The existence of a knob to explain the presence of the Cane River resting on caprock in Cane River time is a logical hypothesis, but alternative theories should be explored. Might the dome have pierced the intervening sediments between caprock and Cane River in the area of water well No. 7? If the dome pierced pre-Cane River sediments, the absence of these sediments could thus be explained.

Exploration and speculation are needed on the time in the history of dome development when the top of the salt first came in contact with essentially fresh ground-water conditions subjecting the upper portions of the dome to dissolution and collapse. It would be useful in this regard to establish the geologic age of the formation of the topographic low above the dome or the age of the "anomalous" sands that underlie the known Quaternary at Vacherie and are thought to fill depressions formed by collapse of the underlying salt. There is fairly good evidence that a modest amount of collapse has occurred over the western end of Vacherie dome during Quaternary time. Significantly more salt dissolution and collapse in Quaternary time appears to have occurred over the Rayburn's dome where the salt is at much shallower depth. It might even be possible to determine the rate of salt dissolution during the past million years of Quaternary time by comparing Quaternary thicknesses with the elevation of the caprock and the salt.

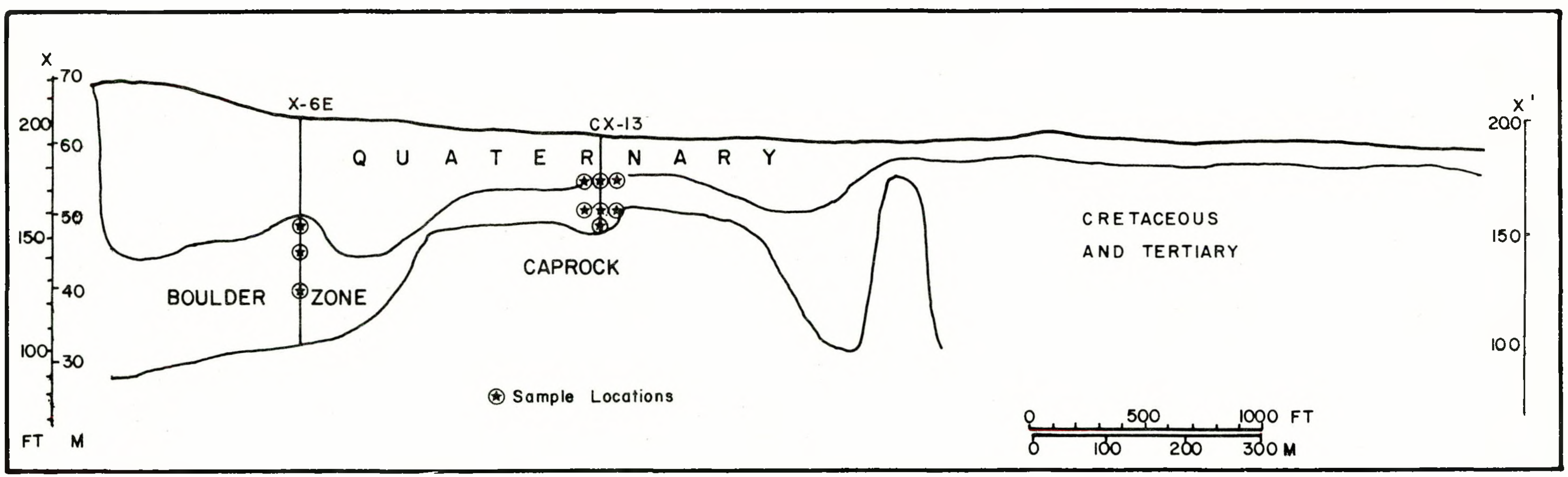
Isotopic Evidence for the Origin of the Rayburn's Boulder Zone

Because of the configuration of the boulder zone and its stratigraphic relationship to the anhydrite caprock of Rayburn's salt dome and the overlying veneer of Quaternary alluvium, it was initially hypothesized that the boulder zone represents residuum formed by the weathering of calcite caprock during Quaternary time (Figure 7). Until the present, efforts to verify this hypothesis have been inconclusive. Examination of thin sections of limestone boulders by Martinez and Rovik (Martinez et al, 1979) led to disagreement as to the origin of the limestone. Rovik suggested that the boulders represent marine limestone carried up with the salt as it intruded the overlying formations. Martinez et al (1978) concluded on the other hand that the boulders are probably caprock, though unlike caprock specimens he had previously examined. Furthermore, efforts to test whether the boulder zone had been exposed in the subaerial environment during past geologic time were conducted by the IES palynology staff, but the results were inconclusive. Examination of 28 boulder zone samples during FY 79 yielded no significant pollen, indicating either that this lithologic unit had not been exposed at the surface or that any pollen that had been deposited had been subsequently destroyed because of unfavorable geochemical conditions. To further pursue this question, a new direction of study was sought.

Previous isotopic studies of caprock by Thode, Wanless, and Wallouch (1954), Feely and Kulp (1957), and Cheney and Jensen (1967) have shown that the calcite caprock of Gulf Coast salt domes is formed by a process greatly different from that of marine or freshwater limestone; consequently, calcite caprock has a distinct isotopic composition reflecting this origin. Working independently, these authors have presented convincing geochemical, mineralogic, geologic, and isotopic evidence that calcite caprock is the product of the



(a) Section A–A′



(b) Section X–X′

FIGURE 7. RAYBURN'S DOME SHOWING LOCATIONS OF SAMPLES SELECTED FOR $\delta^{13}C_{PDB}$ ANALYSES

breakdown of petroleum hydrocarbons by bacteria in the subsurface environment, yielding CH_4 and CO_2 which is finally oxidized to form the carbonate radical, CO_3. The most compelling evidence for the organic origin of caprock carbonate is the isotopic composition of the carbon present in these limestones. Similar isotopic measurements were performed on 20 samples from both the Vacherie calcite caprock and the Rayburn's boulder zone limestones to provide results for comparison with the results published by these authors.

The parameter $\delta^{13}C_{PDB}$ is used to define the isotopic composition of carbon present in limestone. For geochemical purposes, this parameter is not measured directly to yield a result of, say, 98.89897 percent ^{12}C and 1.10103 percent ^{13}C. Instead, each sample to be analyzed is converted to CO_2 and compared, using a mass spectrometer, with the CO_2 used as a standard. The experimental data are converted to the parameter $\delta^{13}C_{PDB}$ using the formula

$$\delta^{13}C_{PDB} = \frac{(^{13}C/^{12}C)\text{sample} - (^{13}C/^{12}C)\text{PDB}}{(^{13}C/^{12}C)_{PDB}} \cdot 1000 \text{ per mil},$$

where $^{13}C/^{12}C$ is a value based on the ratio of the two isotopes of a given sample and where PDB stands for CO_2 derived from Cretaceous-age belemnites of the Peedee Formation of South Carolina. Examination of this formula shows that any sample having relatively more ^{13}C than the standard will have a positive value for $\delta^{13}C_{PDB}$. These differences are expressed in parts per thousand.

In Figure 8 the $\delta^{13}C_{PDB}$ values of various limestones are compared with those from other sources of organic and inorganic carbon. Note that the standard used (PDB) has a $\delta^{13}C_{PDB}$ value of zero and all of the $\delta^{13}C_{PDB}$ values for other geologic materials are plotted relative to this standard. It can be seen that the compiled $\delta^{13}C_{PDB}$ values for calcite caprock do not overlap with those values measured for marine or freshwater limestones. The $\delta^{13}C_{PDB}$ values of calcite caprock overlap with those measured for petroleum and methane, which is strong evidence that caprock limestone is derived from these organic materials. Marine limestones, on the other hand, have $\delta^{13}C_{PDB}$ values that compare favorably with marine HCO_3, from which this kind of carbonate rock forms.

In Figure 9, measured $\delta^{13}C_{PDB}$ values for six samples of Vacherie calcite caprock and 14 samples of Rayburn's boulder zone limestone are compared with $\delta^{13}C_{PDB}$ values obtained for other kinds of limestones. The deep corehole at Vacherie penetrated 22 feet of calcite caprock; the six samples used in the isotopic analyses were taken from continuous, 4-inch core returns at depths of 543.5, 552.5, 555.5, 556.5, 559.0, and 563.0 feet. The mean $\delta^{13}C_{PDB}$ value for the six Vacherie samples equals -25.4 per mil, which is considerably enriched in ^{13}C, compared with the mean $\delta^{13}C_{PDB}$ value of -36.2 per mil observed for the 35 Gulf Coast salt dome caprock samples reported by Cheney and Jensen (1967). It is interesting that the mean $\delta^{13}C_{PDB}$ value for the Vacherie calcite caprock is very close to that observed for typical petroleums, as shown in Figure 8, indicating perhaps that methane, which is believed to be the precursor of strongly ^{13}C depleted calcite caprock, was not present during oxidizing conditions.

The results of the $\delta^{13}C_{PDB}$ measurements obtained for the 14 Rayburn's boulder zone samples are greatly different from those observed for the six Vacherie calcite caprock samples. The boulder zone $\delta^{13}C_{PDB}$ values range between -6.2 and -24.9 per mil and average -15.5 per mil. Considered as a single lithologic unit, the boulder zone values are distinctly different from both $\delta^{13}C_{PDR}$ values expected for marine limestones or terrestrial carbonates and the $\delta^{13}C_{PDB}$ values measured for calcite caprock. Fortunately, evidence exists that several generations of calcite are present in the boulder zone limestone fragments, and isotopic measurements show

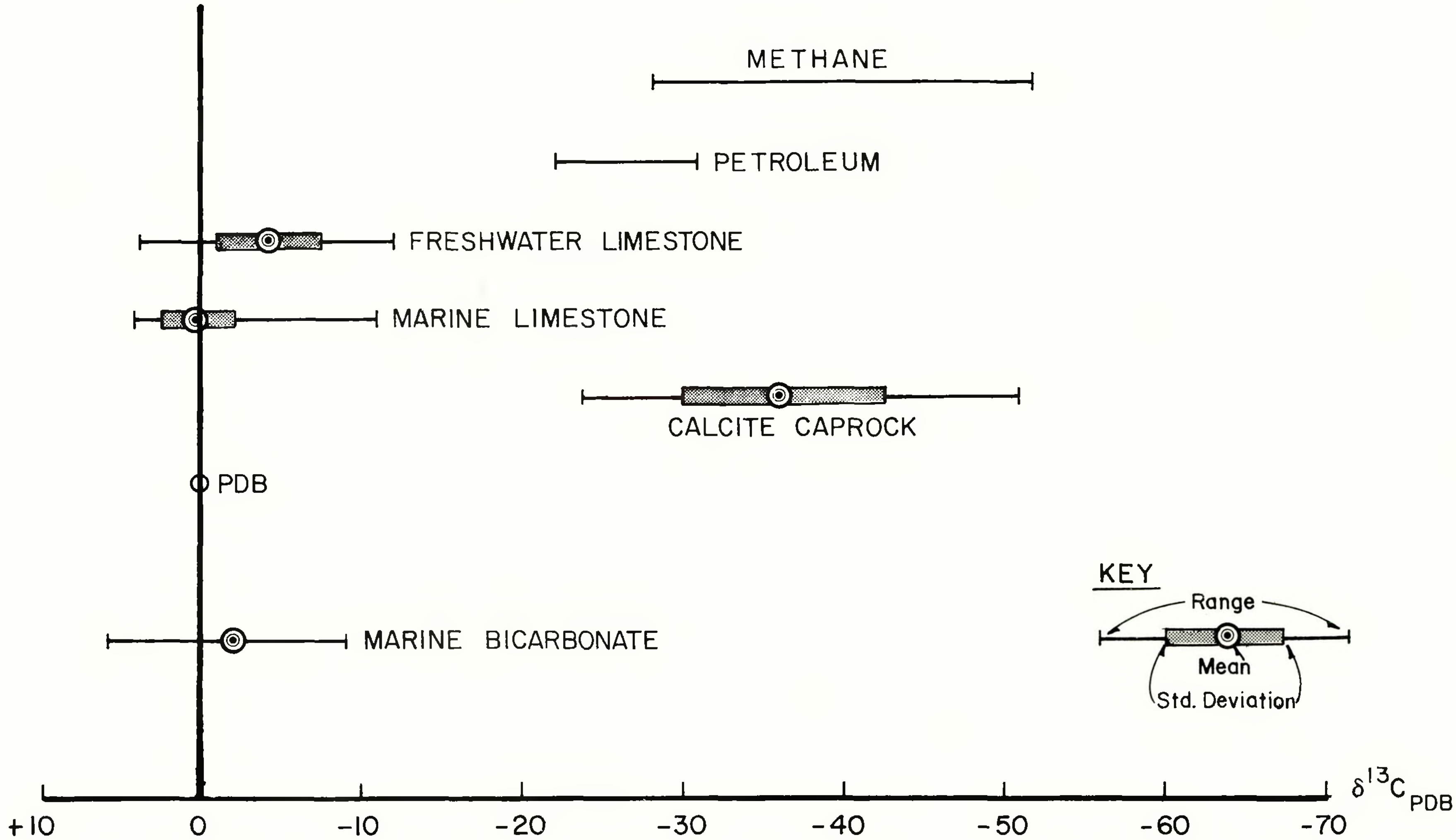


FIGURE 8. $\delta^{13}C_{PDB}$ VALUES FOR SELECTED LIMESTONES AND THE CARBONACEOUS MATERIALS FROM WHICH THEY ARE DERIVED

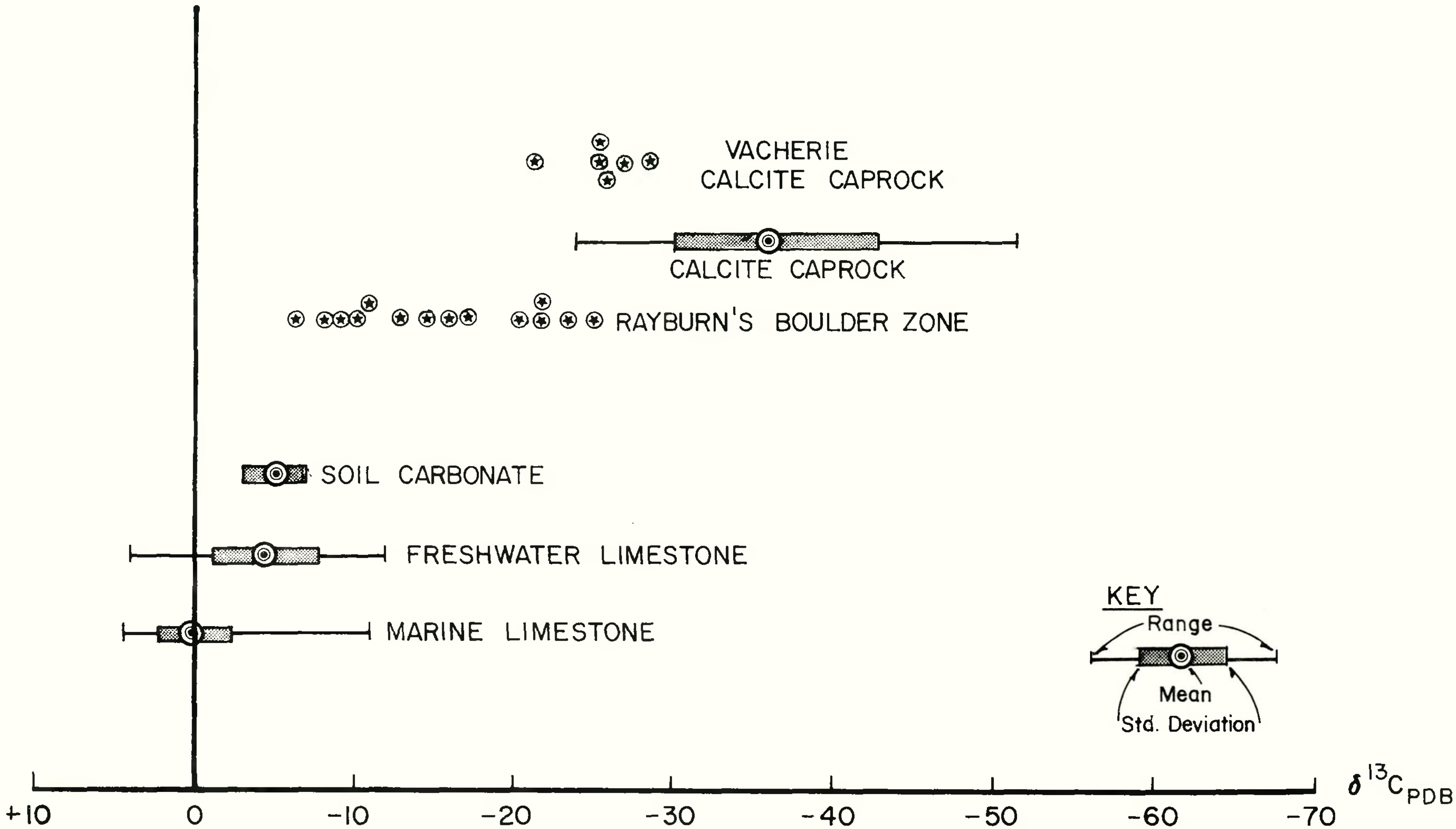


FIGURE 9. $\delta^{13}C_{PDB}$ VALUES OF 20 SAMPLES SELECTED FROM THE VACHERIE CALCITE CAPROCK AND RAYBURN'S BOULDER ZONE LIMESTONE

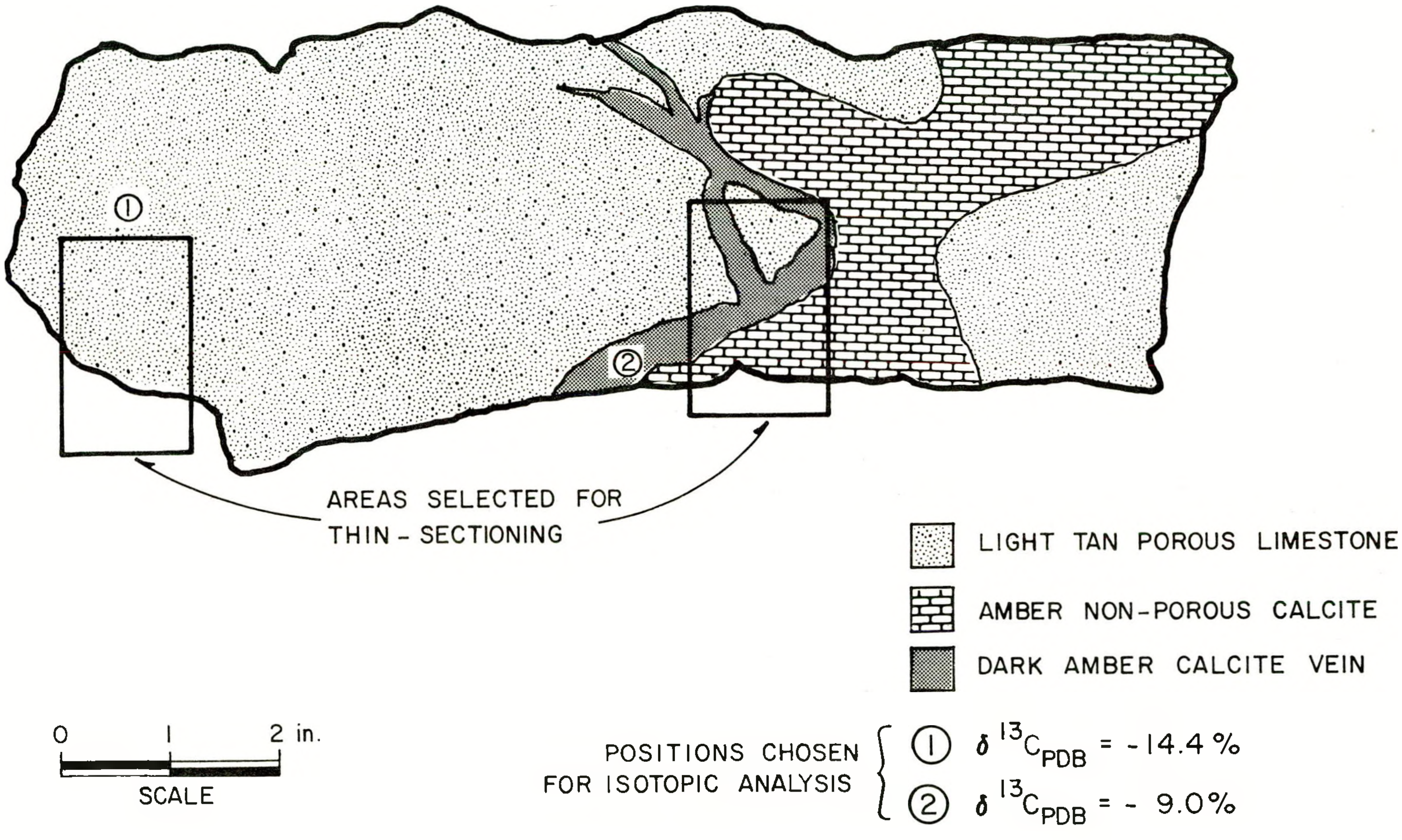


FIGURE 10. COMPOSITE DRAWING OF CROSS SECTION OF LIMESTONE BOULDER FROM CX-13 (32 ft) SHOWING POSITIONS USED FOR ISOTOPIC ANALYSES AND THIN-SECTIONING

that the less-altered primary calcite has $\delta^{13}C_{PDB}$ values that are more "caprock-like" than the younger secondary calcite veins and cement. The example of this relationship was observed in a single boulder from calyx hole CX-13 (see Figure 10) at a depth of 32 feet. Several large veins of amber-colored calcite intrude the lighter colored tan calcite which makes up the bulk of this boulder. The $\delta^{13}C_{PDB}$ value of the vein was 5.4 per mil more enriched in ^{13}C than the surrounding tan calcite and is similar to $\delta^{13}C_{PDB}$ values measured for soil carbonates derived from ground water.

Thus, it appears that the boulder zone is caprock with an isotopic composition which has been altered by contact with carbon from ground water. The $\delta^{13}C_{PDB}$ values for the CX-13 (32 ft) samples are shown separately in Figure 9, along with the remainder of the boulder zone $\delta^{13}C_{PDB}$ values. Thin sections are being prepared for each sample for which isotopic analyses have been performed so that this relationship can be further explored.

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WBS 1.4.3

Project: Evaluating the Potential of East Texas Salt Domes for Isolation of Nuclear Waste

Principal Investigator: The University of Texas at Austin, Bureau of Economic Geology (C. W. Kreitler)

ONWI Project Manager: O. E. Swanson

Objective

The objectives are: to evaluate the potential of East Texas salt domes as hosts for the management of nuclear wastes; to determine whether salt domes and their environs will remain tectonically stable during the active life of nuclear wastes; and to determine whether domes will remain hydrologically stable over the same period of time.

Progress Reported Previously

The Bureau began activities in January, 1978. Initial studies concluded that three domes in East Texas (Keechi, Palestine, and Oakwood) merited further study. Since then the Bureau has recommended that Palestine dome no longer be considered as a candidate dome because of the extensive brining that had previously occurred there. Dome-specific studies have continued on Oakwood and Keechi, as well as generic studies on the rest of the basin.

Activities During the Reporting Period

HYDROGEOLOGY

Dome-Specific Studies

The following work was conducted in regard to the caprock studies:

- The base of the Oakwood Dome caprock core, from 1155 to 1163 feet, was split, described, and sampled for thin sections. The salt/caprock contact is very sharp. No cavity is present at the base of the caprock, and there is little or no porosity between grains. A 1 to 2-mm-wide band of salt-cemented anhydrite grains separates the salt stock from the tightly compacted anhydrite caprock. Veins of salt extend 2 to 3 cm up into the anhydrite in places.

  Above the salt-cemented anhydrite, the caprock consists of a mosaic of interlocking crystals 0.1 to 1.0 mm long. Interpenetration of the anhydrite grains was probably caused by pressure solution, which has resulted in a tight fabric with low porosity and permeability. Zones of fine-grained (0.015 to 0.04 mm) "crushed" anhydrite surround larger anhydrite crystals in some samples.

- Six Oakwood caprock samples were X-rayed to confirm petrographic determinations of mineralogy. Minerals identified by X-ray are: calcite, dolomite, celestite, gypsum, anhydrite, pyrite, and quartz. This agrees with petrographic identifications.

- Porosity and permeability tests have been completed on 23 samples from the Oakwood caprock. Plugs were taken mainly in the horizontal direction, but vertical permeability was measured in representative anhydrite, calcite, and transition zone samples. In the upper, calcite section, porosity ranges from 1.3 to 13.0 percent and permeability from <0.01 to 43 microdarcies. Vertical permeability at 820 feet, in a typical banded calcite sample, is 16 microdarcies, whereas horizontal permeability is only 0.01 microdarcy. At 907 feet, in the transition zone, vertical permeability of 0.29 microdarcy and horizontal permeability is <0.01 microdarcy.

  Porosity and permeability are significantly lower in the anhydrite section. Porosity ranges from 0.7 to 3.3 percent and permeability from <0.01 to 0.02 microdarcy. Vertical and horizontal permeabilities at 1100 feet are both <0.01 microdarcy.

- Trace element analyses of 44 samples from Gyp Hill caprock were completed for the elements Na, K, Mg, Ca, Al, Mn, Ba, and Sr. The concentrations of the trace elements fall at a depth of about 400 feet, the depth of the transition from anhydrite to gypsum. Lower partitioning of these elements in gypsum than in anhydrite may release them into the meteoric ground-water system.

- Trace element analyses for Na, K, Mg, Ca, Al, Sr, Ba, Mn, and U_3O_8 were completed on 33 samples of caprock from the Oakwood Dome. The concentration of Ca, Na, Mg, Ba, and Mn is higher in the calcite samples than in the anhydrite. K, Al, and U_3O_8 remain about the same, and Sr concentrations decrease in the calcite.

  Within the calcite section, there are variations in trace element distribution between the fine-grained and coarse-grained calcite. The fine-grained calcite contains higher concentrations of Mg, Na, Mn, and Al. The coarser calcite crystals have higher Ba and Sr concentrations.

During the quarter, 49 sections of the Wilcox core from LETCO TOH-2Ao were selected for plug extraction and porosity and permeability analysis. Ten of these plugs have been tested and yield reasonable values of porosity and permeability. Permeability values are of the same order of magnitude as those obtained from the pumping tests. A 7-inch length of the core was prepared for Kd analysis. This "whole" core is being permeater-tested using fluids representing the actual chemistry and temperature for the interval from which the core was selected. The same will be done for additional sections of Wilcox core, and the results will be the basis for Kd inputs in numerical modelling of transport.

Water level and weather monitoring around Oakwood Dome is continuing, with continuous recording of water levels in three wells and weekly or biweekly measurements in all other wells. During the recent dry period in June, several water levels have been declining, apparently because of less recharge. A tipping bucket, continuous-recording rain gauge was set up near site TOH-5 at Oakwood Dome to monitor local recharge events that might be indicated in the shallow piezometers.

Detailed mapping of Total Dissolved Solids (TDS) distribution in the Wilcox around Keechi Dome (similar to that completed for Oakwood) is ongoing.

Analysis of pumping test data from the Oakwood drilling program was completed for all but the shallow borings. Each test appears successful in providing good measurements of transmissivity and hydraulic conductivity. Hydraulic conductivity (K) for the Carrizo is fairly consistent around 8 meters/day, reflecting its homogeneous nature. Two tests in two different types of sands in the Wilcox yielded significantly different K's, as expected. One of these sands appeared almost as "clean" on electric logs as the Carrizo and, accordingly, yielded a K of about 5 meters/day. The other sand appeared relatively silty on electric logs and, accordingly, yielded a K of about 0.2 meter/day. Barrier boundary conditions appear to have affected rates of drawdown in TOH-2Ao, an upper Wilcox well located just south of the dome, and TOG-1WS, a Carrizo well near the salt core. Cone of depression of TOG-1WS presumably intersected one of the numerous faults that have been mapped over the Dome. TOH-2Ao intersected either a fault, sand pinchout, or the dome. No leakage through adjacent aquitards was detected. Pumping of TOH-5D demonstrated hydraulic connection between the Carrizo directly over the dome and the Carrizo tapped by TOH-5D more than 1 mile east of the dome. As a result of pumping this well at 280 gpm, approximately 1 foot of drawdown was observed in a Carrizo piezometer located over the Dome, 5865 feet away (after 24 hours).

Plans for flow modelling around Oakwood Dome were finalized and model construction was begun. The area is the Upper Keechi Creek watershed, excluding the Wilcox-Carrizo outcrop. Boundary conditions and nodal distribution in the horizontal plane were designed. Structure maps for the Midway, Wilcox, and Carrizo are nearly complete and will be used to set up vertical node spacing in the mesh.

A computer program for automatically constructing three-dimensional integrated finite-difference meshes (OGRE) was successfully brought on-line and tested for use in modelling flow around Oakwood Dome with the program TERZAGI.

The Wilcox aquifer studies involved core slabbing. The water-saturated and unconsolidated nature of the Wilcox core posed problems that necessitated the development of specialized core handling and slabbing techniques. Experiments with various methods of core slabbing showed that excellent results were obtained when cores were frozen prior to slabbing. Large-scale slabbing operations are scheduled to begin after cold storage facilities have been renovated.

Stratigraphic studies entailed work on the following:

- Local studies around Oakwood Dome—The Wilcox Section was correlated in three strike sections and two dip sections covering 200 km^2. A fence diagram connecting these sections was constructed to show sand-body geometry around the dome.

- Regional studies around Oakwood Dome—The Wilcox Section is also being studied over a larger area (1500 km^2) in order to model the ground-water hydrodynamics around Oakwood Dome. Data on structure top and base and isopach of Reklaw, Carrizo, and Wilcox have been picked from regional cross sectons, off line well and other available wells. Maps are being constructed at 1 inch = 1 mile. To input natural inhomogeneities into the ground-water model, genetic units within the Wilcox are being picked by compressed cross sections. One cross section is completed. The structure top, structure base, and isopach of each genetic unit will then be input into the model.

Regional Studies

Carbon-14 age dating analyses are indicating significantly different age distributions for Wilcox waters in the central part of the basin (the Keechi Dome region) in comparison with the ages of ground waters in the Oakwood Dome area. The corrected ages of ground waters in the Oakwood area are in the 10,000 to 15,000 range, whereas the waters in the central part of the basin range from 4,000 to 12,000 years old. Selected wells have been resampled to check validity of the initial analyses.

SUBSURFACE GEOLOGY

Dome-Specific Studies

The following work pertained to the studies on salt cores. Detailed logs of the Oakwood salt core were prepared, and photographing and slabbing of the core were completed. Eight thin sections were successfully prepared, together with six polished slabs. Thin-section and polished slab studies confirmed the presence of fine-grained halite in anhydrite-bearing layers. The mean length of the long areas of halite in the entire section of foliated salt core is ~25 to 30 mm, as compared with ~0.5 mm for anhydrite. In transmitted light, grain boundaries in anhydrite-bearing layers are characteristically dark, particularly where parallel to the foliation. Prior to microscopic study, this darkness was thought to be due to concentration of anhydrite along halite grain boundaries. Thin-section and polished slab studies, however, revealed that anhydrite is commonly located within halite crystals, with only low to moderate concentrations along halite grain boundaries. In many of the polished slabs, a lacework of fluid inclusions is present along halite/halite grain boundaries, but not at anhydrite/halite interfaces. The nature of these inclusions is variable, although it is not known as yet whether they are related in some way to the presence of anhydrite. If so, this would account for the dark appearance noted above. However, there is a strong possibility that the fluid was introduced during preparation of the samples and/or during coring of the salt. This possibility is indicated by the mobility of the fluid on heating, and by the localized introduction of grinding paste along grain boundaries during the polishing phase.

From measurements of the orientation of the foliation and layering made during core logging, the large-scale structure of the salt has been analyzed. A structural profile has been constructed on this basis. Two geometric and kinematic models are proposed for the flow of salt during diapiric emplacement of Oakwood Dome. A simple model of salt intrusion cannot account for the structures observed in the core. These can be explained by multiple emplacement of salt spines as overthrust recumbent folds. Structural relations indicate that the crest of the diapir has been truncated. Dissolution by ground water is a likely cause. Estimates of the amount of truncation depend on what assumptions are made about the vertical and lateral extent of the observed structures in the absence of other boreholes nearby. Accordingly, estimates range from about 100 feet (30 meters) to many hundreds of feet.

Calculations of the type (i.e., flattening, constriction, or plane strain), magnitude, and orientation of finite strains at various points down the core will provide additional information on flow patterns of salt within diapirs. On the basis of measurements of grain orientations and axial ratios, a program of strain analyses has been initiated. The following four methods are being used: (1) Shape Factor Grid, (2) Random Point Distribution, (3) Harmonic Mean, and (4)

Rf/Θ. Methods (3) and (4) are computational methods and have been computerized. All four methods are capable of analyzing the effects of strain in initially elliptical or circular particles; all four require that the strain be homogeneous and that there be no previous preferred orientation; two of the methods test whether these assumptions are correct and are capable of mathematically "unstraining" the deformed rock, thus working backwards in time. Initial results on one part of the core indicate that the strain here is moderately high, strongly oblate, and characteristic of the middle to upper part of the head of a diapir. The salt grains have been squeezed in a ductile manner to approximately half their prestrain thickness.

Regional Studies

A study of the Travis Peak-Cotton Valley clastic complex, the first major clastic input into the basin, was initiated during the previous quarter. This study began with the realization that the Travis Peak-Cotton Valley Group deposition was instrumental, if not deterministic, in the formation of salt structures in the central portion of the East Texas Basin. This relationship was initially hypothesized after reviewing the thickness variations apparent on seismic sections in post-Cotton Valley Lime clastics in contrast to the thickness regularity in pre-Cotton Valley sediments.

During this quarter 14 cross sections have been constructed to interpret the relationship of depositional systems and salt tectonics. In addition to the cross sections, four isopach maps and four structure maps are being constructed: Isopach maps—(1) Top James-Top Pettet, (2) Top James-Top Travis Peak, (3) Top Pettet-Top Cotton Valley Lime, and (4) a revision of Top Travis Peak-Top Cotton Valley Lime; structure contour maps—(1) Top James, (2) Top Pettet, (3) Top Travis Peak (revision), (4) Top Cotton Valley Lime.

In the Upper Cretaceous section, the Upper Cretaceous interval from 49 regional cross sections has been compiled to study the depositional facies and stratigraphic relationships as they are affected by salt tectonism.

A program was previously instituted to evaluate the petroleum resources of the basin. During the present reporting period, petroleum statistics were organized into a form emphasizing formation, facies, and genetic relationships. Petroleum production statistics were tabulated alphabetically by field name. These data were reorganized to list the same statistics by producing formation. Histograms of yearly field discoveries have been graphed for Upper Cretaceous sandstone sequences including Nacatoch, Wolf City, Blossum, Tokio, Subclarksville, and Woodbine. Petroleum production maps have been made for Upper Cretaceous sandstone reservoirs. Analysis of hydrocarbon production around salt structures in East Texas has shown that most shallow piercement diapirs are barren of hydrocarbons.

SURFACE GEOLOGY

Dome-Specific Studies

Morphologic mapping of Keechi, Oakwood, and Palestine Domes has been done to help compare the geomorphic maturity of the domes and also to supplement drainage analysis studies. The geomorphic mapping deals primarily with distinguishing (1) different slopes (0 to

2, 2 to 5, and 5 to 15 degrees, etc.) due to erosional processes and (2) slopes due to recent deposition. Mapping was done utilizing USGS topographic maps, scale 1:214,000, and field checking. Preliminary results indicate that higher slopes are more common at Oakwood Dome than at Palestine Dome. Slopes at Keechi Dome rarely are greater than 5 degrees. The data suggest that Oakwood Dome may be in a less mature geomorphic stage than Keechi and Palestine Domes. This assumption also corresponds with the results of the domes drainage analyses. All three of the domes have recent deposition occurring at their central area.

Aerial photograph lineaments were field checked at both Oakwood and Keechi Domes to gain insight as to the significance of these linear features. Of the 26 lineaments field checked at Oakwood Dome, 15 are related to segments of stream channels or gullies and 11 are covered with vegetation, while none proved to be fence lines, old roads, or any man-made features. Most of the channels associated with lineaments have recent or very weathered Claiborne sediments exposed on the banks, but other channel exposures over the dome show closely spaced joints or fractures and faults, possibly influencing the channel course. Faulting having no relationship to aerial photograph lineaments or stream channels has also been recognized.

At Keechi Dome, 82 aerial photograph lineaments were field checked in a 5-mile radius of the dome. Of these, 60 were related to channels or gullies, 20 were covered with vegetation showing no morphologic expression, and two were found to be man-made features (power line and road). Only one lineament corresponds with the numerous faults mapped by Ebanks (1965).

At Oakwood Dome, nine shallow boreholes have been proposed to supplement the data obtained from initial drilling. The principal objective of these additional borings is to determine the thickness of the modern floodplain alluvium over the dome.

Regional Studies

The statistical analysis of lineament peaks from aerial photography and Landsat imagery was completed and all vectors were plotted. A study of the effects of land use and surficial deposits over an area covered by thirty-six 7½-foot quandrangles was completed and analysis of the data is in progress. This revealed a very low positive correlation coefficient (0.183) between percentage of natural vegetation and the total length of lineaments in each quadrangle. This suggests that identification of lineaments was unaffected or only weakly influenced by the presence of pastures and plowed fields. This can possibly be accounted for, in part, by the high proportion of lineaments defined by drainage channels (~70 percent for the areas around Oakwood and Keechi Domes), which are generally unaffected by cultivation. A significant negative correlation coefficient (-0.370) was found to exist between the percentage of floodplains and the length of lineaments in each quadrangle. This tendency for lower lineament densities in areas covered by surficial deposits is to be expected.

At Palestine Dome, surface mapping, hand augering, and shallow power augering determined that a terrace surface is exposed from the Trinity River to the western flank of the dome. Topographic profiles of this terrace surface show no upward warping on the western flank of the dome as compared with areas northwest and southwest of the dome. Palestine Dome is the only East Texas dome with well-developed Quaternary deposits overlying the dome, and no evidence of uplift of the Quaternary deposits has been determined.

Results

(1) The Oakwood caprock appears to have formed in a nonmeteoric ground-water environment. It is not the result of low-TDS ground-water dissolution in the Carrizo-Wilcox aquifer.

(2) Strain analyses of salt core may provide a new approach towards understanding the deformation history of diapiric salt.

(3) Studies of Quaternary gravels along the Trinity River in the Palestine Dome area do not show evidence of uplift.

(4) Shallow piercement salt domes in the East Texas Basin are generally barren of hydrocarbons.

REFERENCE

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WBS 1.4.3

Project: Mississippi Hydrology

Principal Investigator: U.S. Geological Survey, Water Resources Division (WRD), District Office, Jackson, Mississippi (C. A. Spiers)

ONWI Project Manager: O. E. Swanson

Objectives

The objectives are to review literature and hydrology data to develop a framework for the Northern Mississippi Salt Dome Basin and to assist in the drilling and hydrologic testing of proposed test wells.

Progress Reported Previously

The aquifer tests have been completed.

Activities During the Reporting Period

Objectives

Preparation of potentiometric maps and completion of the chemical analyses were the objectives for the quarter.

Results

No results or conclusions were reached during the quarter.

WBS 1.4.3

Project: Well Log Digitization, Central New York

Principal Investigator: Syracuse University (J. E. Robinson)

ONWI Project Manager: W. E. Newcomb

Objective

The major objective of this program is to digitize, correct, and compile in a computer data file information on the geologic structure, deep hydrologic systems, and potential for petroleum and natural gas within the 16-county area of Central New York State for potential use in analyzing for rock porosity, fluid content, and fluid flow using techniques currently employed in the petroleum industry.

Progress Reported Previously

The program began in July of 1979 when equipment was ordered. During the first two quarters, the equipment was purchased and installed, operating personnel were hired, and processing programs were written. Interfacing and equipment bugs were also worked out and log digitizing was started on a production basis.

Activities During the Reporting Period

Objectives

The objectives were to:

- Digitize the basic network of wells needed to determine the parameters for standardization
- Start the systematic digitization of all suitable logs in the area
- Produce geologic cross sections indicating cleanest formations to be used in standardization calculations
- Continue programming to improve playback and correction programs
- Ensure that digitization and correction procedures produce logs that not only fulfill the accuracy requirements but also are efficient tools for working geologists.

Procedures

The initial emphasis during the first part of this quarter was to digitize as many logs as possible. Consequently, equipment was operated up to 20 hours a day, capturing log information. During this time, programming was at a minimum. As of 30 June, 1980, sets of logs from 135 wells had been digitized.

As of 30 June, 1980, 130 logs have been played back and checked for accuracy. Of these, 58 have been accepted as meeting all requirements; 64 will be acceptable with corrections; and 26 have been returned for complete redigitization. Of the 26, 6 have been redigitized acceptably, and 12 still need corrections and have been included in the category of being acceptable with corrections. The remaining logs will be redigitized shortly.

The initial reject rate has been rather high because digitizers must not only fulfill the quality assurance requirements, but also must follow the minor log variations in order to reproduce the line character of the original curve. This is important for acceptance by geologists.

Preliminary cross sections have been completed and those formations suitable for standardization parameters have been specified.

A new data channel Versatec interface was installed to speed up the playback of the digitized log displays. Digitizing and display programs have been improved to eliminate minor problems with paper stretch and curvature in the original logs. A full solution has been reached for all digitized points, ensuring accuracy of reproduction regardless of the orientation of the log when placed on the tablet for digitization. The original recorded digits for all logs have been retained so that changes in the display programs do not affect the ability to reproduce logs or to compute the final corrected versions. Attempts were made to streamline the digitizing procedures in order to operate as efficiently as possible.

Results

Results of the work this quarter are:

- The digitizing equipment has been working reasonably well, and we have completed approximately a quarter of the contract.
- The operators have been gaining experience, and the reject rate of logs has improved considerably.
- Displays of reproduced logs are accurate and realistic.

WBS 1.4.3

Project: Louisiana Hydrology

Principal Investigator: U.S. Geological Survey, District Office, Baton Rouge, Louisiana (G. N. Ryals)

ONWI Project Manager: O. E. Swanson

Objective

The objective is to compile regional geohydrologic maps for the North Louisiana Salt Dome Basin and to conduct hydrologic field studies, data collection, and analyses near Vacherie and Rayburn's Salt Dome.

Progress Reported Previously

Seventeen regional geohydrologic maps have been completed. The maps represent an area of more than 16,000 square miles in north-central Louisiana and southern Arkansas. They are intended for use in a proposed regional multilayered ground-water flow model. All major hydrologic features that might noticeably affect flow patterns are within the mapped area. Other maps and data necessary for the model cannot be made without data input from a regional test-drilling program.

Activities During the Reporting Period

Objectives

During the past quarter, work objectives were: (1) to prepare a small report presenting all data collected to date as part of the study, (2) to maintain the ongoing ground- and surface-water data-collection network, (3) to collect geologic and hydrologic data from test-drilling activities, (4) to prepare potentiometric surface maps of the Sparta and Wilcox aquifers, and (5) to prepare a base-of-freshwater map of northern Louisiana and southern Arkansas.

Results

The data report has been approved for publication. Fourteen of the proposed sixteen test wells for area characterization have been completed. Pump tests have been completed for eight of the test wells and the eight wells were sampled for inorganic, radioelement, and trace-metal determinations. The potentiometric-surface and base-of-freshwater maps have been completed and submitted for review.

WBS 1.4.3

Project: Permian Basin

Principal Investigator: Texas Bureau of Economic Geology (T. C. Gustavson)

ONWI Project Manager: W. E. Newcomb

Objective

The objective is to evaluate the potential of the Palo Duro and Dalhart subbasins for siting of a deep geologic repository for high-level radioactive wastes.

Progress Reported Previously

Nuclear waste isolation feasibility studies in the Texas Panhandle region were initiated in FY 77. Centered in the Palo Duro and Dalhart Basins, these studies had evolved by FY 80 through three phases: (1) 6 months of preliminary data collection and initiation of basic research tasks (late FY 77); (2) 1 year of intensive research to produce a basic stratigraphic/structural/facies framework for the basins and to initiate ongoing studies of surficial and near-surface processes that affect erosion, denudation, and salt solution (FY 78); and (3) 1 year of research aimed at initial analysis of deep cores, initiation of basin resource studies, calibration of subsurface logs (using cores), discrimination of general depth/salt/thickness fairways, initiation of deep-basin hydrologic studies, and continuation of surface and near-surface analyses of erosion, denudation, and salt solution rates (FY 79).

Studies initiated in FY 80 involved specific discrimination and determination of salt character, natural resources potential, hydrologic integrity, host rock properties, and surface and near-surface process rates, among others. The Basin Analyses/Subsurface Geology group focused much of its attention in FY 80 on systematic collection of stratigraphic data and interpretation of facies from calibrated well logs through the San Andres Formation. Subsurface descriptions have been keyed to outcrop descriptions. In addition to these San Andres studies, two topical studies initiated during the past quarters dealt with stratigraphic intervals that presented unique problems in correlation.

The study of resources was in progress in a number of areas. Studies of San Andres oil and gas emphasized systematic correlation and tabulation of stratigraphic data as well as organic geochemistry of San Andres hydrocarbons. Studies of hydrocarbon resources of granite wash facies on the Amarillo Uplift were in progress both on a regional scale and as a more detailed topical study of the Mobeetie oil field. Regional studies of uranium resources were completed.

The previous quarter's work under the Remote Sensing/Surficial Analyses group involved: identification of sinkholes and undrained depressions in Hall County by aerial photographic interpretation; construction of regional cross sections depicting salt dissolution zones; and continued evaluation of erosion and stream incision rates. Estimates of stream incision rates of 1.45 mm/yr over the past 7900 to 9530 years were obtained in Caprock Canyon State Park. Scrap retreat rates in the Little Red River Basin were estimated to have been 0.71 mm/yr over a 380,000-year period.

The Hydrology/Geochemistry group sampled the Randall county core for whole-rock chemical analysis and clay mineralogy studies. Efforts have been directed at data collection and plotting, and generation of preliminary hydraulic head maps, cross sections, etc. Various computer programs have been obtained and/or modified to aid in identification of regional geochemical/hydrologic trends and in interpreting flow directions, states of saturation, etc. Water salinity data completed from self-potential (S.P.) logs have been plotted throughout the Palo Duro Basin. The Host Rock Analysis group was organized in FY 80. Activities through its first 6 months included photographic analysis of thin sections from the Randall County core. That study concluded that the 3400-foot Permian interval was 6 percent dolomite, 19 percent anhydrite, 25 percent massive salt, 24 percent chaotic mud-salt, 24 percent claystone/siltstone, and 2 percent sandstone. Thermal maturity studies indicated that although the organic contents were relatively great, middle and upper Permian evaporites of the Palo Duro Basin did not reach temperatures high enough to generate hydrocarbons. The Host Rock group also initiated studies to evaluate the paleosalinities of Permian brines, sabka, depositional environments, and granite-wash arkosic sequences. Each study was designed to provide a better understanding of the salt bed setting and surrounding rock resource potential.

Activities During the Reporting Period

BASIN ANALYSIS (SUBSURFACE GEOLOGY)

Objective

The objective of this task is to describe the subsurface geology of the Palo Duro and Dalhart Basins, with special emphasis on stratigraphy and facies of the salt-bearing interval, analysis of resources, and structural and seismic activity.

Activities

Facies and Stratigraphy of Individual Salt-bearing Units. During the reporting period a set of seven regional cross sections through salt-bearing strata of the Palo Duro and Dalhart Basins was prepared. Systematic collection and tabulation of stratigraphic data for the lower San Andres was completed. Maps are in preparation.

Pinch-out of Salado salt beds in the western Palo Duro Basin is believed to be a result of ancient dissolution processes. Core of the Salado interval shows fractures possibly resulting from salt dissolution. Studies of the Glorieta Sandstone in the northwestern Panhandle and the western Palo Duro Basin were continued.

Studies on facies of the lower Clear Fork Formation and a coastal sabkha salt-pan depositional model were completed. Major environments/facies, recognized in the lower Clear Fork, are largely based upon modern depositional settings and include: wadi or desert alluvial-eolian plain red beds which occur in updip regions and pass basinward into chaotic mudstone-salt of an inner sabkha saline mud flat; followed by banded to massive salt and laminated anhydrite deposited in shallow salt pans across the inner sabkha; and nodular anhydrite, laminated dolomite-anhydrite, and dolomite deposited in marginal sabkha terrain.

Geophysical Log Facies Interpretation. Geophysical well logs from Randall and Swisher Counties, Texas (DOE-Gruy, Federal No. 1 Rex White; DOE-Gruy, No. 1 Grabbe) were computer-digitized for use in statistical log facies analysis.

Maturation of Basin Hydrocarbons. Geochemical tests of core samples from the Pennsylvanian section in the Palo Duro Basin were completed this quarter. The results show no significant difference from thermal maturity values obtained from cuttings. Average vitrinite reflectance in the core samples was 0.52 percent.

San Andres Oil and Gas Studies. New log data for the San Andres oil and gas study area was obtained to fill significant gaps identified in the original data base. Generation of maps from these data was initiated. Cross sections illustrating facies as well as lithology were constructed and studies of facies interpretations continued. An extensive study of organic geochemistry of the San Andres Formation in the southern Palo Duro and northern Midland Basins was completed. Results suggest that organics within San Andres carbonates in the Palo Duro Basin never attained the thermal maturity necessary to generate significant quantities of hydrocarbons. Oil presently produced from San Andres reservoirs in the southern Palo Duro Basin probably migrated to its present position from a source area to the southeast.

Clear Fork Oil and Gas Studies. A six-county study area in the southern Palo Duro and northern Midland Basins was selected. A base map was prepared showing available data, and a literature survey on Clear Fork oil and gas fields in the study area was initiated. Five cross-section lines were selected.

Hydrocarbon Resource Analysis of the Granite Wash. Descriptive logging of a total of 1644 feet of granite wash core from seven wells in Mobeetie Field was finished. Eight electric-log cross sections through the field have been constructed. Construction of strike and dip facies cross sections, which combine electric log and core data, are in progress. Isopachous maps of alternating carbonate and clastic units within the producing interval have been completed. These units consist of coarse-grained fan delta clastics alternating with algae-foram wackestones and packstones.

Regional cross sections of granite-wash units are being extended over the Amarillo Uplift to connect with existing Palo Duro Basin sections.

REMOTE SENSING/SURFICIAL ANALYSIS

Objective

The objective of this task is to ensure that the integrity of a potential nuclear waste management site is secure from erosion, stream incision, and salt dissolution.

Activities

Climatic conditions were monitored throughout this quarter at climatic monitoring stations in Caprock Canyon State Park, Palo Duro State Park, Lake Meredith National Recreation Area, Buffalo Lake National Wildlife Refuge, and Muleshoe National Wildlife Refuge.

Erosion pin monitoring also continued throughout this quarter. All climatic and erosion measurement data through March 1980 have been entered into the computerized data bank.

On the basis of studies of the Little Red River basin in Briscoe and Hall Counties, Texas, four additional small drainage basins have been selected for morphometric analysis. These are: (1) Dixon Creek in Carson and Hutchinson Counties, Texas, a tributary to the Canadian River; (2) McClellan Creek in Carson and Gray Counties, Texas, a tributary to the North Fork of the Red River; (3) Duck Creek in Dickens and Kent Counties, Texas, a tributary to the Salt Fork of the Brazos River; and (4) Alamagordo Creek in Guadalupe and De Baca Counties, New Mexico. All basins will be analyzed with the objective of estimating their rules of development and hence rates of retreat of the High Plains margin. Similarities and differences in materials and climate will be considered and results compared with those for the Little Red River Basin.

Suspended sediment discharge data have been received from the U.S. Geological Survey for the gaging stations on the Little Red River near Turkey, Texas, and the Prairie Dog Town Fork of the Red River near Lakeview, Texas. The dry weight of suspended sediment discharged from the Little Red River Basin was 375,496 tons/year (340,642 metric tons/year) and that from the gaged portion of the Prairie Dog Town Fork was 1,407,793 tons/year (1,277,122 metric tons/year).

The Bureau of Reclamation has initiated a sedimentation survey of the Lake Meredith Reservoir on the Canadian River. All original land lines have been resurveyed to determine subaerial deposition or erosion. All original survey lines that are now under water have been resurveyed using a precision depth recorder. Sediment sampling is also complete. Data analysis is expected to take several months.

Geomorphic Mapping. The distribution of geomorphic features on the High Plains was mapped on 1:24,000-scale topographic map bases. A total of 227 7½-foot topographic quadrangles were mapped (C F files). The materials from which geomorphic map units were discriminated include 1:24,000 black and white aerial photo mosaics, County Soil Surveys, and toporaphic maps.

Land Use/Land Cover Mapping. During this quarter, 7869 square miles (19,737 sq. km) of land use/land cover mapping was completed.

The Landsat lineament analysis of the Texas Panhandle was completed, with a total of 12,294 miles (19,785 km) of lineaments delineated. The distribution of lineament length by azimuth frequency was computed for areas on and off the High Plains within each sheet of the 1:250,000-scale National Map Series covering the study area. Data from the High Plains show the least scatter; playa alignments and shallow drainage lines retain the same preferential northwest and northeast orientation across most of the High Plains. Exceptions are the High Plains data from the Amarillo, Tucumcari, and Perryton sheets, which show greater diversity in orientation. This diversity may be related to dissolution of bedded Permian salts in the subsurface of these areas. Processes of deflation and localized dissolution of the caprock caliche have probably influenced the development of playa lakes across all of the High Plains. Over these areas of greater lineament diversity, however, examples of playa lakes overlying salt dissolution at depths of 800 to 1,000 feet (240 to 300 meters) have been documented. The diverse orientation of lineaments and the greater frequency of larger playas (over 8,000 feet or 2,400 meters in diameter) in the northeast part of the Texas Panhandle may be one consequence of regional salt dissolution.

Total lineament lengths in each 10-degree sector for areas off the High Plains show a northerly peak trend for data plotted on Perryton, Amarillo, and Plainview 2-degree topographic sheets. This trend may merge with a northeasterly trend, as on the Big Spring sheet, or may be subordinate to the northeasterly trend, as on the Lubbock sheet. North-west and east-west lineament orientations also occur in the Rolling Plains, Pecos Plains, and Canadian Breaks.

Studies and topographic surveys along the Little Red River clearly show the multiple levels associated with various flow stages within the river. Changes in bedload particle size and composition were also noted in a reconnaissance of the upper part of the drainage basin. A decrease in the size of light gray sandstone clasts (Dockum Group?) and an increase in rounding of these clasts were noted within the first 12 km of thalweg length. Locally, the largest gravel clasts consist of blocks of gypsum, much of which is derived from gypsum-bedrock controlled apices of the meander bends. Elsewhere the stream is reworking alluvial gravel deposits, accounting for sudden increases in gravel within the active stream bed. Many platy gypsum clasts 30 cm or more in intermediate axis are imbricated, which is indicative of significant stream competence under the present climatic conditions and the present period of basin development.

Salt Dissolution and Surface Collapse. Four regional cross sections have been completed which show the extent of salt dissolution and collapse along the northern margin of the Palo Duro Basin and into the adjacent Dalhart and Anadarko Basins.

A new sinkhole, the Wink Sink, was observed during its formation on June 3, 1980. The hole, located about 5 miles southwest of Kermit, Texas, grew from 1 meter to about 110 meters across within a 24-hour period. Maximum depth of the hole was 110 feet (34 meters) 2 days after the sinkhole began to form and the volume of material displaced was estimated at 6.9 x 10^6 cubic feet (196,250 cubic meters). Blocks measuring up to 33 feet (10 meters) in length have continued to fall into the hole at irregular intervals since its discovery. The sinkhole is surrounded by annular cracks which extend up to 330 feet (100 meters) away from the hole. The south rim has subsided about 10 feet (3 meters) relative to the north rim and the subsided area is bounded by fissures which are tangent to the east and west sides of the sinkhole.

Preliminary investigations of the geology in the vicinity of the sinkhole indicate that dissolution of Permian Salado Formation salts was the probable cause of the sink. This event, plus subsurface evidence that salt dissolution has occurred during the Quaternary, suggests that other collapse features are likely to form in the future in this area. Unfortunately, complex patterns of ground-water movement, especially in cavernous or brecciated rock, makes prediction of when or where dissolution and collapse will occur very difficult, and sinkholes may continue to form in this area without warning.

An analysis of the process of Karst development in Hall County, Texas, is complete. Karstification in the rolling plains of the Texas Panhandle due to dissolution of Permian evaporates is summarized below.

Over 400 collapse sinks and depressions occur in Hall County, Texas. Of these, as many as 36 sinks and 2 depressions formed between 1940 and 1972. Collapse sinks are typically circular and range up to 100 meters in diameter and 15 meters in depth. Collapse depressions are irregularly shaped, internally drained depressions up to 1.5 miles (2.4 km) in length. Surface fractures up to 0.9 miles (1.5 km) in length are associated with certain collapse depressions. Six of 11 recognized fractures have formed since 1970.

Karst features are forming as a result of regional dissolution of Upper Permian evaporites — primarily halite and secondarily gypsum from the Queen, Grayburg, Upper and Lower San Andres Formations. Halite dissolution and overburden collapse are evident from geophysical log cross sections, and dissolution occurs at depths ranging from 740 to 850 feet (225 to 260 meters). Estimated mean dissolution rates for salt beds in the Hall County area range from 1.7 to 2.4 cm/yr (horizontal) or from 0.052 to 0.082 mm/yr (vertical). Evidence from geophysical log cross sections indicates that as much as 220 feet (68 meters) of halite has been removed.

The valley of the Prairie Dog Town Fork of the Red River in Hall County is an area of regional ground-water discharge for flow systems moving eastward from topographically high areas of the Rolling Plains and from the eastern rim of the High Plains. Halite beds in contact with these waters undergo dissolution. Salt springs and brine seeps, some associated with sinkholes and depressions, occur in the discharge area and indicate that dissolution is an ongoing process.

HYDROLOGY/GEOCHEMISTRY

Objective

The objectives of this task are to determine the hydrodynamics of fluid migration within the Basin and in the shallow ground-water aquifers, and to determine the effects of fluid/rock chemical interactions as they contribute to an understanding of long-term stability of a nuclear waste repository.

Rock Properties Investigations. Preparations were made for an investigation of the moisture content of bedded salt. The samples to be used in the study are from the DOE-Gruy Federal No. 1 Rex White well in Randall County, taken from 3-foot-long core sections that had been sealed in core tubes at the drilling site for rock-property investigations. These sections were then sampled by removing whole core slabs approximately 2 inches in length and cut with a salt-saturated solution as lubricant.

For this study the samples were split in half. One half is being analyzed by vacuum decrepitation; the other half is being subsampled by removing a 1 x 2 x 3-cm slab for optical determination of fluid inclusions. The final stage will be done at the Texas Bureau of Economic Geology and will include petrographic, X-ray, and chemical analysis, as well as a final moisture content determination by Karl-Fisher titration. Data are also being provided on the composition of the fluid inclusions.

The chemical analyses of the Randall County core are completed and will be compiled in the near future.

Clay mineral assemblages were identified by chemical analysis and X-ray diffraction of 73 samples taken from the Randall County Core. Illite and chlorite have been identified as well as mixed-layer clays typical of marine evaporite sequences. Upper Seven Rivers, Yates, and Salado Formations of Late Guadalupian age typically contain smectite-dominated mixed-layer clays. Older Permian deposits have both chlorite-vermiculite mixed-layer clay, which is a swelling phase, and regularly ordered mixed-layer chlorite-swelling chlorite of the corrensite type. These older Permian deposits have minor amounts of associated illite, with a trend towards increased illite with depth.

Even though many of these clastics were deposited in a saline, chemically reactive coastal sabkha environment, no distinct relationship exists between clay mineralogy and host lithofacies or depositional environment. Smectite-chlorite dominance of Late Guadalupian samples suggests a source change at that time.

Geochemistry Investigations. Published chemical analyses of brines collected from drill stem tests have been tabulated according to region and formation. These data will be plotted on cross sections being constructed by the Basin Analysis Group for interpretation of fluid/rock reaction state and flow path determinations. The stable isotopes ^{18}O, D, and ^{13}C are being analyzed and ^{14}C is being measured.

Two field trips have been conducted for the purpose of sampling ground-water and brine discharge points in the region of known salt dissolution on the eastern edge of the Palo Duro Basin. These water samples are being analyzed for their inorganic constituents, stable isotopes, and ^{14}C content. These data will be compared with other published chemical and hydrologic data to determine the flow path of fluids through this region.

A computer model (AQ/SALT) has been developed for use in the geochemical evaluation of brines in the Palo Duro Basin (Bassett and Griffin, 1980). Model computations have been compared with solubility data and with published computations done by others, and results are in excellent agreement (Wood, 1975; Harvie and Weare, 1980).

Contrary to previous assumptions and calculations using other geochemical models, calcium sulfate phases in many parts of the Palo Duro Basin are in equilibrium with the brine, and the fluctuation of absolute concentrations reflects the interionic effects of the high ionic strength brines. In addition, the deep formation brines are undersaturated with respect to halite but appear to be in stable or metastable equilibrium with anhydrite.

Methods of computing the activity of water in brines, a requirement for an accurate determination of the saturation state for hydrous minerals such as gypsum, are now being investigated. It is anticipated that this model will aid in identifying the solubility controls and zones of active dissolution or secondary precipitation. It may be possible to gage the rate and amount of infiltration in portions of the Texas Panhandle by using nitrate from the ammoniated fertilizer as a tracer.

The spatial variations in ground-water composition can indicate the flow path. Regional X, Y, Z plots using longitude, latitude, and composition indicate that Ogallala water may be dissolving anhydrite to saturation and then precipitating gypsum. In addition, there is apparently a substantial amount of mixing in the Permian aquifers with waters containing high concentrations of sodium chloride.

A plotting package called CPS 1 has been used to display the regional variations in chemical compositions of ground-water systems. The majority of the plotting has been done for the Prairie Dog Town Fork drainage basin.

Recent analyses have shown that the Ogallala and Permian ground-water systems are chemically distinct; Ogallala water is typically of a $Na\text{-}HCO_3$ type with local variations, and the Permian waters are of a $Ca\text{-}SO_4\text{-}Na\text{-}Cl$ composition. A regional potentiometric surface for these two aquifers indicates that even though there may be significant discharge into the surface drainage system, the ground waters are hydraulically connected, and the distinct water compositions are a result of water/rock interactions. There may also be a significant component of recharge by infiltration through the thin Quaternary alluvium and eolian sands that locally cover the Permian sediment.

Deep Basin Hydrodynamics. Permeability was calculated from all records where the necessary parameters had been reported. Permeability data computed from these records and collected from industry files are being posted to the appropriate lithologies and locations on the structural/lithologic cross sections. These sections will be used to construct the framework of a computer simulation of the flow system.

Evaluation of methods for determining the hydraulic properties of samples of non-fractured rock matrix in the evaporite section has begun . Two hundred and twenty-two cylindrical plugs (~2.5 cm x 4.5 cm) have been drilled at intervals in the DOE-Gruy Federal No. 1 Rex White core to obtain multiple, representative samples of each lithologic type of rock matrix in each formational interval. The porosity and the permeability to gas and liquid of a small pilot group of 21 samples were measured. The methods employed are the standard means of evaluating single-phase permeability of petroleum reservoir rocks. The results show that permeabilities to gas and liquid vary widely, even among samples with a similar lithology, and there is no constant ratio between the two types of permeability.

Permeability values of tens of millidarcies are suspect since thin sections of rock in adjacent core intervals exhibit no visible porosity. Several samples are being retested because of the inclusion of an unauthorized alcohol rinse in sample preparation. The retests include procedures designed to evaluate the possibility of leakage around the rubber sleeve in the test apparatus. Another group of samples has been submitted for similar tests.

Compilation of lost-circulation zones noted on available sample logs has been completed. The data were digitized for inclusion on computer-plotted maps and cross sections that show permeability and hydraulic head. The correlation between such zones and tracts of highly permeable lithofacies is being investigated.

Fluid potentials have been computed from shut-in pressures measured by drill-stem tests listed on magnetic tape. These apparent potentials are fresh water heads, which represent the elevation of the top of a column of pure water that would balance the recorded pore pressure at the point of measurement.

All calculated values of hydraulic head greater than 500 feet elevation were computer posted on 1 x 1-degree quadrangle plots. Computer posting allows rapid sorting of data into maps corresponding to individual hydrogeologic units, combinations of adjacent units, or specified elevation intervals. A map of fluid potentials in Wolfcamp-age strata in the Palo Duro Basin is complete. The map is composed of 1 x 1-degree quadrangle plots joined to make a regional map and then hand-contoured. Machine contouring was not used since equipotential trends are partly obscured by data from faulty tests. Data coverage is adequate to tentatively identify a relationship between areas of low potential and trends of highly permeable lithofacies such as granite wash. The Amarillo Uplift oil and gas field, which overlies a basement high at the basin margin, has the lowest fluid potentials of Wolfcamp strata in the Palo Duro Basin.

Calculated fluid potentials have been posted to lithologic/structural cross sections, and interpretation and contouring of traces of equipotential surfaces is under way.

Drill-stem-test data have been used to generate pressure versus elevation plots. A division of ground waters into deep and shallow hydrodynamic systems by intervening low-permeability evaporite beds is evident. The pressure gradients of waters in all of the deeper formations are greater than the hydrostatic gradient for either fresh water or a brine with 100,000 ppm total dissolved solids. This suggests the presence of an upward-directed vertical component of flow.

HOST ROCK ANALYSES

Objective

The objective is to conduct chemical and physical analyses, including petrography of rock samples, in cooperation with the Basin Analysis and Geohydrology Groups.

Activities

Work continued on preparation of a comprehensive report on the Randall County core. Facies relationship diagrams and facies models were constructed for two genetically related types of sequences: mud-rich and mud-poor. The results show that predictable facies sequences recur throughout the Permian cored interval and are useful in facies modelling and predicting laterial facies changes.

Field reconnaissance and laboratory work were completed for the purpose of developing a facies model of Bristol Dry Lake, a modern playa basin thought to be analogous to certain aspects of the Palo Duro Basin evaporite facies. Beds of chaotic mud-salt up to 16 feet thick are present near the surface of Bristol Dry Lake and are nearly identical to much of the halite from the Randall core. Evidence suggests that chaotic mud-salt is a product of halite precipitation from ground-water discharge at or near the surface of the playa basin. A similar diagenetic origin may be inferred for Permian chaotic mudstone-salt. The overall facies mosaic of Bristol Dry Lake is most useful for understanding the mechanisms of deposition and facies prediction in updip portions of the sabkha terrain in the Palo Duro Basin.

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WBS 1.4.3

Project: Geologic Project Manager Program—Salina Basin

Principal Investigator: Stone & Webster Engineering Corporation (D. S. Pierce)

ONWI Project Manager: R. R. Nicks

Objective

The objective of the Geologic Project Manager (GPM) program for the Salina Basin is to plan and manage a systematic investigation of the geologic and hydrologic characteristics of the bedded salt deposits and their enclosing rocks within the basin. This investigation will provide fundamental information necessary to evaluate the basin as a whole, and areas within it, for nuclear waste repository siting.

Progress Reported Previously

The GPM program was initiated on 21 July, 1977. The results of the regional study show that salt beds within the Salina Basin occur at adequate depth and in sufficient thickness to meet initial screening specifications. Based on criteria described in the report, certain areas favorable for further study and evaluation have been recommended in Ohio and New York.

Detailed information obtained for New York and Ohio indicates that New York is structurally more complex than Ohio. Faulting in the New York study area is more widespread than previously thought. Besides thrust faults within and above the salt section, the salt basin in New York is cut by strike-slip tear faults and other nearly vertical faults which represent potential conduits for ground-water circulation.

Salt beds tend to be more laterally continuous in Ohio, and although generally thinner than in New York, the salt bed thicknesses are more predictable in Ohio. Seismicity studies show that there have been few earthquakes recorded within the basin and all were of low to moderate intensity. Seismic design for repositories within the Salina Basin does not appear to be a problem.

Well log data for Ohio and New York study areas have been incorporated into a free field data storage program to facilitate retrieval and use in future studies.

Activities During the Reporting Period

The *Draft Generic Program for the Geological Characterization of Candidate Sites* was completed and is in review.

Tapes and associated documentation of the Geologic Well Data File computer program and report printouts were sent to ONWI.

Documentation of the Finite Element Analysis Salt Transport Program was completed.

WBS 1.4.3

Project: Paradox Basin Geological Exploration

Principal Investigator: Woodward-Clyde Consultants (F. R. Conwell)

ONWI Project Manager: N. A. Frazier

Objective

The objective is to plan and conduct geological work required to identify, investigate, characterize, and license a repository in salt.

Activities During the Reporting Period

General

Program planning proceeded for the next phase of drilling, coring and testing through salt at Gibson Dome-1 (GD-1). Technical requirement planning was also carried out. The planning and implementation of an additional short-term seismograph station microearthquake recording network at the north end of the area (including Salt Valley) were undertaken.

Drilling

Coring at GD-1 continued from a depth of 1,508 to 4,348 feet. The first holdpoint was reached on 26 April at a depth of 2,727 feet for hydrogeologic testing. Prior to testing, the following geophysical logs were run: dual induction guard, temperature, fracture-finder microseismogram, sidewall neutron, compensated acoustic velocity, and compensated density neutron. The hydrogeologic testing was done at eight different levels between 600 feet and the bottom of the hole. A surface resistivity survey was conducted and testing with gross gamma neutron neutron logs, a caliper log, and a KUT log were completed.

Hole opening began on 11 May through use of drilling mud to the 12-1/4-inch size and was completed on 18 May at a depth of 2,500 feet. The 17-1/2-inch hole opening was started. This opening was completed on 31 May at 2,495 feet. A 13-3/8-inch-diameter casing was installed and cemented on 1 June. A cement bond log was run before coring began again. Results showed an adequate bond. The well head equipment was rerigged for the 13-3/8-inch well head and coring began again on 6 June using air. On 13 June, coring was stopped with air because the salt core was blown into small pieces. A calcium chloride brine was mixed for use as a drilling fluid, with a concentration of about 400,000 ppm. Coring began again on 16 June. The calcium chloride concentration was increased to 525,000 ppm by the end of the quarter.

Hole deviation ranged between 1/4 and 1-1/4 degrees and core recovery was generally around 96 percent. A change in equipment improved core recovery.

Geomorphology/Quaternary History

The Geomorphology/Quarternary history activity continued regarding geologic events and the paleoclimate which characterize the Quaternary time period. Studies included a literature review of erosion rate studies for the Colorado Plateau, compilation of photogeologic maps for the study areas and vicinity, the continued assessment of age-dating methods that may be used on the Quaternary deposits in the Paradox Basin, and preparations for the field studies.

The review of erosion rates was focused on studies that measured the filling of small reservoirs. These studies are commonly carried out near the headwaters of a drainage and encompass only one rock type. Many were conducted on rock formations that are easily eroded, such as the Mancos shale. The depth of denudation calculated from these data for a 500,000-year period ranged from 40 feet to 3,990 feet. Further evaluation of data will be directed at defining which studies were for lithologics comparable to those in the study area.

Photogeologic Quaternary maps of the Elk Ridge and Gibson Dome study areas and of the Abajo Mountain area were compiled from the following types of photos: 1:12,000 black and white in a portion of the Gibson Dome study area; 1:20,000 natural color on the National Forest land; 1:35,000 color infrared photo coverage on the BLM land in the Elk Ridge area; and 1:60,000 black and white photos for the remainder of the area. These maps will be used to direct the field mapping effort next quarter, and will be altered, as necessary, based on the field data.

In the evaluation of age-dating techniques that may be applicable to the Paradox Basin, uranium series data have been derived from caliche rinds in cobbles. Ages tended to be younger than expected, and additional studies will be done next quarter to further evaluate these results. Other dating methods that will be utilized include paleomagnetic studies, amino acid dating, pedogenic development, carbonate building in soils, Carbon-14, and relative weathering characteristics.

Stratigraphy

The major activity of this reporting period was the recovery of core from the GD-1 boring and the geologic logging of that core. An additional activity was the mapping of the Gibson Dome study area.

Hole boring had previously progressed to a depth of 1,577 feet, which was within the Honaker Trail formation. On 25 April, 1980 the boring penetrated into the first major anhydrite bed in the Paradox Formation and the boring was stopped at a depth of 2,727 feet below the Kelly bushing. At this point the activities of the first scheduled hold point began. The activities included: (1) geophysical logging of the boring; (2) hydrologic testing, including drill stem testing and water sampling; (3) a hole-to-surface resistivity survey in cooperation with the USGS; (4) reaming of the hole to 17-1/2 inches; and (5) setting and cementing of a 13-3/8-inch casing to a depth of 2,492 feet. Coring operations resumed on 6 June, 1980 in the Paradox Formation.

The first salt encountered was in Salt Cycle 4. The upper contact with the overlying anhydrite was sharp and clean, and no evidence of salt dissolution was present. This sharp upper contact of the salt was typical of all the salt cycles penetrated to date.

The only significant core loss was approximately 37 feet in the lower part of Cycle 5 while drilling with air. Because of this, brine was then used as a drilling fluid and recovery has been excellent (approximately 98 percent).

The only potash salts encountered to date (other than scattered crystals of sylvite that occur at numerous horizons) are in the upper part of Salt Cycle 13, where a thin sequence of interbedded halite and potash salts with minor anhydrite is present. The salt core is generally "banded" with thin stringers of anhydrite or anhydrite sand at 1 to 3-inch intervals.

The color of the salt is variable, with orange, white, clear and light gray all being common. The interbeds are predominantly anhydrite and dark siltstones and shales. Some carbonate beds are present, particularly in the upper part of the Paradox section.

Core samples for hydrocarbon analysis are being collected between all salt cycles or as deemed appropriate by the geologist collecting and logging the core. The core bled small quantities of gas at approximately 3,845 feet, 4,342 feet, and 4,400 feet and samples were collected at these intervals.

Structural Geology

The objectives of the structural geology activity this quarter were to prepare for and begin field mapping of faults, folds, lineaments and collapse structures. Previously mapped faults (from the literature) were plotted on 7-1/2 foot topographic maps in preparation for field mapping. Included were all faults inside the Gibson Dome and Elk Ridge study areas, and also those faults that trend toward these study areas. The low-sun-angle black and white aerial photos acquired last November were analyzed for expressions of faults and collapse structures. The fault mapping procedure was written and finalized.

Field mapping included mapping of faults, lineament reconnaissance, and some preliminary reconnaissance of breccia pipes. Faults mapped include the northeastern one-third of the Shay Graben, the Lockhart fault and nine related faults in the Lockhart Basin, the Trough Springs fault and related faults of the Cane Creek anticline, the west terminus of the Verdure graben and the northeast terminus of the north fault of the Hammond Graben.

Fault mapping to date has indicated that the typical surface expression of normal faults includes a brecciated zone that is frequently bleached and that is often cemented with calcite and/or limonite. Mapping of the Shay Graben (northeast end) has suggested that there are several small splays or subparallel faults within the zone that were previously unmapped.

Reconnaissance was also completed on 8 of the 48 remaining selected lineaments from last year's aerial reconnaissance. Six of the eight lineaments were found to be fault-related but are outside the study areas.

Some preliminary reconnaissance studies of breccia pipes/collapse areas were done to compare the three known collapse feature areas in the Paradox Basin, including Lockhart Basin, the San Rafael Swell (Temple Mt. area) and the Spanish Valley collapse structure. Comparisons were made between their surface expressions, stratigraphic involvement, and faults or other structures related to the features.

In addition to field work, analysis and selection of geophysical data were started. Selection of seismic reflection data, gravity, and aeromagnetic data will take place during the first few weeks of next quarter.

Seismology

The majority of studies and work performed this quarter was associated with operation and modification of the 12-station, long-term Gibson Dome and Elk Ridge microearthquake networks. Conversion to long-term facilities and telemetry of the seven-station Gibson Dome subnetwork was completed and data are now being recorded at the recording center in Moab. Two of the seven stations were relocated to optimize seismographic coverage of Gibson Dome as well as Lavender Canyon and the area of previously observed microearthquake activity in the vicinity of the Colorado River northeast of the confluence with the Green River.

The five-station Elk Ridge subnetwork continues to require every-other-day visits for data retrieval. The possibility of three new station locations will improve the present seismographic coverage of Elk Ridge and allow complete telemetry of the subnetwork into Moab.

During the period from 15 February, when the long-term network began operation, to 1 June, 100 seismic events above approximate M_L 0.0 were detected. Of these, 23 were microearthquakes occurring in an approximately 15 km-long segment of the Colorado River northeast of the confluence with the Green River. The remainder are suspected blasts. Seismic activity in the area of the confluence, which was at a moderate level in the first few months of the temporary microearthquake monitoring, was almost nonexistent for 6 months prior to mid-May. On 16 May, an approximate M_L 1.9 mainshock occurred followed by 14 aftershocks. This sequence has been followed by single events every few days, thus apparently signaling the reactivation of moderate-level seismicity in this area. A possible relationship between this microseismicity and the Colorado River is being investigated. A temporary station, Colorado River Lookout, was installed soon after the 16 May earthquake a few kilometers south of its epicenter.

Efforts are presently under way to install a recently acquired develocorder and drum recording system in the recording center in Moab.* The Gibson Dome subnetwork and, soon thereafter, the Elk Ridge subnetwork, will then be recording on 16 mm film (develocorder film) as well as ink-recorded paper drums. This new instrumentation will free 12 instruments for use in the 12-station Salt Valley microearthquake network, which will be installed and monitoring in mid-July. Site selection for the Salt Valley network has been completed. The objective of this monitoring is to identify and evaluate any microearthquake activity that may be associated with Salt Valley, Cache Valley, the Moab fault, and the Uncompaghre uplift.

Other activities this quarter were: (1) an investigation into blasting sources (mine, quarry, or construction-related) to aid in blast-earthquake discrimination; (2) preliminary analysis into recent seismic activity (largest events M_L 3.6) in the area of Capitol Reef and the Waterpocket fold; and (3) preliminary studies into mining-induced seismicity.

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*This type of recording system is a standard one used by the USGS and universities engaged in microearthquake network studies. It requires much less time for maintenance and is less costly to operate than the present MEQ-800.

Tectonic History

Activity this quarter consisted of continued literature review and compilation of paleotectonic maps of the Colorado Plateau for the Cenozoic Era. Aquisition of a 1 to 50,000-scale residual Bouguer gravity map of Colorado and Utah is well advanced and should be completed by fall. This map will be combined with published maps of Arizona and New Mexico to provide a comprehensive overview of major basement structures in the Colorado Plateau and surrounding regions.

Hydrogeology

The Paradox Basin Project hydrogeologic activities this quarter included field work in the Gibson Dome study area, procurement of appurtenant equipment, analyses of the data collected in the field, and compilation of hydrogeologic data in the region encompassing the Elk Ridge and Gibson Dome study areas. The Gibson Dome field activities and equipment procurement focused on the GD-1 borehole monitoring and hydrogeological testing. Data from all tests completed in GD-1 this quarter were analyzed, and interpretation and compilation of the regional hydrogeochemistry data continued.

A comprehensive hydrogeologic monitoring and testing program is under way at GD-1. To date, this program has included several activities that were continuous during coring, plus a series of tests that was conducted during a period when coring was temporarily suspended. Downhole water conditions were monitored as coring progressed. Selected intervals of core were sampled for lab tests on porosity and permeability. During the air-mist drilling to the top of the Paradox Formation, specific conductance and the rate of discharge of the return flow were monitored at the end of each core run. Several samples of water were also collected for complete chemical analysis. These data indicated an increase in salinity of formation water with depth until a productive zone was encountered midway through the Elephant Canyon. Flow from this interval obscured any further downhole variations in water chemistry that could be monitored during subsequent drilling to the first hold point.

A fluorinated anionic tracer was added to drilling fluids used in GD-1. Comparisons of the tracer concentrations in the input and output mist lines corroborated measurements of the rates of discharge in both lines, indicating that the tracer was functioning properly (i.e., not being bound to cuttings, foam, or the borehole wall). At a predetermined hold point depth of approximately 2,700 feet, which is stratigraphically near the top of the Paradox Formation, coring was suspended and drill-stem testing of the stratigraphic section above the Paradox Formation proceeded. The zones selected for testing were judged to be the most permeable ones encountered within the strata above the Paradox Formation. Information used to select the zones included lithologic logs, fluid travel logs, porosity logs, and acoustic "fracture-finder" logs. Porosity and permeability values for the lower permeability zones will be determined by laboratory analysis of core samples. Seven drill-stem tests were successfully completed utilizing a specially designed straddle-packer test tool. The performance of this tool is exceptional because it allows real-time monitoring and surface recording during testing of pressure changes induced in the interval above, below, and within a test zone, which is isolated by the inflated packer elements. Conventional flow-in/shut-in tests and air-lift pump-out tests were performed to obtain data on permeabilities (hydraulic conductivity) and potentiometric levels.

Only two of the seven zones tested produced significant quantities of water. The most productive zone, found midway through the Elephant Canyon, produced approximately 14 gallons per minute after approximately 1 hour of pumping with 330 feet of drawdown. The other water-producing zone, a relatively porous zone within the middle Honaker Trail Formation, was much less capable of yielding water; it produced only about 0.7 gallon per minute after 1 hour of flow time with a drawdown of about 1,700 feet. Even though both of these zones were capable of only relatively low production, a methodology was devised that resulted in obtaining excellent, uncontaminated water samples for geochemical testing. The other four test intervals could not be sampled because of their extremely low flow capacity. Sampling methods used included purging the drill stem of contaminated (nonformational) water using high-pressure nitrogen. A wireline sampler was lowered to trap the sample downhole and transport it up to the drill site field lab. Field determinations were made immediately after the water sample was released from the sampler chamber to avoid obtaining spurious data for parameters that are sensitive to pressure/temperature changes and degasification of the samples. Additional aliquots of the water sample were preserved and bottled onsite, then transported to Missouri for complete chemical analysis.

Preliminary chemical analyses of water from the three discrete zones that could be sampled substantiate an increase in chloride with depth (increasing from approximately 2,000 mg/l Cl in the Elephant Canyon Formation to over 70,000 mg/l Cl in the Honaker Trail Formation). Concentrations of the fluorinated tracer in these samples indicate that the water samples represent from about 99 to 99.7 percent formational water.

A critical issue raised by these preliminary data is whether the increase in chloride concentration with depth is indicative of active solutioning of the Paradox salt. (No evidence of dissolutioning was detected in field examination of the core.) Comprehensive chemical analyses being performed on the formation water samples will be evaluated in conjunction with geochemical data to be collected subsequently from deeper intervals in GD-1. This information will, in turn, be compared with the regional hydrogeology and geochemistry information to ascertain if dissolution of salt is occurring.

Preliminary analyses of the straddle-packer test data indicate that the permeability of the most productive test zone is approximately 20 millidarcies. Permeabilities of the other test zones range from 0.4 to 0.001 millidarcies. The calculated potentiometric levels approximate a normal hydrostatic pressure gradient within the strata penetrated down to the middle of the Honaker Trail Formation (about 1,850 feet below ground surface). Two tests in the lower Honaker Trail indicate subnormal formation pressures and extremely low permeabilities.

Continued efforts in compiling the data necessary to define the regional ground-water flow system produced a series of hydrogeologic maps. A structure contour map of the top of the Mississippian Leadville Formation provides essential information on the configuration of the hydrostratigraphic unit occurring beneath the salt beds. Areal trends in the geochemical data from springs and wells located on a regional map provide useful indications of ground-water directions and salt dissolution areas. Trilinear diagrams show the relative ionic proportions of water samples collected from springs within the study areas. In general, the only springs sampled (excluding those in the caprock) that indicate a significant sodium-chloride component occur just above the low flow level of the Colorado River in Cataract Canyon. These springs issue from the Honaker Trail and Paradox Formations, or the alluvium blanketing these formations, and are probably covered most of the year by higher stages of the river. Discharge from these springs and other seep areas that may occur below the lowest stage of the river does not appear great enough, however, to increase the specific conductance of the Colorado River as it flows through this area. Further field work is planned to quantify this critical aspect of the flow system relative to the Gibson Dome area, especially with regard to salt dissolution.

Geotechnical Engineering

Logistic planning and test procedure development for borehole expansion tests were completed during this quarter. These tests will be conducted during the next quarter in the Paradox Formation using drill stem test equipment; the tests are expected to provide estimates of in situ properties and hydraulic fracturing susceptibility for selected lithologic units (primarily salt beds) in GD-1.

A borehole expansion test is similar in concept to a borehole pressure meter test (used in in situ soil testing) in that a portion of the borehole will be subjected to pressure changes while simultaneously monitoring the deformation response of the hole. However, as no pressure meter device exists that can both pressurize rock materials at 3,000 to 5,000-foot depths and monitor their deformations, a novel test procedure has been planned utilizing drill stem test equipment.

The drill stem test tool has inflatable packers to isolate selected test zones. The test zone and tubing extending upward from the zone will be filled with fluid to a height of several hundred feet above the zone. As pressure in the test zone is varied, diameter (and thus test zone volume) of the borehole increases or decreases; correspondingly, fluid level in the tubing falls or rises. The measurement of this fluid level change while the tubing is under pressures of up to 6,000 psi presents major difficulties, but it is expected that measurements can be made either by a dual pressure transducer or by a water level sensing device lowered down the tubing with a wire line. The pressurization of the test zone will be continued until the rock (i.e., salt) fractures.

Other geotechnical activities during the past quarter included planning for laboratory permeability testing to be conducted in conjunction with the hydrogeology discipline. Laboratory-measured permeability values will be considered together with in situ measurements to estimate subsurface hydrogeologic parameters.

Geotechnical efforts during the next quarter will emphasize the in situ borehole expansion testing. Some preliminary observations from this testing should be available by the next reporting period.

WBS 1.4.3

Project: Paradox Basin Studies

Principal Investigator: U.S. Geological Survey, Denver, Colorado (R. J. Hite, Coordinator)

ONWI Project Manager: N. A. Frazier

Objective

The objective of this project is to conduct geologic studies related to siting of a repository in bedded salt in the Paradox Basin.

Geology

PROGRESS REPORTED PREVIOUSLY

Cuttings from Salt Valley drill holes DOE No. 1 and No. 2 were analyzed to bromine by X-ray fluorescence. Plots of these data show that both holes penetrated the same halite bed, which is overturned and nearly vertical. A method was developed to determine the water content of halite rock. This involves dissolving the halite sample in methanol and then determining the amount of water in the methanol using a Karl Fischer titrator. Methodology for determining the chemical composition of the brine inclusions in halite rocks is being developed. The distribution of trace bromine in halite from DOE No. 3 indicates that this hole penetrated the same bed found in DOE No. 1 and No. 2 and that it is also overturned at this location. The determinations of water-insoluble material in the halite rock of DOE No. 3 show that it is very low, averaging about 1.5 weight percent. X-ray diffraction (XRD) examination of these residues shows that they generally consist of about 95 percent anhydrite, with the remainder being made up of quartz, dolomite, calcite, and trace amounts of illite. A longitudinal section through Salt Valley anticline shows that the caprock overlying the salt is sealed off to the northwest by a thick cover of Mancos Shale. Additional geologic barriers to hydrologic flow paths from the caprock are the deep and structurally closed synclines flanking the structure.

ACTIVITIES DURING THE REPORTING PERIOD

Objectives

The objectives are to: (1) determine the water content of halite core from DOE No. 3 and the amounts of certain ions (Ca, Mg, and K) in the inclusion water, (2) continue sampling all halite units for determination of trace bromine and the weight percent of insoluble residues, (3) determine mineralogy of insoluble residues by XRD, (4) reexamine DOE No. 3 core to identify overturned sequences and to prepare a fracture log, and (5) develop a methodology to determine whether kerogen remaining in the black shale interbeds is capable of generating additional hydrocarbons when heated. The established technique of pyrolysis fluorescence (PF) will be used for Item 5. Also, halite samples from other deposits will be analyzed for H_2O content as a cross check on the methanol technique.

Results

All of the work on bromine and insoluble residues has been completed for DOE No. 3. Hydrocarbon analyses for select samples of canned core from DOE No. 3 is about 75 percent complete. Approximately 150 samples taken from the core have been analyzed by PF. A geologic cross section was completed through the Elk Ridge area. About 3,300 feet of core from the DOE Gibson Dome No. 1 corehole was received and racked at the storage facility.

Conclusions

Analyses of Paradox halite continue to show a very low H_2O content, generally less than 400 ppm. In contrast, some of the halite samples from the Palo Duro Basin in west Texas show as much as 20,000 ppm. Insoluble residues of Paradox halite in DOE No. 3 average less than 2 percent for the entire thickness of the penetrated evaporite sequence. Surprisingly, certain halite intervals contain as much quartz as anhydrite. PF analyses through the marker beds suggest that pyrolysis of organic matter yields only very small amounts of additional hydrocarbons. Bromine analyses of halite rock in DOE No. 3 indicate the presence of several fault planes, which on close inspection of the core have proven to be well healed. The cross section through the Elk Ridge study area reveals the presence of faulting in the evaporite sequence. Furthermore, in one control well, the thickness of the evaporite sequence is nearly tripled by a complex zone of flowage.

Hydrology

PROGRESS REPORTED PREVIOUSLY

A report on Green River-Moab was prepared for colleague review. Data reduction, preparation of illustrations, and writing were done for the Moab-Monticello, San Miguel, San Juan, and Dolores areal reconnaissance reports, as well as for the report describing the hydrologic testing of wells DOE-4, -5, -6, -7, -8 and -9 in Salt Valley.

ACTIVITIES DURING THE REPORTING PERIOD

Objectives

The objectives of this program are to: (1) revise the upper potentiometric head map and complete the manuscript for the Green River-Moab reconnaissance report; (2) reduce data, prepare illustrations, and write for the Moab-Monticello, San Juan, San Miguel, and Dolores areal reconnaissance reports; and (3) map phreatophytes for the San Juan and Dolores reconnaissance areas.

Results

(1) The report *Results of Hydraulic Tests of Wells DOE-1, -2, and -3, Salt Valley, Utah,* was printed and distributed. (2) The Green River-Moab report has been reviewed and revisions are being made. (3) The report describing the hydrology of the Moab-Monticello area has reached

98 percent completion. (4) The report describing the hydrology of the San Miguel area is approximately 75 percent complete. (5) The report describing the hydrology of the San Juan area is approximately 30 percent complete. (6) The report describing the hydrology of the Dolores River area is approximately 10 percent complete.

Conclusions

The aquifer tests in Salt Valley indicate extremely low permeabilities for the caprock across the valley. Water levels since the pumping tests have recovered to prepumping levels and show essentially no fluctuation with time.

Electrical and Electromagnetic Surveys

PROGRESS REPORTED PREVIOUSLY

Conclusions from the electromagnetic studies at Salt Valley are: (1) Slingram, a ground-based moderate penetration method, can detect anomalies that appear to be related to near-surface perched water pods; (2) extremely low-frequency loop-loop soundings revealed no widespread, continuous dissolution at the top of the salt but there could be small, isolated areas below the detection limit; (3) Schlumberger sounding (DC resistivity) is probably not a good method for investigating caprock above the salt because of the inhomogeneity of the caprock unit, and it cannot penetrate below the salt; and (4) a helicopter-borne electromagnetic (EM) survey revealed long anomalies within Salt Valley that are probably controlled by caprock lithology.

Seismic studies showed that the top of the salt dips toward the northeast limb of the anticline, and indicated the presence of blocks of sandstone that have foundered into the salt.

Geophysical well logs from Salt Valley were successfully interpreted; such logs can be used to give a positive identification of most rock types in an evaporite sequence. Interpretation of the caprock from geophysical well logs will require further correlation between cores taken from the caprock and the geophysical well logs.

ACTIVITIES DURING THE REPORTING PERIOD

Further examination of the data from the helicopter-borne EM survey has revealed consistent anomalies on the flanks of Salt Valley Anticline. These are probably expressions of splay faults, but this hypothesis needs to be confirmed by ground geophysics and/or mapping. The interpretation methods used by the contractor are not suitable for the Paradox sedimentary environment. The digital data tapes from the survey have been read into a USGS computer in preparation for more intensive analysis. Programs that model the effects of layered earth structure in this type of survey have been coded and are being debugged.

Three short lines of VLF (very low frequency, 17.8 KHz) magnetic field tilt data were obtained at Hatch Point (northeast extension of Lockhart Basin fault system), at Shay Graben, and near Rustler Dome (southwest extension of Lockhart Basin fault system). They revealed significant anomalies due to the faults, although additional unexplained anomalies were observed. These are likely to be due to small associated faults or shear zones. A tentative conclusion is that the fast, inexpensive VLF method may be a useful tool for mapping faults and fault extensions where they are hidden by Quaternary aeolian cover. The method's penetration is limited to a few tens of feet.

Hole-to-surface resistivity measurements were made from the Gibson Dome drill hole. Surface measurements were made along radial lines at 20-degree intervals around the drill hole out to a distance of 2000 meters away from the drill hole. Measurements were made with the source at depths of 518 and 760 meters. Approximately 1000 measurements were made (in less than 2 days) with the help of Woodward Clyde personnel. Preliminary interpretation of these data indicates a very uniform distribution of the electric field away from the drill hole. This implies uniform layering of the geologic strata above 760 meters.

Remote Sensing

PROGRESS REPORTED PREVIOUSLY

An open-file report, *Some Geomorphic Aspects of the Breached Salt Anticlines of the Paradox Basin, Utah and Colorado,* was completed, technically reviewed, and revised. A followup to this work has resulted in a narrow range of estimates of the minimum rate of downcutting (>0.006 to 0.019 cm/yr) in the northern Paradox basin since Early to Middle Pleistocene time, and a concomitant range in minimum rate of valley-floor lowering in areas of the diapiric anticlines. Additional valley-floor lowering might have occurred, depending on vertical uplift or continued diapirism of the anticlinal cores. Landsat Multispectral Scanning (MSS) and Return Beam Videcon (RBV) images and X-band radar images were used in conjunction with field investigations in preparation of this report.

A 22-unit colored terrain map for three contiguous 2-degree quadrangles (Grand Junction, Moab, and Cortez) was produced from digitized topographic data, using a color Optronics system. The map units show the distribution of terrain above specified hypsometric levels. The visual effect is to show the topographic grain very clearly. The Uncompahgre block, the La Sals domal uplift, the cross-axial breached anticlinal valleys, and the landforms of the Grand Valley of the Colorado are well demarcated. This map is an ideal terrain base for gravity and magnetic field data and for plotting lineaments in relation to landforms.

ACTIVITIES DURING THE REPORTING PERIOD

Objectives

In addition to field investigation, activities during the reporting period have been aimed at producing a series of remote-sensing data products and interpretations useful to the Radwaste program for the Paradox basin, including X-band radar image analyses.

Procedures

Preparation of a preliminary uncontrolled slant-range X-band radar image mosaic of the northern Paradox basin with an accompanying USGS open-file report was completed, and field investigation of lineaments and landforms was continued during this quarter.

Results

A draft USGS open-file report, *Uncontrolled X-band Radar-Image Mosaic of the Western Part of the 2-degree Moab Quadrangle, Utah,* was completed and is being prepared for technical colleague review. This mosaic product is suitable for geomorphic interpretations and identification of fracture traces, but because of lack of a ground-range data presentation, true azimuthal bearings are not available for the fracture traces mapped from the mosaic, in contrast to previously studied and reported rectified Landsat MSS images.

Conclusion

A radar image rectification procedure involving an optical-transfer process is necessary to convert the radar slant-range presentation mode to a planimetrically rectified, ground-range presentation giving true azimuthal bearings, but the present uncontrolled mosaic shows many previously unreported fracture traces and is a significant contribution to the understanding of the fracture pattern of the region.

Seismic Profiling

PROGRESS REPORTED PREVIOUSLY

Description of the Method

To test the applicability of computer processed vertical seismic profiles, which is essentially a new technique, a seismic source is placed in one drill hole and the waveform is recorded at many depths in the other. The data are then processed, analyzed, and interpreted to identify, resolve, and profile-map lithologic units of the geologic section between the source and geophone holes.

Because the seismic source and detector are both in the salt, much higher frequencies can be generated than are usually possible when surface sources and detectors are used. Since some of the interbeds are quite thin, the higher frequencies (or shorter wavelengths) offer a considerable advantage over surface methods. In addition, having source and receiver relatively close to the reflecting interbeds may yield better resolution.

Complicated structures, extraneous reflections (from the ground surface for example), unwanted wave modes (shear waves for example), and ambient noise make the interpretation of actual data difficult. Extensive computer processing of the actual field data is usually required to suppress unwanted seismic events and enhance desired reflections before an adequate interpretation can be made.

Summary of Previous Work

A vertical seismic profile (VSP) experiment was conducted at the Salt Valley test site from 7 January to 27 January, 1979, but only one complete, fair quality profile was obtained. The field data were extensively edited and processed to enhance coherent events.

On the basis of results of the first shoot, the second shoot was planned and accomplished utilizing improved field parameters and equipment. A new time-break system was employed as well as a different source setup. The geophones and locking arm in the downhole receiving tool were modified. These changes were made to enhance the data in ways that will permit a better final interpretation. The shoot was carried out in 21 consecutive 12-hour days in November and December.

Two aspects of this reshoot are most valuable. First, it was possible to shoot from both DOE 1 and DOE 2, which gave data along the strike of the salt structure as well as along the dip. Second, repeating the shooting of DOE 1 will provide some confirmation of the results of the first shoot, which will greatly aid in the confidence of the final geological interpretation.

ACTIVITIES DURING THE REPORTING PERIOD

The main activity has been to computer process the VSP data acquired in December, 1979. The reformatted data were plotted and each of the several thousand recordings was checked for quality and accuracy. Approximately 10 percent of the traces were discarded to improve overall data quality. Shots recorded under identical source-receive conditions were summed and composited to improve signal-to-noise ratio. Frequency analysis was performed. The recorded data appear to have frequency components up to about 500 Hz; it is not known how much true reflected signal is in the high-frequency portion of the data. The data were test deghosted because it is suspected that ghost reflections from the top of the salt obscured the interbed reflections. The results of the test were inconclusive. For the most part, surprisingly little improvement was obtained. This means that either the parameters used to deghost were in error, or that ghosting is not a serious problem, as previously supposed.

A velocity-filtering operation was carried out in two steps. First, a wave number-frequency (f-k) type of filtering operation was performed to generate two data sets: one containing only upward-traveling events, and one containing only downward-traveling events. There were two wells and three components of motion for each well, yielding six data sets to be f-k filtered. Next, the data sets were velocity filtered, using multichannel time domain filters, in increments of 1 msec per trace. These results were recombined to produce a maximum-coherency-type plot which retains only the events with the greatest space-time coherency. The upward and downward maximum-coherency versions were merged and plotted. These results were subjected to a variety of frequency filtering operations to improve signal-to-noise ratio with a minimal loss in resolution.

The most important feature in the plots is the multiplicity of upward-traveling events, or reflections. These events are very much in evidence, and in several cases correspond to places in the hole where marker beds are known to intersect the hole. The consistency of the appearance of these events and their coherence give a good deal of confidence that these events are true reflections and not just artifacts of the data.

Not all the events originated as compressional waves directly from the air gun. It is now believed that a compressional and shear wave came directly from the source, another pair of p and s disturbances came from the bottom of the source hole, and still a third pair was generated when a tube wave in the source hole encountered the air gun after reflection off the bottom of the hole. This multiplicity of sources causes a redundant tendency in the data.

Seismic Refraction Surveys

No progress report was submitted for this period.

Gravity Surveys

No progress report was submitted for this period.

WBS 1.4.3

Project: Southeast Disposal Site Studies

Principal Investigator: Savannah River Laboratory (I. W. Marine)

ONWI Project Manager: R. B. Laughon

Objective

The objective is to conduct regional reconnaissance surveys of (1) igneous and metamorphic rocks of the Piedmont Province, (2) mudstones, shale, and sandstones of the Triassic Basins, and (3) unconsolidated-to-semiconsolidated sands and clays of the Coastal Plains in parts of the coastal states east of the Blue Ridge Mountains between Maryland and Georgia. The task to be completed is to review the literature and current knowledge of the entire southeastern region to facilitate designation of areas for further study.

Activities During the Reporting Period

Preliminary copies of the eight reports produced as part of the Southeast Disposal Site Studies were issued for DOE, ONWI, and DuPont review prior to sending them to the state geologists for their review.

WBS 1.4.4

Project: Environmental Characterization

Principal Investigators: NUS Corporation (J. DiNunno, W. Belter)
Bechtel National, Inc. (N. Norman)

ONWI Project Managers: NUS—D. A. Waite, BNI—R. B. McPherson

Objective

The objective is to conduct environmental characterization studies at the region, area, and location as a means of identifying environmental aspects of concern or interest in relation to the geologic formation of interest. The studies provide a means of identifying sites that may be potentially the most suitable for a repository as well as documenting base data to be used in subsequent licensing documents such as Environmental Reports.

Progress Reported Previously

These tasks were begun on 7 July, 1977. Documentation for the area environmental characterization phase was completed in the Permian, Paradox, and Gulf Interior Regions. The final Regional Environmental Characterization Reports and the final Regional Summary Report for the Salina Basin were released. Environmental evaluations in the Gulf Interior Region were reported for area study Drill Holes LH-2, LH-8, LVH-6, LH-7, LRH-13, and LH-17 in Louisiana; MH-8, MRIG-9, MRIG-10, and MRIH-11 in Mississippi; and TOG-1, TOH-2, TOH-3, TOH-4, and TOH-5 in Texas. Environmental evaluations in the Paradox Region were reported for area study drill holes at Gibson Dome and Elk Ridge in Utah.

The Site Evaluation Committee continued to evaluate and rank the seven domes in the Gulf Interior Region. No environmental field activities were conducted during this quarter.

Preparation of the National Site Characterization and Selection Plan (NSCSP) continued. A special three-man task force was appointed to redraft the plan for review.

Activities During the Reporting Period

The final Gulf Interior Regional Summary and Area Recommendation Report was transmitted to DOE for review, as was the Draft Permian Area Environmental Characterization Report. The proposed Utah Wilderness Areas were reviewed for possible impacts on Utah Study Areas. Evaluation and ranking of the seven domes in the Gulf Interior Region continued. A study entitled "Transportation Routing Study for the Gulf Interior Region—Comparative Radioactive Dose Commitments for Seven Repository Scenarios" was completed for use in evaluating transportation risk among the seven domes. No environmental field activities were conducted during the quarter.

Preparation of the NSCSP continued. Schedules for preparing the plan and for preparing National Environmental Policy Agency (NEPA) documents were established and a revised working draft of the plan was completed and reviewed. A new outline was prepared and the plan is being revised accordingly. Final drafts of the guide for preparing environmental evaluations for deep drilling, the NWTS geologic and geophysical exploratory activities document, and the document describing environmental effects of deep drilling were prepared. NWTS workshops were held to discuss the Site Characterization Plan, NEPA implementation, and the contents of Environmental Assessments and Environmental Impact Statements required during the site selection process.

SUMMARY

1.5 FACILITIES ENGINEERING

The scope of Facilities Engineering investigations covers Repository Engineering (Pre-Title I), Test facilities, and Spent Fuel Packaging Facility Engineering. The prime objective of this task is to develop the conceptual engineering and design bases and criteria necessary to allow Titles I and II design and eventual construction of repositories.

The detailed reviews of repository and prerepository designs have resulted in information and data that allowed characterization of the pertinent waste handling systems to subsystem and equipment levels of detail. These characterizations facilitated a systematic comparison and review of waste handling systems components that have analogous inputs, functions, operations, procedures, and outputs. From these comparisons and reviews, an extensive array of component standardization candidates based on similarities and differences has been assembled. The parametric analysis of the alternative candidates will identify the components considered most suitable for waste handling system standardization.

WBS 1.5.1

Project: NWTS Conceptual Design Study—Salt Dome Assessment

Principal Investigator: Stearns-Roger Services, Inc. (J. C. Mattern)

ONWI Project Manager: N. J. Dayem

Objective

The objective of this project is to evaluate the engineering feasibility of developing a repository in seven sites. The sites are: Lampton (Mississippi), Cypress Creek (Mississippi), Richton (Mississippi), Rayburn's (Louisiana), Vacherie (Louisiana), Keechi (Texas), and Oakwood (Texas). All of the engineering evaluations will be based upon existing geotechnical and environmental data which have been, or are being, developed by other contractors. This study will also evaluate the adequacy of this existing data base.

Progress Reported Previously

During the previous quarter the main activities were the organization of the project and the assembling of data for the study.

Activities During the Reporting Period

The overall product of this study will be a final report describing the engineering evaluations performed and the conclusions reached regarding the engineering feasibility of a repository located at each of the seven sites. During this reporting period the following activities were performed to accomplish this objective:

- Evaluating geological/geotechnical data
- Evaluating environmental information published by Bechtel
- Evaluating creep and creep-related problems associated with deep (~ 3,000-foot) repository levels
- Selecting preferred and alternate repository depths
- Developing layouts for underground facilities at preferred and alternate depths
- Developing stratigraphic sections for shaft locations
- Producing site arrangement sketches and geopolitical maps for all sites
- Evaluating salt disposal methods
- Developing comparative cost estimates for each site.

WBS 1.5.1

Project: Standardization of Waste Handling Systems

Principal Investigator: Los Alamos Technical Associates, Inc. (R. J. Kingsbury)

ONWI Project Manager: T. Tewksbury

Objective

Conceptual designs have been prepared for National Waste Terminal Storage (NWTS) repositories intended to receive, handle, transfer, emplace, and retrieve nuclear wastes. These repositories are designed to store wastes underground in selected geologic media. Surface and underground repository facilities include waste handling systems and equipment required to perform operations under the rigorous constraints necessary to assure safety, protection of the environment, and achievement of operational objectives. This project is intended to identify viable alternatives for these systems and equipment and to develop recommendations for waste handling systems standardization.

Progress Reported Previously

This project was started on 1 March, 1980. The work performed previously consisted of preparation and initiation of detailed reviews of the conceptual design reports for the NWTS Repository 1 (dome salt) and Repository 2 (bedded salt). These reviews identified the waste handling systems, subsystems, and components; pertinent functions, objectives, constraints, and design/performance parameters; and the interfaces between waste handling systems and the repository facilities, services, and other systems. The data and information extracted by these reviews and stored in a computerized data base serve as the basis for development of repository-specific flow diagrams, component alternatives, and alternative evaluation parameters.

Activities During the Reporting Period

Objective

The work performed during the reporting period was intended to:

- Complete reviews of conceptual design data for repository waste handling systems and equipment
- Review additional data for waste handling systems and equipment in operations similar to the repositories
- Identify similarities and differences in waste handling systems and equipment between repository designs and others

- Establish waste handling flow paths through the repositories and identify major and ancillary components
- Identify and review waste handling system component alternatives.

The technical effort necessary to accomplish these objectives will establish the basis for development of recommendations for waste handling system component standardization.

Procedures

The detailed reviews of the repository conceptual designs and data on similar waste handling operations from other waste management programs were conducted in accordance with prescribed reviewer instructions by a multidisciplinary team. These reviewer instructions included identification of the materials to be reviewed, definition of terms, systems engineering formats, and forms for recording results.

The functional, operational, and procedural data extracted during the detailed reviews serve as a basis for establishing flow diagrams of waste handling systems for Repository 1, Repository 2, prerepository operations, and for certain repository-similar programs. These flow diagrams have been assembled using a common format to facilitate comparisons.

Corresponding flow diagram components from repository, prerepository, and other waste handling operations have been compared and functional, operational, and procedural similarities and differences identified. These similarities and differences have been reviewed and alternatives suitable for further study were selected.

Results

Principal results through the reporting period are:

- Identification and selection of significant candidates for waste handling system component standardization based on repository conceptual design similarities
- Identification and selection of alternative candidates for waste handling system component standardization based on repository conceptual design differences and other system differences
- Specification of the parametric analysis methodology and evaluation parameters to be used in the multidisciplinary review and selection of standardized waste handling system components.

Conclusions

The detailed reviews of repository and prerepository designs have resulted in information and data that allowed characterization of the pertinent waste handling systems to subsystem and equipment levels of detail. These characterizations facilitated a systematic comparison and review of waste handling systems components that have analogous inputs, functions, operations, procedures, and outputs. From these comparisons and reviews an extensive array of component standardization candidates based on similarities and differences has been assembled. The parametric analysis of the alternative candidates will identify the components considered most suitable for waste handling system standardization.

SUMMARY

1.6 SITE QUALIFICATION AND LICENSING

Work conducted under this program element includes the development of licensing strategies, criteria, and guides necessary for the identification of required information for, and the preparation of, licensing documents. The ultimate objective is the granting of an operating license for a geologic repository by the Nuclear Regulatory Commission.

Work included assisting the Department of Energy in completing its Statement of Position on the Confidence Rulemaking and forwarding it to the NRC on 15 April 1980. Continued assistance was provided to DOE in reviewing the statement, developing errata, and working on document control/logistical planning for subsequent rulemaking phases.

Extensive workshops were held with the regulatory project managers to review comments received on the PIR and to redraft the PIR to incorproate those comments. The majority of the PIR was modified to incorporate such comments during the third quarter. The PIR will be forwarded to DOE for review in the fourth quarter.

An Advanced Notice of the Proposed Rulemaking on 10 CFR Part 60 was published in the *Federal Register* by the NRC. An extensive review of the Advanced Notice was initiated which included NWTS participants from each major office and a large number of outside reviewers. An integrated set of comments based on that review was prepared and transmitted to DOE for its use in preparing the DOE comments on the proposed rulemaking.

Preparation of Part II of the NWTS Licensing Plan was initiated. Part II will identify significant licensing issues and provide guidance for their resolution through such mechanisms as the PIR and the Licensing and Topical Report programs.

The Decommissioning Report was reviewed, revised, and forwarded to NPO.

WBS 1.7.2

Project: Evaluation of Implications of Future Human Activities on Nuclear Waste Repositories

Principal Investigator: Envirosphere Company (J. A. Franco)

ONWI Project Manager: J. R. Finley

Objective

The objective is to provide required institutional information on future human activities regarding nuclear waste repositories to groups involved in site qualification and licensing, facility design, and communications and public affairs.

Progress Reported Previously

Work began on 1, May 1980. To date, work has centered on background literature review, subconsultant identification, and initiation of specific analyses.

Activities During the Reporting Period

Objective

The purpose of the work undertaken during this quarter was to identify and evaluate background materials necessary to conduct the analyses required for each work task.

Procedures

The objectives are being accomplished through: (1) consultation with ONWI personnel; (2) review of literature produced to date by the NWTS program; (3) identification and review of other information related to each work task; (4) review of pertinent regulatory criteria (EPA, DOE, NRC); and (5) preparation of topical report sections for each task.

Activities

Review of EPA Standard. Research for this task is nearing completion. Completion will involve making EPA contacts regarding development of the standard.

Human Intrusion Scenarios. Existing scenarios have been identified and analysis of them has begun. Development of supplemental scenarios is under way.

Repository Record Preservation. Basic information in this area is being gathered. Specialists in archives management are being sought.

Institutional Barriers. Work has concentrated on an analysis of the potential for an effective site marker. Several international organizations involved with the development of cross-cultural symbols have been contacted. Services of specialists in this area will be utilized.

WBS 1.7.5

Project: Social Science Research and Support Services

Principal Investigator: HARC (Battelle) (H. Schilling)

ONWI Project Manager: D. Keller

Objective

The broad objective is to enhance solution of commercial nuclear waste problems by providing analyses of social science issues in nuclear waste and assisting ONWI in using the results of such analyses. Much of the analytic work is directed toward public issues in nuclear waste. Some analysis is more specifically focused on social science aspects of licensing. Finally, there is general support to ONWI in the social science area including general advice; review of plans, reports, and intended actions; and dissemination of research findings.

Activities During the Reporting Period

HARC activities for the quarter focused on Tasks 2 and 3.

Task 2 work included further progress on studying the institutional characteristics of various states.

Under Task 3, an analysis of consultation and concurrence activities by stage of repository site and selection and characterization was prepared. The major focus of Task 3 activity, however, was directed toward providing support to the State Planning Council. HARC assisted in preparing a docket book of materials in low-level waste and consultation and concurrence for the June State Planning Council meeting.

Finally, an additional task was added to HARC's work. This work entails preparation of a state-of-the-art paper on consultation and concurrence.

ABBREVIATIONS

AEC	U.S. Atomic Energy Commission
AEGIS	Assessment of Effectiveness of Geologic Isolation Systems program (program replaces WISAP)
AFR	away from reactor
ANL	Argonne National Laboratory
ANS	American Nuclear Society
ANSI	American National Standards Institute
ASTM	American Society for Testing Materials
BEG	Bureau of Economic Geology (Texas)
BLM	Bureau of Land Management, U.S. Department of the Interior
BNI	Bechtel National, Inc.
BNL	Brookhaven National Laboratory
BNW	Battelle-Northwest
BPMD	Battelle Project Management Division
BPNL	Battelle Pacific Northwest Laboratories
BWIP	Basalt Waste Isolation Project
BWR	boiling water reactor
CFR	Code of Federal Regulations
Ci	Curie
CSM	Colorado School of Mines (Golden, CO)
D/D; D&D	decontamination and decommissioning
DOD	U.S. Department of Defense
DOE	U.S. Department of Energy
DOT	U.S. Department of Transportation
EIS	environmental impact statement
EPA	U.S. Environmental Protection Agency
ERDA	U.S. Energy Research and Development Administration
FR	Federal Register
FRG	Federal Republic of Germany
FY(TD)	fiscal year (to date)
GIR	Gulf Interior Region
GPM	Geologic Project Manager
HARC	Human Affairs Research Centers (Battelle-Seattle)
HEDL	Hanford Engineering Development Laboratory
HLW	high-level waste
HWR	heavy water reactor
IAEA	International Atomic Energy Agency
ILW	intermediate-level waste
IWG	Interface Working Group

KBS	Kärnbränslesäkerhet, Swedish Nuclear Fuel Supply Co.
LASL	Los Alamos Scientific Laboratory
LATA	Los Alamos Technical Associates, Inc.
LBL	Lawrence Berkeley Laboratory
LETCo	Law Engineering Testing Company
LLL	Lawrence Livermore Laboratory
LLW	low-level waste
LSU	Louisiana State University
LVDT	linear variable displacement transducer; linear variable differential transformer
LWR	light water reactor
MIT	Massachusetts Institute of Technology
NASA	National Aeronautics and Space Administration
NBS	National Bureau of Standards
NEA	Nuclear Energy Agency; National Energy Act
NEPA	National Environmental Policy Act; National Environmental Protection Agency
NOAA	National Oceanographic and Atmospheric Administration
NPO	NWTS Program Office (formerly RL-C)
NRC	U.S. Nuclear Regulatory Commission
NTS	Nevada Test Site
NUS	NUS, Inc. (Nuclear Utilities Services, Inc.)
NWTS	National Waste Terminal Storage (program)
ONWI	Office of Nuclear Waste Isolation
ORNL	Oak Ridge National Laboratory
OSHA	Occupational Safety and Health Administration
OWI	Office of Waste Isolation (predecessor of ONWI)
PNL	Pacific Northwest Laboratories (Battelle)
PSU	Pennsylvania State University
PWR	pressurized water reactor
QA	quality assurance
R&D	research and development
RHO	Rockwell Hanford Operations
RL-C	Richland Operations, Columbus Program Office, now NPO
SF	spent fuel
SL	Sandia Laboratories
SRP	Savannah River Plant
TASC	The Analytic Sciences Corporation
TBEG	Texas Bureau of Economic Geology
TRU	transuranic (contaminated) waste
TSCA	Toxic Substances Control Act

USBM	U.S. Bureau of Mines
USGS	U.S. Geological Survey
WES	Waterways Experiment Station, Corps of Engineers
WIPP	Waste Isolation Pilot Plant
WISAP	Waste Isolation Safety Assessment Program (replaced by AEGIS and WRIT)
WRIT	Waste/Rock Interactions Technology program (program replaces WISAP)

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