

Earth Sciences Department

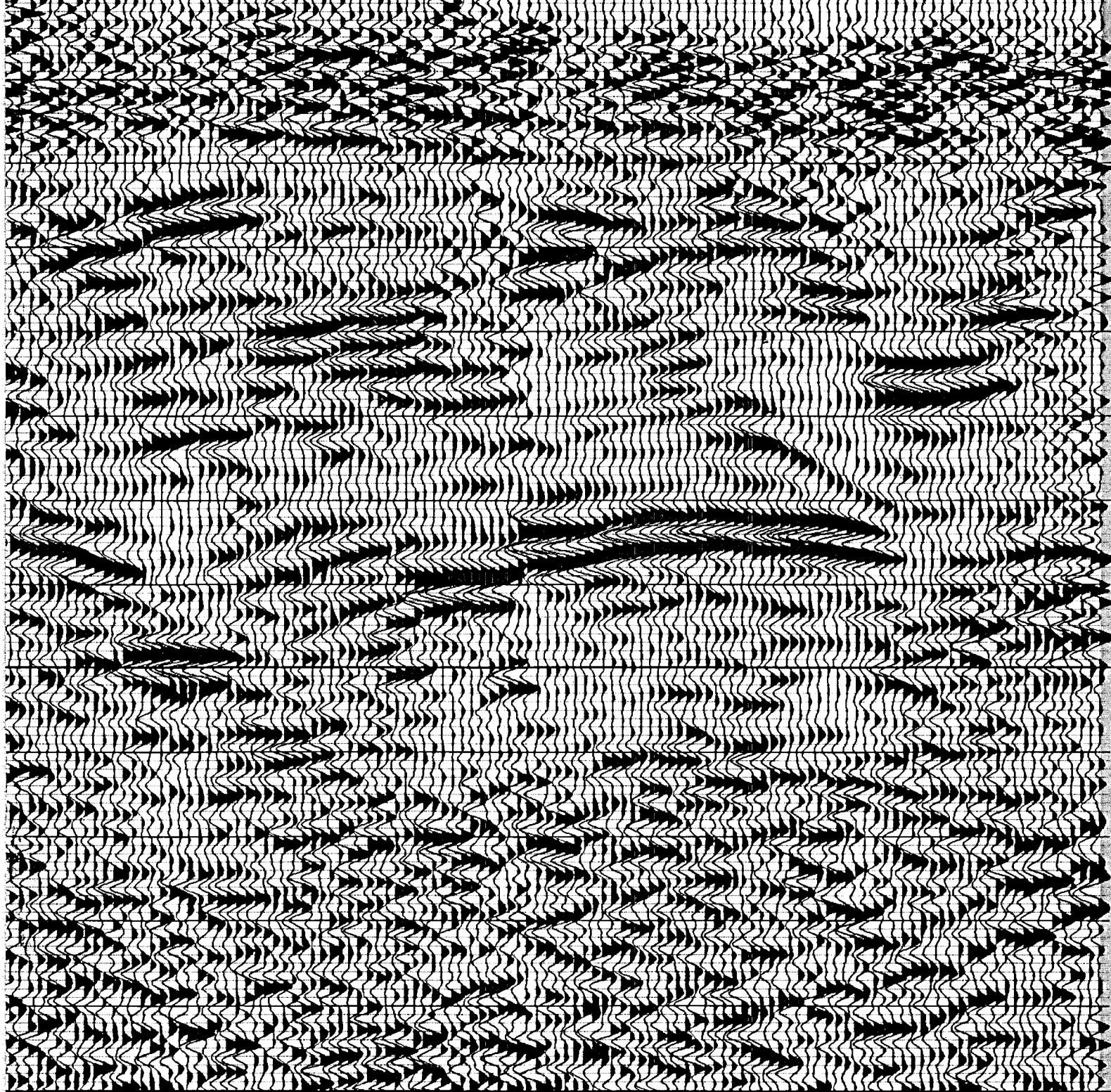
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Cover

Seismic reflection data shot in Area 8 of the Nevada Test Site using Primacord as a seismic source. These data are used to determine subsurface structure to help select suitable sites for underground nuclear tests.

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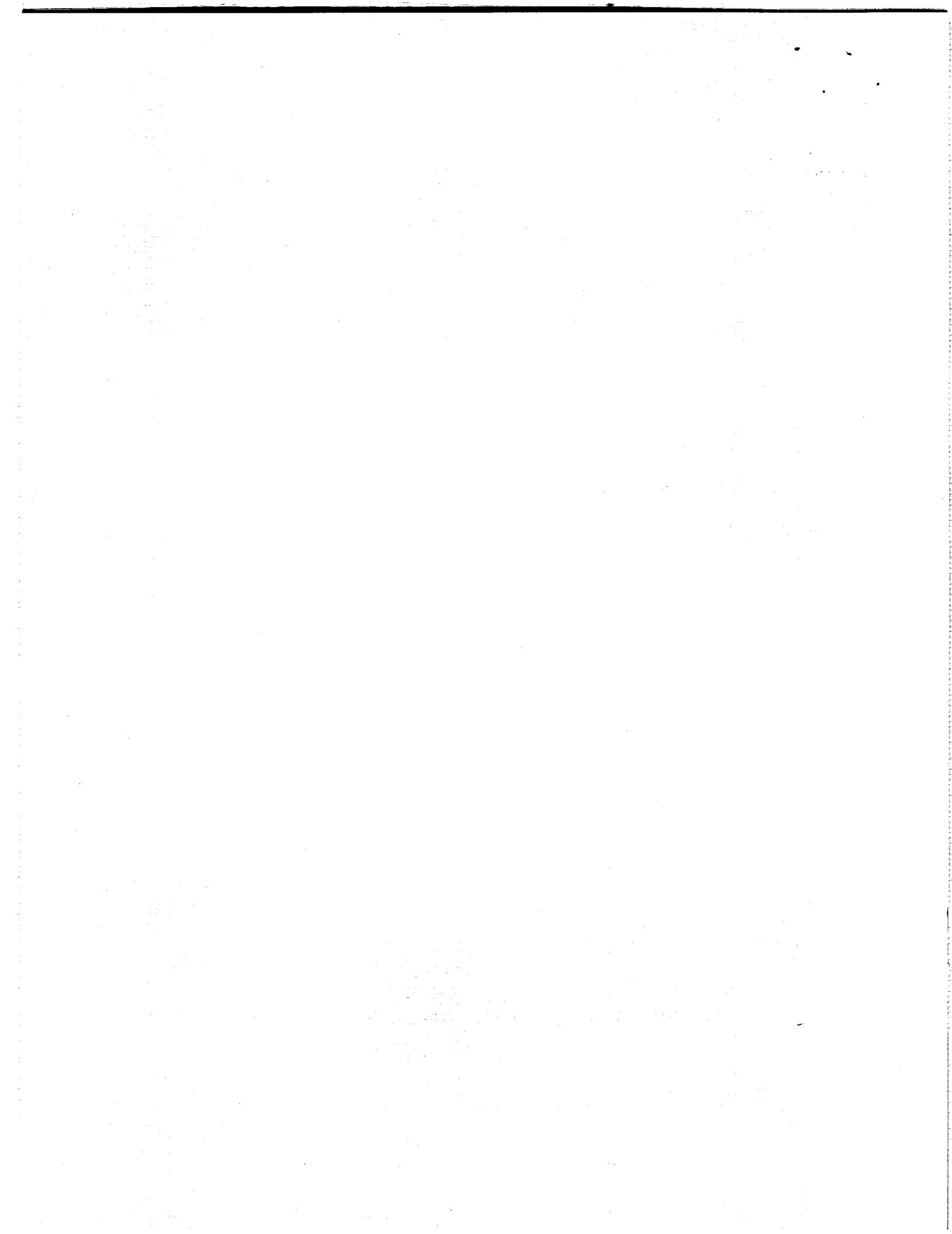
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Earth Sciences Department Annual Report 1984

Abstract

The Earth Sciences Department at Lawrence Livermore National Laboratory comprises nine different disciplinary and programmatic groups that provide research in the geosciences, including nuclear waste management, containment of nuclear weapons tests, seismic treaty verification, stimulation of natural gas production by unconventional means, and oil shale retorting. Each group's accomplishments in 1984 are discussed, followed by a listing of the group's publications for the year.

Introduction

The Earth Sciences Department at Lawrence Livermore National Laboratory (LLNL) is one of the largest geoscience research groups in the nation. It comprises about 100 professional scientists from a wide variety of disciplines: geology, seismology, physics, geophysics, geochemistry, hydrology, engineering geology, mining engineering, chemistry, chemical engineering, and mechanical engineering.

Interest in the earth sciences at the Laboratory began in the 1950s with the Plowshare Program, which researched how nuclear explosives could be used to peacefully provide large-scale excavation for the creation of harbors, canals, or underground storage facilities, and the fracture of earth materials deep underground to stimulate natural gas reserves or to aid in the recovery of other natural resources. The Plowshare Program is no longer active, but it brought to the Laboratory a creative group of earth scientists who took the knowledge gained from that program and, with a perceptive understanding of the nation's needs, developed a wide variety of research efforts.

Today the role of the Department at LLNL is to provide research capability in the earth sciences to any Laboratory program that needs it, to man-

age projects assigned to the Department, and to develop and maintain capability in the earth sciences to meet the present and anticipated needs of LLNL programs. The result of this broad responsibility is that the Department works on a wide variety of programs, some large and some small, develops new programs, manages some programs, and provides its disciplinary capability to others. The programs the Department is now managing include: nuclear waste management, containment of nuclear weapons tests, seismic treaty verification, stimulation of natural gas production by unconventional means, and oil shale retorting.

This is a report of research accomplished by staff members of the Earth Sciences Department at LLNL during calendar year 1984. It includes a description of each of the organizational groups in the department. These descriptions include details of the discipline capability of each group, the programs supported by members of the group, and laboratory, field and computational equipment available to complete the research. Each group has also included a bibliography of publications by group members during the year, and some have included brief summaries of research projects completed by the members.

Experimental Geophysics Group

The high-pressure geophysics group has the capability to measure physiochemical properties of materials to temperatures of 2000°C and pressures up to 70 GPa. During this past year, we have used these capabilities to investigate a wide range of physical and chemical phenomena, which are applicable to several major LLNL programs, including radioactive waste management, test containment, physics, seismic verification, and basic energy sciences.

We have studied wave propagation in pressed NTS fine-grained alluvium using multiple-turn velocity gauges and a newly developed magnet system capable of studying samples as large as 1.5 m in diameter. The resulting data are of high quality down to strains of less than 10^{-5} , permitting us to cover a wider range of scaled distance than has been heretofore possible in our study of equation of state at high strain rates.

Our thermal properties measurement capability was extended by two new systems. One measures thermal conductivity and diffusivity of samples as large as 100 mm in diameter and 250 mm long to 300°C and 50 MPa. The other measures only thermal conductivity on samples 75 mm in diameter and 150 mm long to 200°C and 100 MPa. These add substantially to our existing capability to measure thermal diffusivity of samples 25 mm in diameter by 63 mm long to 400°C and 200 MPa.

Our cryogenic creep and constant strain rate apparatus, which operates routinely between 77 and 258 K to 500 MPa and at strain rates from $3.5 \times 10^{-4} \text{ s}^{-1}$ to $3.5 \times 10^{-6} \text{ s}^{-1}$, has been modified to work at strain rates of $3.5 \times 10^{-7} \text{ s}^{-1}$. During the past year results from strength and frictional sliding experiments have been reported in the ice I_h, II, and III fields at 77 K.

Our semi-automated technique using the SEM for quantitative measurements of crack structure in rocks was used on samples of Climax granodiorite for the Spent Fuel Test—Climax. A correlation between micro-fracture density and tectonic features was documented with this technique.

With our high-temperature viscometer we have made measurements of the rheological properties of Kilauea Iki basalt under controlled oxygen fugacity at temperatures to 1250°C. Activation energies for viscous flow over two temperature ranges have been reported.

We improved our ultrasonic velocity measurement system to obtain simultaneous measure-

ment of both P and S wave velocities to 1.0 GPa in six directions. The measurements were performed on Mesaverde sandstone for the unconventional gas program.

We have measured fluid permeability, electrical resistance, capacitance, and ultrasonic velocity of rocks to 5.0 MPa and 140°C. A report on results for Topopah tuff found differences in all these properties between fractured and unfractured samples.

Our diamond anvil cell has been used to measure pressure/volume of actinides to the megabar range. Our rotating anode x-ray source has significantly reduced the time required for such studies. We have also demonstrated the feasibility of doing positron annihilation studies in the diamond anvil cell. A new electrical resistance measurement technique has been developed and the resistance of several metals measured.

Simultaneous measurement of electrical conductivity and Seebeck coefficient in olivine to temperatures of 1500°C under controlled oxygen fugacity indicates that a change in charge carrier occurs around 1400°C. The variation of conductivity as a function of oxygen fugacity at 1200°C has been interpreted as an indication that conduction at this temperature is via small polarons.

We have measured, to 500°C and 200 MPa at strain rates from 10^{-3} to 10^{-7} s^{-1} , the creep of salt samples doped with known impurities. Our results show that impurity levels can account for the observed differences in creep behavior of natural salts, and that small amounts of such impurities can increase the stability of underground openings by factors up to 10^{10} . This work demonstrates the way in which experimental work can have an impact on significant national problems, such as radioactive waste management and the strategic petroleum reserve.

For 40 years, ever since the first nuclear reactor was started, high-level radioactive waste has been accumulating. The debate over what to do with these wastes has been going on for almost as long. The Department of Energy has indicated that construction of the first nuclear waste repository could begin in 1993. One of the geologic mediums under consideration for long-term isolation of high-level reactor waste is deeply buried rock salt. Bedded and domal salt deposits have survived hundreds of millions of years, so they presumably will endure a few thousand years more. Furthermore, because rock salt is weaker and

more ductile than most other rocks, cracking would be suppressed in the repository region because any voids would tend to heal (fill back in) rather than grow larger.

However, the Nuclear Regulatory Commission requires that any proposed method of waste management include a provision for retrieving the waste canisters for at least 50 years after emplacement. Hence, it is vitally important to be able to accurately predict how fast underground workings in rock salt will close. There is wide disagreement among different investigators over the rheological behavior (time-dependent flow under stress) of salt.

We have been investigating the possibility that the origin of this disagreement may lie in the variable composition of natural rock salt. Upon mechanical testing and chemical analysis, we found that salt from most sources was relatively pure and weak, with less than 0.01% each of potassium and magnesium. However, salt from two sources had about 0.1% of potassium and about 0.6% of magnesium, respectively; and were two to three times stronger than pure salt. Studies on metals and ceramics suggest that the strength of rock salt might be strongly influenced by such relatively minor impurities.

To investigate the effects of such trace concentrations of cations on the strength of salt, we prepared synthetic samples using pure chlorides of sodium, potassium, and magnesium. In this way we avoided the inclusions and other defects likely to be present in natural rock salt which might have interfered with our measurements. When we examined the rheological behavior of these samples at ambient to moderate temperatures, the results were strikingly different from those for pure sodium chloride (Fig. 1).

Translated into a practical example, these results show that, at normal temperatures, a cavern mined at a depth of 850 m in rock salt containing 0.6% of magnesium would close up 10 million times more slowly than a similar cavern in pure salt. For salt containing 0.1% of potassium, the

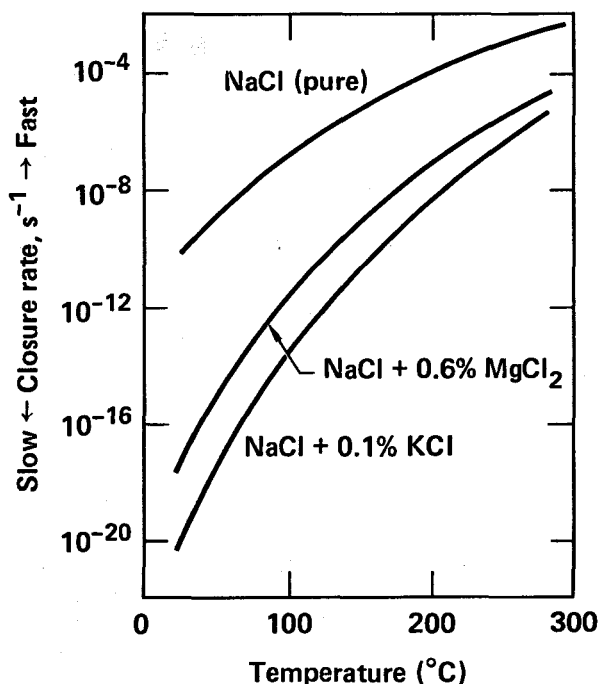


Figure 1. Closure rates (logarithmic scale) for cavities in salt at depth with various levels of impurities. Pure sodium chloride deforms relatively quickly, but minor amounts of magnesium or potassium chlorides can slow deformation by a factor of as much as 10,000 at 200°C and 10,000,000,000 at room temperature.

corresponding figure is 10 billion times slower. At a temperature of 200°C, about the highest repository temperature envisioned, the corresponding rates are 1000 and 10,000 times, respectively.

On the basis of these results, it appears vitally important to repository design and operation to determine exactly what kind of salt is present in any proposed location, and to design with that salt's particular properties in mind rather than to rely on measurements that may have been performed on a quite different material.

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Fossil Energy Group

Present energy projects include research in oil shale retorting, the granular flow of solids, production of gas from unconventional gas reservoirs, and technical assistance to INTEVEP, the National Venezuelan Oil Company. These projects are operated in close cooperation with other departments as well as with other groups in the Earth Sciences Department. As is customary at LLNL, each project is led by a project leader, and participants include members from other departments as well as other groups in Earth Sciences (in addition to those in the Fossil Energy Group).

Research in oil shale retorting has been a major program in the department for about a decade. We are active in mathematical modeling of the chemical and physical processes important in retort processes, in research on the chemistry of oil shale and shale oil, and in experimental operation of retorting processes. Contributions in these areas and in improved concepts for retorting are helping to advance the technology for producing liquid fuel products from the nation's vast oil shale deposits.

The granular flow of solid material has broad application of interest to the earth sciences in the

areas of soil mechanics, landslides and avalanches, and sedimentation. It has even broader applications in industry wherever granular solids must be moved or processed. Mathematical modeling of particle interactions is becoming practical with advances in computer technology, and promises to bridge the gap left by limitations in our ability to measure interparticle forces and other properties essential for advancement of the science. Our efforts in mathematical modeling of granular material are at the forefront of this exciting new science.

The study of the production of gas from unconventional reservoirs is led and carried out in the Geotechnical Group and includes research on western gas sands and on eastern Devonian shale. See the Geotechnical Group section for more information on this subject.

INTEVEP, the research arm of the Venezuelan national oil companies, is engaged in a cooperative program to study subsidence related to production of oil from their oil fields.

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Seismic Monitoring Research Group

Introduction

The Seismic Monitoring Research Program (SMRP) uses LLNL's seismic expertise, geological and seismological data bases, and classified national defense and intelligence information in selected projects designed to verify compliance with test ban treaties, interpret intelligence data, and support DOE personnel as they participate in the formulation of arms control agreements and treaty negotiations.

During 1984 the program was responsible for the following projects, each discussed in more detail:

- Evaluation of the Regional Seismic Test Network (RSTN);
- Array design and signal processing efforts;
- Analysis of source and path effects on regional seismic signals;
- Analysis of data from foreign sites;
- Systematic analysis of Comprehensive Test Ban Treaty issues.

Evaluation of the Regional Seismic Test Network

A key provision of the seismic verification of a comprehensive test ban treaty is the use of networks of in-country seismic stations. To ensure the ability of the U.S. to install and operate such a network within the Soviet Union, the Department of Energy has installed and is maintaining the Regional Seismic Test Network (RSTN). We have carried out seismological studies designed to test engineering aspects of the system and we are examining the detection, location, and capabilities of the network.

In Fig. 2 we show a technique we used to determine the crustal structure beneath the RSTN stations. We took advantage of the fact that transitions between the crust and upper mantle have frequency-dependent effects. Sharp transitions affect long- and short-period waves equally, whereas gradual transitions have a greater effect on shorter period waves. Panels a-c in Fig. 2 show calculations of the effect of a gradation in the shear wave velocity on the amplitude of the shear wave (P_s), which is generated by conversion of a compressional wave striking the base of the crust

from below. The effects of increasing thickness of the transition region are shown. Panel d in the figure gives the observations at Cumberland Plateau, TN. These indicate a transition zone between 5 and 10 km thick at the base of the crust at that station.

Array Design and Signal Processing Efforts

Effective monitoring of a comprehensive test ban will require the detection, location, and identification of the sources of small seismic signals. Using these small seismic signals requires extending the present envisaged network of in-country seismic stations to include seismic arrays or other instrumentation capable of achieving improved signal-to-noise ratios. Arrays offer significant advantages over simple three-component stations: improved signal-to-noise for detection, discrimination of seismic waves using velocity, and across-the-array estimates of source location made by individual sites.

We have defined an optimal design for an experimental regional seismic array, and have conducted deployments to test our concepts and define site selection criteria and procedures. In the process of doing so, we: (1) developed the geometrical design of the Norwegian Regional Seismic Array; (2) developed effective processing algorithms for array and three-component seismic data; (3) developed an automatic method for calibrating and correcting instrument responses; (4) developed a method using a single seismic phase, R_g , to estimate distance for nearby events with overlapping seismic phases. Using the Tennessee array to detect small NTS events, we demonstrated the considerable improvement that is possible with regional seismic arrays.

Analysis of Source and Path Effects on Regional Seismic Signals

Seismic verification of nuclear test ban treaties requires inferring the source properties from the characteristics of the observed signals. The ideal approach would be to use detailed studies using sources and stations within the Soviet Union. Without access to the Soviet Union, we

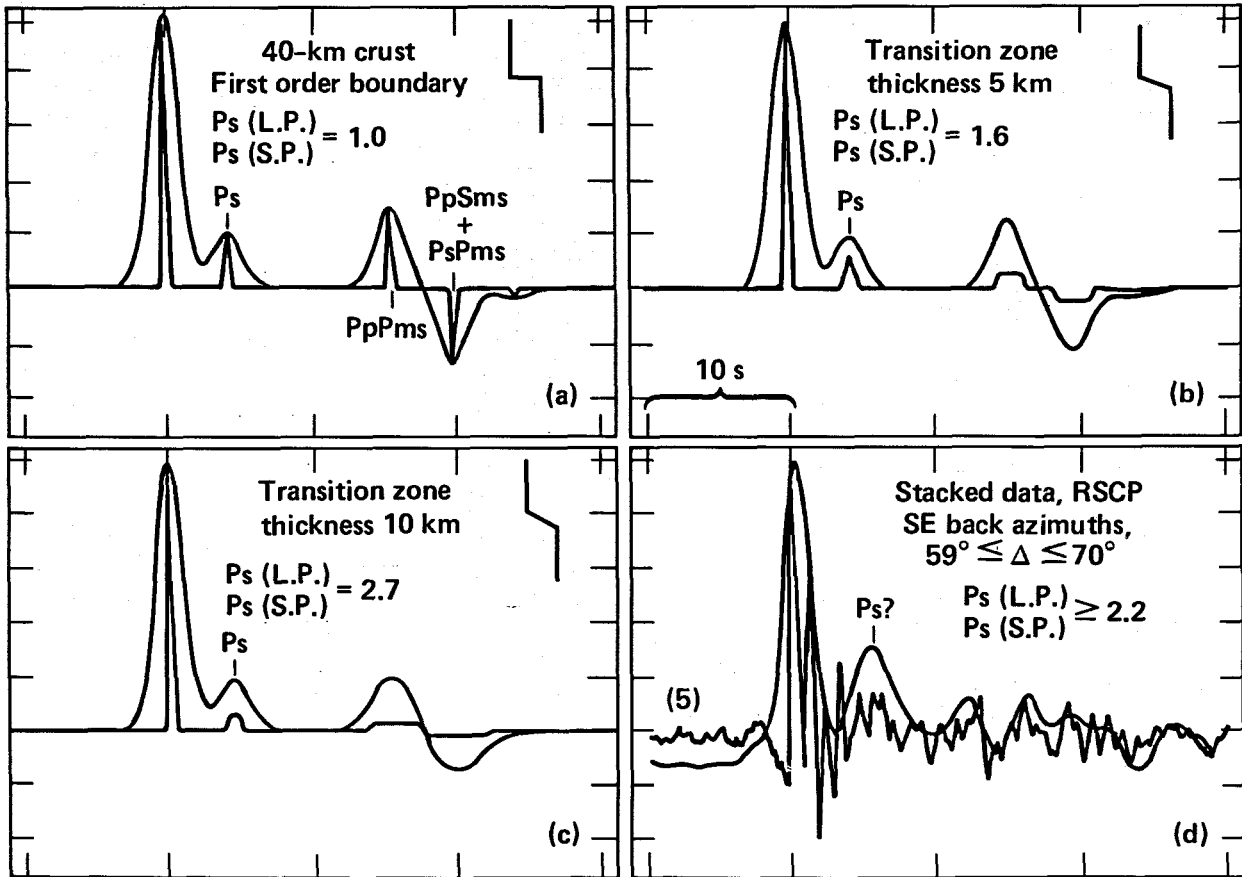


Figure 2. Technique for determining crustal structure beneath RSTN stations.

must isolate the fundamental processes by analyzing U.S. sources and paths and then use this understanding to predict Soviet phenomena.

We have used our close-in and regional recordings of U.S. explosions to examine a variety of phenomena, including variation of free-field, surface ground zero, and regional wave (P_n , P_g , L_g , R_g) amplitudes and energy with different yield and emplacement conditions. We have also measured discrimination parameters for NTS explosions. In addition, we have studied the reversal of Rayleigh wave polarity seen from some Soviet explosions.

Studies of Soviet Explosions and Geology

We have gathered selected subsets of the information available and attempted to develop a view of Soviet geology and test practices. Two

projects in 1984 addressed specific issues related to the current Soviet test program, while two additional studies described important geological and geophysical properties needed to estimate monitoring capabilities within the Soviet Union. These studies drew upon expertise developed during research carried out within the previous sections.

Systematic Evaluation of Comprehensive Test Ban Treaty Issues

Finally, we have attempted to develop a framework for evaluating decisions related to the design and development of a regional seismic verification system for verifying a Comprehensive Test Ban Treaty. The framework stipulates both a logical and an analytical approach to: (1) evaluating these systems; (2) determining their benefits to

the verifier, and (3) assessing their deterrence effect on a potential evader. These results can be used to examine decisions for Regional Seismic Verification System design, and to evaluate alternate strategies for treaty negotiations and their influence on research and development.

We have developed an initial framework in some detail. For demonstrations the framework is implemented as a highly aggregated model on a microcomputer. We plan to reference the model and exercise it using input data provided by technical experts from LLNL and other organizations.

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Containment Group

Introduction

Complete containment of radioactive debris from underground nuclear testing at the Nevada Test Site is the primary goal of the Containment Group. Group members must understand the complex phenomena resulting from the nearly instantaneous release of a great amount of energy in a nonhomogeneous, geologic setting. Each proposed site is carefully studied to determine material properties and geologic structure. The drill holes, which are 8 ft or more in diameter and 600 to 2100 ft deep, are studied using special geophysical logging tools developed for use at NTS. The geologic structure is deduced using numerous surface exploration measurements as well as borehole data.

The explosive device to be tested and its associated diagnostics hardware are evaluated, and a safe location and depth-of-burial are chosen. A stemming design—the plan for materials to be used to backfill the hole after hardware emplacement—is developed, as are diagnostics to determine the behavior of containment features and the phenomena related to the interaction of the explosion with its environment.

The group interacts strongly with the Geotechnical Group, where we maintain our phenomenological computations capability, with the Geochemistry/Geology Group, where we obtain structural geology support and x-ray diffraction analyses; with the Seismology/Applied Geophysics Group, where we obtain exploration support, especially seismic surveying; and with the Experimental Geophysics Group, where we obtain the mechanical properties of geologic material. There is also considerable interaction with other parts of the Laboratory outside the Earth Sciences Department, particularly with Nuclear Test Engineering Division, L-Division, Nuclear Chemistry, and the LLNL-Nevada personnel.

The Containment Group is primarily program-oriented and is responsible for managing and coordinating numerous outside activities related to specific tests and R&D, including liaison with the U.S. Geological Survey, the Los Alamos National Laboratory, and several contractors.

Work within the group is diverse, but three functions are concentrated in the group: maintaining the data bank, analyzing diagnostics data, and serving as containment scientists.

Data Bank

The Test Program Data Bank includes statistical data related to drill hole geophysical logs, material properties, and nuclear event parameters. The three classes of information are presently in separate data bases, but they are in the process of being collected in a single data base in a new Containment Program VAX computer. Maintaining, updating, and using the enormous amount of data we have gathered is a major project.

Diagnostics Data

Diagnostics data analysis starts with consideration of the phenomena to be studied and design of the appropriate data gathering system, a job that often involves R&D work in transducer development and calibration. One such project, stress measurement, will be treated in more detail. The data are recorded and digitized by EG&G personnel, and then must be reduced and correlated. Finally, the data are analyzed by comparing records with other data channels, with calculational results, and with results from previous tests to develop a coherent picture of the phenomena in question.

The stress measurement project has been an important part of diagnostic data analysis. During the past decade, an important criterion for the containment of underground nuclear explosions has been the formation of adequate residual hoop stress in the region surrounding the cavity. Using the TENSOR* code, Terhune[†] showed that for an adequately buried explosion in material of typical shear strength (20–100 bars), one should expect a residual hoop stress higher than cavity pressure throughout the volume between one and two cavity radii from the explosion point. In practice,

* A two-dimensional Lagrangian hydrodynamic code that includes the constitutive relations necessary for modeling the response of rock and soil. D. F. Burton, L. A. Lettis, Jr., J. Bryan, and N. R. Frary, *Physics and Numerics of TENSOR Code*, Lawrence Livermore National Laboratory, Livermore, CA, UCID-19428 (1984).

[†] R. W. Terhune, *Analysis of Burial Depth Criteria for Containment*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-52395 (1978).

where geologic features or material properties are somewhat unusual, a TENSOR calculation has been used to predict the stress history and particle motion around the cavity. The adequacy of the site is then determined based on these predicted results. Since there have been no prompt ventings of cavity gases during the past decade, this use of the residual hoop stress concept appears to be conservative. However, the detailed validation of the concept and calculational tools requires the actual measurement of stress and particle motion within the region of interest. For typical explosions at the Nevada Test Site, the near-cavity stress levels of interest are expected to range from tens to hundreds of bars. Consequently, some effort has been dedicated to the development of a stress gauge that would allow the measurement of stresses up to about one kilobar.

The principal problems to be solved appeared to be cable survival, gauge-to-medium coupling, and gauge deformation. Considerable progress has been made in all three areas. Survivability has been enhanced by minimizing cable-gauge interface discontinuities and the use of stretch cable. Coupling effects are being addressed by precasting the gauge elements in material similar to that in which the measurement is to be made. The gauge deformation problem is being addressed by the use of both stress- and strain-sensitive material in the same package such that stress element deformation can be accounted for. In addition, the gauge element is encapsulated in a fluid cavity to minimize strain.

Typical gauge configurations are shown in Fig. 3. Ytterbium is used as the stress-sensitive material with some sensitivity to strain; constantan is used as the strain-sensitive material. Figure 4 shows the results from gauges of this type used in a recent nuclear test. The gauges were located in a gypsum-concrete stemming plug, approximately two cavity radii above the explosion point, and appear to have given quite reasonable data. Detailed calculations have not yet

been performed to relate these results to specific predictions. The peak measured value for radial stress (0.62 kbar) is somewhat more than scaling* would predict (0.4 kbar). The tangential residual stress (140 bars) is within the expected range, 3.2 times overburden (43 bars). Similar gauges have been fielded on two other events of somewhat higher yields. However, these gauges failed before measuring residual stress.

Future efforts will be directed toward survival at higher yields and/or stress levels and measuring both radial and tangential stress at the same point.

Containment Scientists

The role of containment scientist is a demanding one, requiring synthesis of information from many sources into a single, comprehensive document, the Containment Prospectus, which discusses the pertinent features of each event, the containment design and the rationale for it, the expected phenomena, and the provisions for treating the unexpected. The Containment Prospectus is distributed throughout the test program, but in particular, to the Containment Evaluation Panel (CEP), an advisory group to the Manager of the Nevada Operations Office of the Department of Energy. A formal presentation is made to the panel, which must be convinced that the design is one that will lead to satisfactory containment. A successful presentation to the panel is an exceedingly important part of the Test Program, since permission to conduct an event depends on concurrence by the CEP.

* T. R. Butkovich and A. E. Lewis, *Aids for Estimating Effects of Underground Nuclear Explosions*, Livermore National Laboratory, Livermore, CA, UCRL-50929, Rev. 1 (1973).

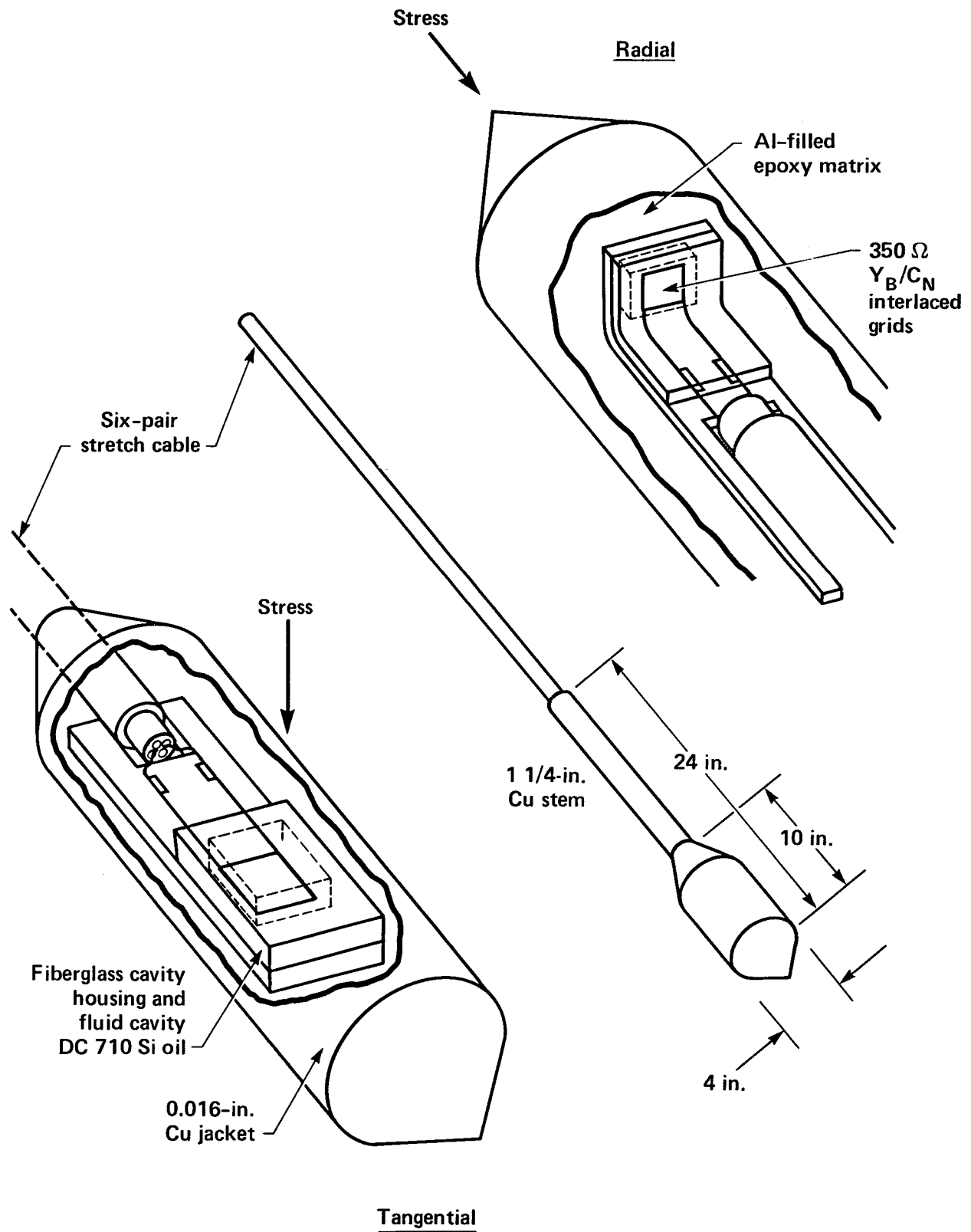


Figure 3. Torpedo stress gauge configuration.

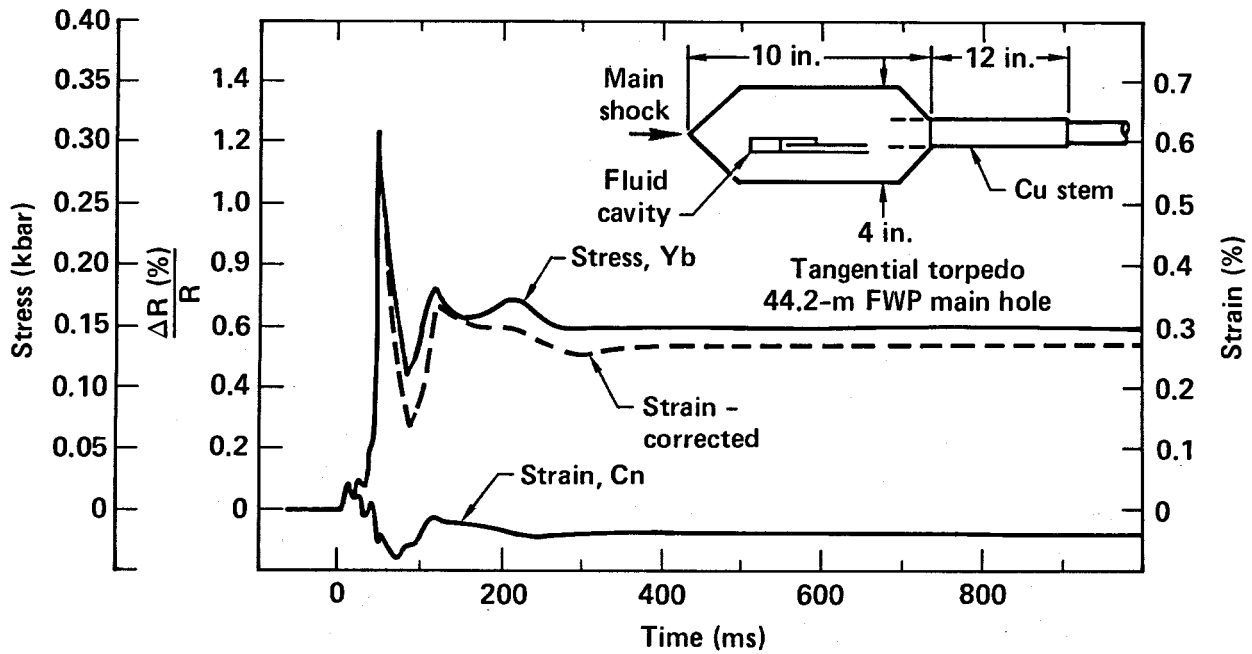
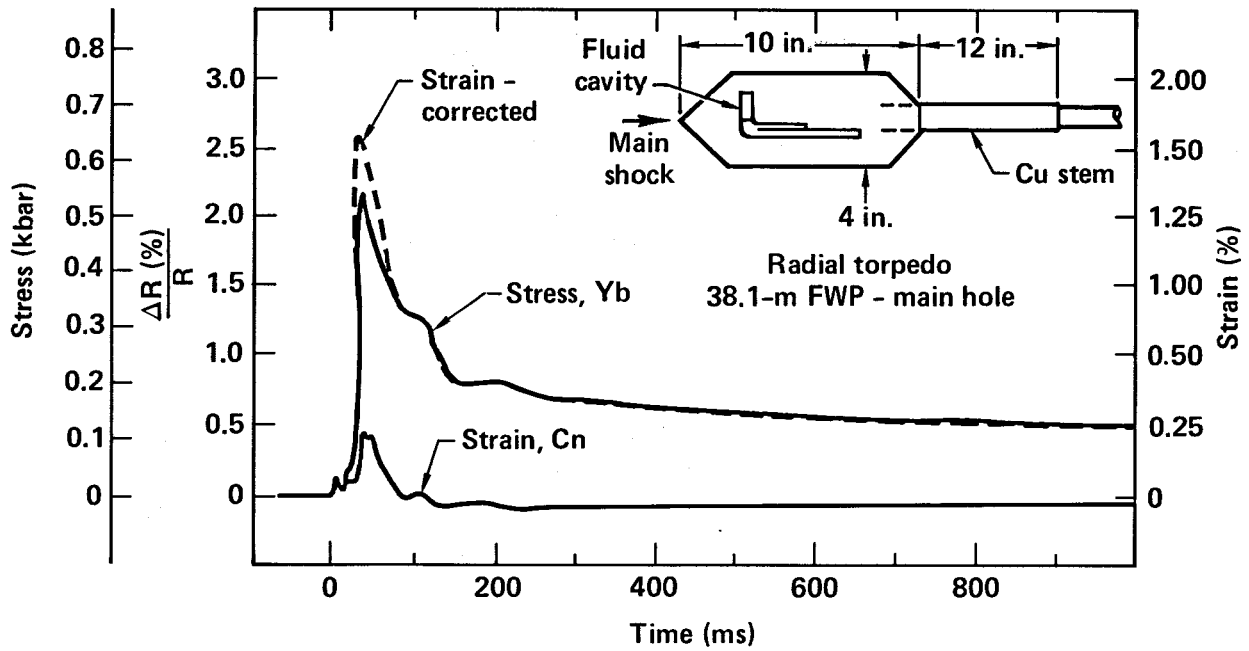


Figure 4. Stress gauge data.

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Waste Management Group

Introduction

The function of the Waste Management Group in the Earth Sciences Department is to provide technical leadership for research and development projects in nuclear and hazardous waste management (the responsibility for actual disposal of LLNL-generated waste lies elsewhere at the Laboratory). All of the group members lead elements of ongoing waste management programs.

Current projects led by the group are in the area of high-level nuclear waste. In the past, there have been low-level nuclear waste projects, and we anticipate hazardous chemical waste projects in the near future. In FY 1984, group members were responsible for projects totaling approximately \$10 million.

During 1984 the majority of the work in the group was sponsored by the Office of Civilian Radioactive Waste Management (OCRWM), and most of that falls within the Nevada Nuclear Waste Storage Investigations (NNWSI). For NNWSI, there are three major projects: Spent Fuel Test—Climax, Waste Package for a Tuff Repository, and Geochemical Modeling. The first two of these are large, interdisciplinary projects involving other departments at the Laboratory as well as numerous subcontractors. The third is a discipline-oriented activity funded by the Waste Management program. In addition, because these projects deal with hazardous nuclear and nonnuclear material, formal quality assurance is a significant group activity. A brief description of the three major programs follows.

Spent Fuel Test—Climax

Beginning in 1978, LLNL designed a test in which a limited number of actual spent fuel assemblies from a commercial nuclear reactor were safely packaged, transported, stored, and retrieved. This generic test was conducted 1380 ft below the surface in the Climax granite stock at the Nevada Test Site.

During April and May of 1980, 11 canisters of spent fuel were emplaced in a storage drift along with 6 electrical simulator canisters. Two adjacent drifts contained 20 electrical heaters, which were operated so that the rock within a repository-model cell of 50 ft by 50 ft was subjected to the thermal

history it would have in a large repository. In addition, each end of the storage drift had six locations where both spent fuel and electrical simulators were interspersed. Within that area, a comparison can be made between the effects of heat alone (electrical simulators) and the effects of heat plus radiation (spent fuel). During March/April 1983, the spent fuel assemblies were retrieved and returned to a surface storage facility at the Nevada Test Site.

Temperatures, stresses, and displacements were monitored continually at more than 750 locations underground before and throughout the 3-year emplacement period and for 6 months after withdrawal of the fuel. Through September 1983, a total of 8.7 million data points were stored on magnetic tape. From test inception to present, more than 8500 visitors have toured the facility in more than 500 tours, with 23 foreign countries being represented among the visitors.

During 1984, post-test calibration and rock monitoring studies continued in the field, and post-test evaluations were carried out at Livermore. During 1985, numerous topical reports and a comprehensive final report on this \$30 million project will be issued. To date, more than 80 LLNL reports have been issued, along with 15 reports by contractors or other agencies. In addition to providing a graphic demonstration to the public of the safety and relative simplicity of handling highly hazardous radioactive material in an underground repository environment, this test also established a significant data base of the physical effects of underground storage of nuclear material. Many improvements were also made in the techniques of monitoring and evaluating the response of rocks to the thermal changes induced by the spent fuel storage.

For the past several years, the Office of Crystalline Repository Development has provided funding for LLNL to transfer data and technology obtained in the Spent Fuel Test—Climax to the Atomic Energy of Canada, Limited, for use in the development of their Underground Research Laboratory near Pinawa, Manitoba. This has included designing, modifying, and evaluating instruments used in the underground environment of the Spent Fuel Test—Climax, as well as consulting on and reviewing Canadian plans based on experience with the project.

Waste Package

LLNL has been assigned responsibility for developing a waste package for storing high-level waste in a repository in tuff at Yucca Mountain near the Nevada Test Site. The following two performance objectives for such a waste package are set forth in the Nuclear Regulatory Commission's rules 10CFR60, entitled "Disposal of High Level Radioactive Waste in Geologic Repositories": (1) a waste canister that will contain the waste within the canister for a time period of 300 to 1000 years, and (2) a waste form that will restrict release of radionuclides into groundwater to no greater than 1 part in 100,000 of the radionuclide inventory per year for 10,000 years. To attain these objectives, the waste package task is organized into the following areas:

- Environment in which the waste package will perform;
- Materials selection and characterization (e.g., metallic barriers, waste form, other materials);
 - Waste package design;
 - Performance assessment;
 - Confirmatory field testing.

In 1984 with a budget of about \$6 million, research was conducted by the Earth Sciences, Mechanical Engineering, and Chemistry and Materials Science Departments; the Nuclear Chemistry Division; and outside contractors including the U.S. Geological Survey, Westinghouse Hanford Engineering Development Laboratory, Argonne National Laboratory, and Battelle Pacific Northwest Laboratory. A cooperative test program was also carried out with the Savannah River Laboratories for defense high-level waste.

Some of the near-future technical milestones scheduled for the waste package task are as follows:

- Environment: evaluate the stability of the emplacement holes (September 1985); establish a reference waste package environment (January 1986).
- Materials: provide a preliminary estimate of the release rate of radionuclides from all waste forms (December 1985); decide on the need for a packing material for control of release (March 1986); and make a final selection of a metal barrier material (October 1987).
- Design: develop advanced conceptual waste package prototype designs (April 1986).
- Performance assessment: complete revision and testing of a waste package system model (March 1986).

- Field testing: complete field test hardware for underground waste package environment tests at Yucca Mountain (September 1986).

By March 1989 we will have developed a tuff waste package design suitable for submittal to the NRC for a license application. By January 1990 we will have a final definition of the radionuclide source term expected from a waste package in the Yucca Mountain environment.

As noted earlier, all of this work is to be carried out under a quality assurance program similar to that in place for the design and construction of commercial nuclear power plants.

Geochemical Modeling Code EQ3/6

The code EQ3/6 is a set of related computer codes that represents the state of the art in geochemical modeling of aqueous solutions. EQ3NR calculates, from water sample analyses, the distribution of ions, ion-pairs, and complexes, and determines whether the water sample is saturated with various minerals. EQ6 calculates dynamic models of rock/water interaction; that is, minerals and other phases can be added to a chemical system such that the state of a new system is predicted. Both codes assume that chemical equilibrium controls most reactions. Although the codes offer a limited ability to handle kinetics, it is insufficient for dealing with complexities that will likely be encountered in a nuclear waste repository.

During 1984 we began to carry out a plan that will upgrade the EQ3/6 code package and supporting data base to allow modeling of chemical processes to determine their relative contribution to the potential transport of radionuclides in groundwater from a nuclear waste repository. The improvements carried out were the completion of a model for systems open to gases (i.e., a fixed-fugacity model); addition of precipitation kinetics to the EQ6 code; addition of a graphics post processor to EQ6, expansion and revision of the data base; and completion of the code documentation with EQ6 and MCRT users' manuals. Future activities include extending the precipitation kinetics model in EQ6; continual upgrading of data base and data base management programs; adding an equilibrium sorption model and supporting data base; and starting a glass/water interactions model. Numerous other improvements are possible over a longer time frame, but many of these will be more evident as the code is further applied to practical problems.

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Geotechnical Group

Introduction

The Geotechnical Group is chartered to provide expertise to programs in the hydraulic, mechanical, and thermal behavior of geologic formations (rocks and soils). This entails primarily geomechanics, some geology, and some geophysics.

The group supports all major Earth Sciences programs (Basic Energy Sciences/Base Technology, Containment, Fossil Energy, Institutional Research, Treaty Verification, and Waste Management), and several additional projects outside of Earth Sciences Department such as Test Program/High-Energy-Density Facility (HEDEF), and Defense Nuclear Agency (DNA) Ground Motion Research. It also provides support to the intelligence community. In all, the geotechnical group has about 20 projects split almost evenly between the

defense and energy areas. Figures 5 and 6, respectively, illustrate a defense and an energy project.

Group Organization and Capabilities

The Group is organized into four teams:

- Ground motion and cratering,
- Solid and wave mechanics,
- Fluid mechanics,
- Engineering geology and geohydrology.

The ground motion and cratering team performs numerical and analytical modeling of nuclear (NE) and high-explosive (HE) tests in terms of ground and surface (crater) effects. It is also responsible for determining the hydrodynamic behavior of geologic materials, doing high-temperature, high-pressure equations of state (EOS), and providing shock modeling.

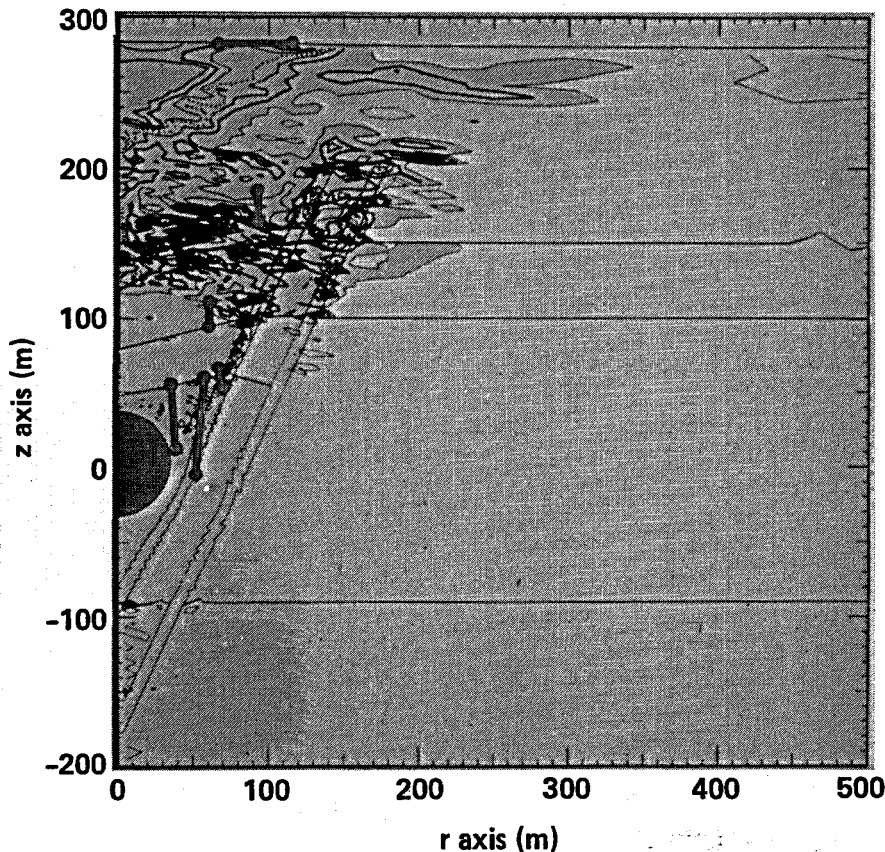
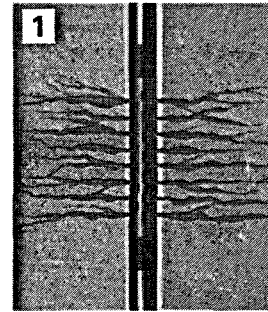
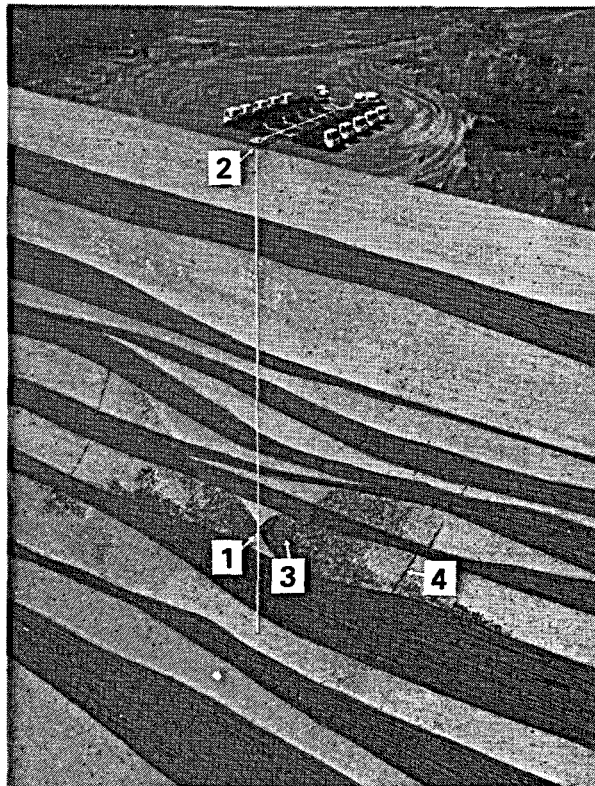
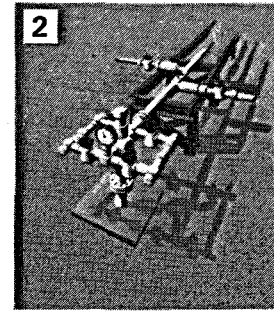


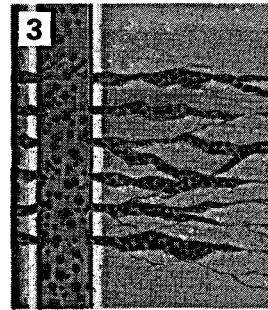
Figure 5. Example of a defense project supported by the Geotechnical Group: calculating the containment of underground nuclear explosions.



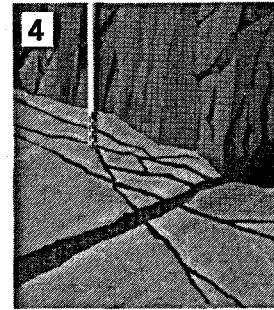
1
Packers set, and casing perforated



2
Controlled fluid flow and pressure



3
Propping agents keep vertical cracks open against tectonic stress



4
Fracture propagation controlled by bedding planes, joints and tectonic stress

Figure 6. Example of an energy project supported by the Geotechnical Group: researching the stimulation of tight gas reservoirs by hydraulic fracturing.

The solid and wave mechanics team provides analytical and numerical studies of the response of geological materials, structural materials, and geological structures to static and dynamic loading. The team is also responsible for rock fracture mechanics, *in situ* testing of rock mass stiffness and strength, physical and kinematic modeling of geological structures, and design of rock structures (mines, pits, shafts, tunnels).

The fluid mechanics team studies fluid flow and transport in continuous and fractured media, provides coupled fracture and flow capabilities and has expertise in reservoir stimulation and production analysis.

The engineering geology and geohydrology team provides geological field mapping, field testing for *in situ* deformations and stresses, hydraulic tests in wells and boreholes, thermal testing of rock masses, subsidence studies, and geomechanics instrumentation development.

Defense and Energy Projects

The Geotechnical Group supports several defense-related projects, including providing containment calculations and research for the Containment Program sponsored by the Earth Sciences Department. The project comprises collapse, gas flow, subsidence, and wave propagation studies. Nonseismic yield evaluations are also provided for the Verification Program of the Earth Sciences Department.

The group also supports other defense-related projects not sponsored by the Earth Sciences Department. These include cratering calculations for the Defense Nuclear Agency; hard-target modeling for LLNL's Weapons Division; and multistage conventional munitions, cavity decoupling, and energy security for various LLNL programs. In addition, the group is studying a

high-energy-density facility for LLNL and is providing shock tracking for the Army Research Office.

With the exception of hydrologic site contamination studies performed at LLNL for LLNL, all of the energy-related projects supported by the Geotechnical Group are sponsored by the Earth Sciences Department. These include tuff waste package and geotomography studies as well as investigations into the feasibility of a Canadian Underground Research Laboratory for the Waste Management program. The Fossil Energy/Gas program is also conducting research into western gas sands and eastern Devonian shale. Finally, the Institutional Research program is doing studies of energy flow and transport.

Summary

The Geotechnical Group offers an expert and diversified mix of engineers and scientists working closely with each other. Their combined expertise covers the areas of field testing, laboratory experiments, and computer simulation of mechanical, hydraulic, and thermal processes in geologic media. They support all major defense and energy programs of the Earth Sciences Department as well as several projects in other divisions of LLNL. The attached list of their publications (more than 50 in 1984 alone) attests to the productivity of the group and its relevance to LLNL's mission.

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Seismology/Applied Geophysics Group

Introduction

The Seismology/Applied Geophysics (SAG) Group has interests and capabilities that span a spectrum from theoretical to experimental studies, from field to laboratory environments, and from "back of the envelope" to computer analyses. A wide variety of geophysical applications can be addressed by the SAG Group because it emphasizes a multidisciplinary approach. The general areas of expertise include regional crustal tectonics and structure; detailed microearthquake/aftershock analyses; strong-motion seismic studies; seismic processing, analysis, and interpretation; general geophysics and geology; borehole geophysics; logging tool design; geostatistical studies; and laboratory measurements. In each of these areas, the SAG Group can and does, whenever appropriate, deploy field equipment and collect, process, analyze, and interpret data.

The SAG Group uses the capabilities to support many programs and projects throughout the laboratory, including the Seismic Monitoring Program, the Nuclear Test Containment Program, the LLNL Site Seismic Program, the Nuclear Waste Management Program, the Unconventional Gas Program, and the Basic Energy Sciences Program.

Seismology Studies

We routinely use our seismological expertise to study crustal structure and tectonics. To carry out these studies, we can design, deploy, process, and interpret seismic data from surveys using manmade or natural seismic sources. The SAG Group has experience with seismic arrays ranging from the very small to the very large. The SAG Group has the capability and resources to process and catalog large volumes of digital seismic data. From these data sets, we are able to determine structure by inversion of the P, S, and surface wave data. These inversions lead to models that address issues related to three-dimensional structure, seismic source mechanisms, microseismicity, and regional geology and tectonics.

Applied Geophysics

For problems addressable with applied geophysical exploration techniques, we use electrical,

gravity, magnetic, well logging, or seismic techniques. We take pride in the effort we make to determine (whenever possible, before data collection) whether or not a particular geophysical technique will address the particular problem at hand, and careful attention is given to the special characteristics of each problem. The measurements we make can address problems whose scale ranges from laboratory size, to engineering dimensions, to large regional pictures. Although we routinely address problems using standard techniques, we can develop unique state-of-the-art geophysical tools and/or techniques whenever the problem or project is best accomplished by these developments.

Computerized Data Collection

In all areas, the SAG Group uses, when appropriate, state-of-the-art computer equipment for data collection, processing, and analysis. These computer facilities enable the SAG Group to gather and process high quality digital data, and to model numerous geophysical or seismological situations. The Seismic Analysis Code (SAC) can process seismic data quickly with a great deal of analytical diversity. Numerous codes have been developed to model seismic, electrical, gravity, and logging data. Codes for synthetic seismograms, density log calibrations, geostatistical evaluations, seismic and gravity inversion, seismic scattering and waveform analysis have been developed.

The following section summarizes work done for the Basic Energy Sciences Program on the Q-structure of the Basin and Range from surface waves. Many of the tools described above were employed.

Q-Structure of the Basin and Range from Surface Waves

The Basin and Range of the western United States is characterized geophysically by thin crust, extensive normal faulting, low seismic velocities in the crust and upper mantle, high heat flow, and recent volcanic activity. In total, these characteristics and plate tectonic considerations constitute strong evidence for a major tectonic rift zone covering a large area of the continental lithosphere.

Studies of the seismic wave velocities in the Basin and Range have indicated the presence of a pronounced low-velocity zone in the upper mantle. In addition, it is well known that the attenuation rate of seismic waves is significantly greater in the western United States than in the eastern United States. Studies of Q as a function of depth have found evidence for a low Q -zone in the upper mantle of western United States. However, there is still considerable uncertainty about Q in the crust and upper mantle of the Basin and Range itself. Study of seismic-wave attenuation within this geophysically distinct region should provide further details about the nature of the low Q -zone. Such details and correlations of attenuation measurements with other geophysical data are important for evaluating possible mechanisms of energy dissipation in the earth. With this in mind, we have undertaken a study of the surface-wave attenuation in the Basin and Range.

Regionalized Rayleigh- and Love-wave attenuation coefficients have been measured across the Basin and Range province of the western United States using the methods of Tsai and Aki (1969) and Yacoub and Mitchell (1977) modified to work on any number of events simultaneously. The epicenters of the events and paths used in this study are shown in Fig. 7. The events consist of six earthquakes and one explosion for which there are reliable information about the source mechanisms and depths. The stations belong to the World-Wide Standard Seismograph Network, and the paths shown in Fig. 7 are for Rayleigh waves that left the sources on azimuths well away from nodes in the radiation pattern. Similarly, we selected Love wave data that avoided complications due to nodal planes.

We divided the western United States into two provinces for the purpose of estimating regional attenuation coefficients. The boundary between the two provinces shown in Fig. 7 was determined by the 1.5 heat-flow unit contour from the energy flux map of Blackwell (1978). Using the relationship between attenuation coefficient and Q , $\eta = \pi/QUT$ where U is group velocity and T is period, we calculated Rayleigh- and Love-wave Q -values, Q_R and Q_L , respectively. The regionalized Q_R are significantly lower than previous measurements for frequencies below 0.08 Hz. This is also the frequency range where regionalization made a difference in reducing the residual variance. This result is an indication that Q at depth, possibly in the lower crust and upper mantle, within the Basin and Range is considerably lower than the average Q for western United States.

The Q_L observations at low frequencies show very high values in contrast to the low values for Q_R . Previous measurements of Q_L also show very high values for the frequency range, 0.04–0.06 Hz, and decrease rapidly at lower frequencies (Solomon, 1972). Several studies point out that in certain earth structures, the group velocities of the fundamental and first higher mode Love waves are quite similar for periods of 30–90 s. Due to poor time separation, the first higher mode interferes with the fundamental mode, causing erratic phases and amplitudes. We calculated phase and group velocities of Rayleigh and Love waves for a Basin and Range earth model. The first higher-mode Love-wave group velocities are quite close to the fundamental-mode velocities for frequencies from 0.025–0.035 Hz, whereas Rayleigh-wave velocities for the two modes are separated over the entire frequency range. In the critical frequency range where velocities are similar, the higher mode amplitude is 20 to 30% of the fundamental mode amplitude. The higher-mode amplitudes may be large enough to seriously affect the measurements of Love-wave attenuation considering that, based on Rayleigh-wave decay at low frequencies, we detected a change in amplitude of about 40% or less over a distance of 1000 km.

Because of the possible complications in the long-period Love waves, we restricted our attention to the Q_R and short-period Q_L observations in order to infer the Q -structure of the Basin and Range. We found that Rayleigh-wave attenuation, $100/Q_R$, in the Basin and Range increases gradually from values near 0.5 at 0.12 Hz to values near 0.8 at 0.06 Hz. Below 0.06 Hz, attenuation is clearly greater in the Basin and Range than in surrounding regions, and increases rapidly to values near 2.5 ($Q_R \sim 40$) at 0.025 Hz. These regionalized attenuation values are significantly greater than previous observations of surface-wave attenuation in the western United States, presumably because the previous studies used long path sampling regions outside of the Basin and Range.

Once the Rayleigh- and Love-wave attenuation observations were made, we inverted them for attenuation as a function of depth. We used a number of initial Q -models based on previous studies in the Basin and Range, which generally led to a set of models with similar characteristics. Constant initial models with $Q_a = 325$ and $Q = 150$ were used for all of the inversions. In consideration of observed errors, the results of our simultaneous inversion show that a frequency-independent Q -model is consistent with both Rayleigh-wave and short-period Love-wave

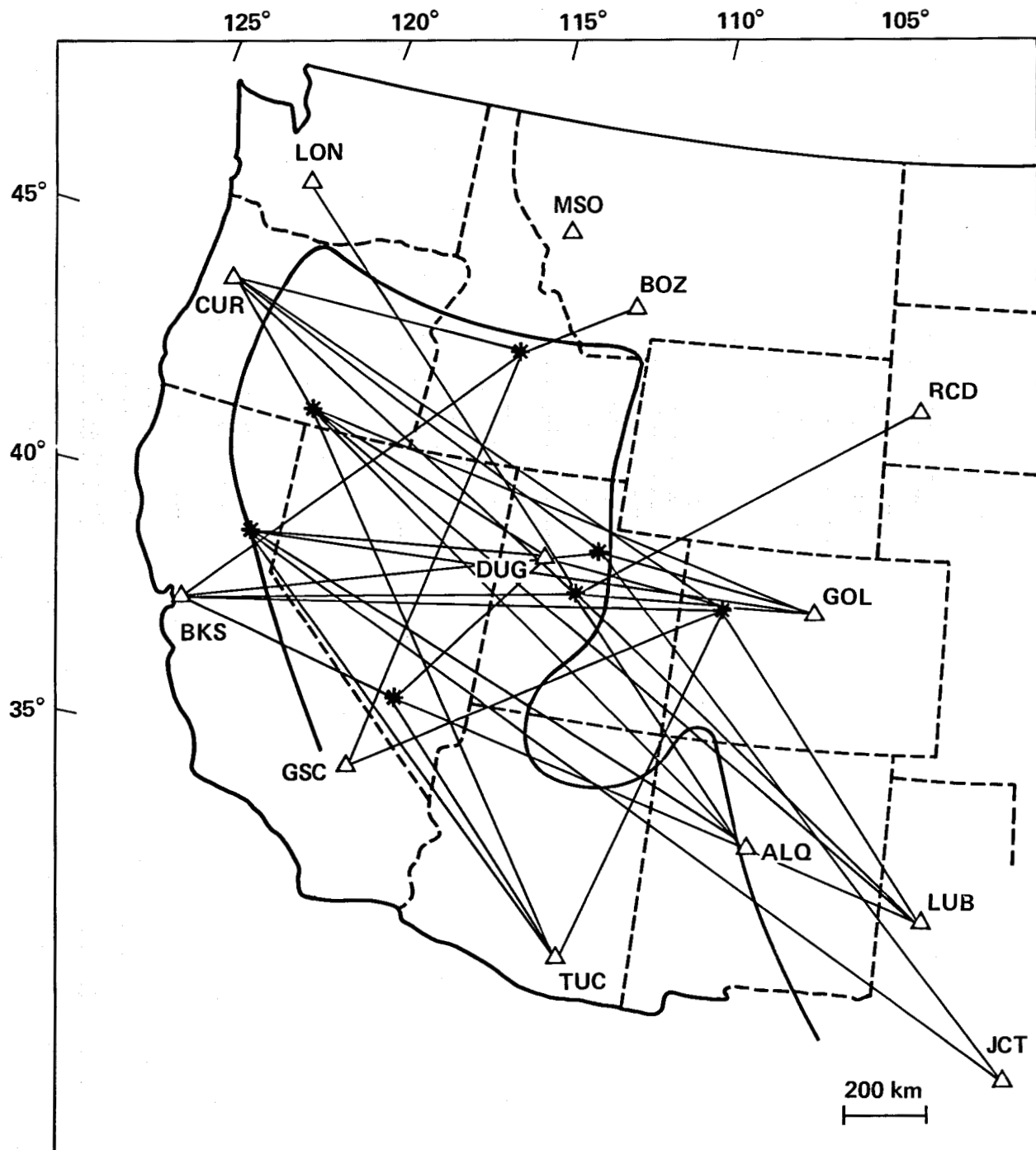


Figure 7. Epicenters (*) of six earthquakes and one explosion studied using regionalized Rayleigh- and Love-wave attenuation coefficients.

attenuation data. The shear attenuation model is characterized by high attenuation in the lower crust ($Q \sim 100$) and increasing attenuation in the upper mantle with maximum values ($Q \sim 30$) below 60-km depth. These results, combined with

resolution plots, allow us to conclude that the top of the highly attenuating upper mantle layer probably lies between 50–70 km. Forward modeling shows that a high Q -lower crust or upper mantle lid is inconsistent with the data. The fit to

the observed surface wave data underestimates the Rayleigh-wave attenuation and overestimates that for the Love waves. A better fit to the observed data might be obtained by allowing for an anisotropic shear-attenuation model (where $Q_{SV}^{-1} > Q_{SH}^{-1}$) or by permitting bulk attenuation. The addition of bulk attenuation to the modeling procedures would increase the calculated Rayleigh-wave attenuation coefficients without affecting those for the Love waves.

Figure 8 shows a comparison of the Q^{-1} model vs a Basin and Range S-velocity structure due to Priestley and Brune (1978) and a range of Basin and Range geotherms from Lachenbruch and Sass (1978). It can be seen that the rapid increase in Q^{-1} occurs at about the same depth as the intersection of the Basin and Range geotherms with the dry basalt melting curve (~ 45 km). This is also the depth at which a rapid increase in electrical conductivity has been observed (Porath, 1971). The shear velocity model based on surface-wave dispersion is characterized by a constant velocity lid with shear velocity of 4.5 km/s and a sharp lithosphere-asthenosphere discontinuity at 65 km. It is important to note, however, the nonunique-ness of this velocity model since recent studies (Sheehan, 1984) have illustrated that structural models with negative velocity gradients in the lid are also consistent with the observed dispersion curves and a sudden jump in velocity is not required. Results of body-wave studies can be found which favor a sharp lithosphere-asthenosphere discontinuity or gradational boundaries, and it is clear that further work is needed on the velocity structure of the Basin and Range. In any case, we believe that the results of this study, particularly the low Q -values required in the lower crust and upper mantle, in conjunction with a host of geophysical evidences suggest that the lithosphere is poorly developed beneath the Basin and Range and that the lithosphere-asthenosphere boundary, whether gradational or abrupt, may extend to the base of the crust.

Because of the numerous attenuation mechanisms proposed in recent years (cf. Mavko et al., 1979), it is difficult to interpret the attenuation models in Fig. 8 without the aid of additional geophysical and geological evidence suggesting the presence of partial melt in the upper mantle (and possibly lower crust) beneath the Basin and Range. However, each observation taken separately can be explained by subsolidus mechanisms or by the existence of only localized melting beneath volcanically active regions. Additional studies are in progress involving a simultaneous inver-

sion of regionalized surface wave phase velocity and attenuation data following the technique of Lee and Solomon (1978). These studies may provide further constraints on physical processes in the Basin and Range and allow the use of predictive models such as those described by O'Connell and Budiansky (1977) to examine the possibility of attenuation mechanisms involving partial melt.

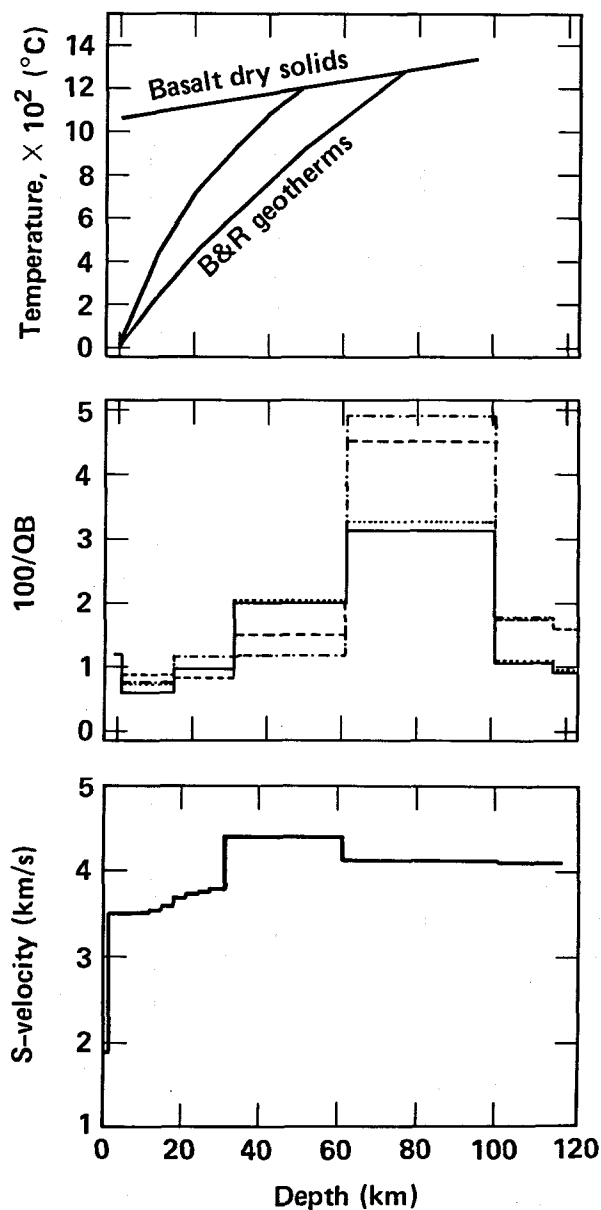


Figure 8. Comparison of Q^{-1} model with a Basin and Range S-velocity structure and Basin and Range geotherms.

Seismology/Applied Geophysics Group Publications

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Geochemistry/Geology Group

Introduction

The Geochemistry/Geology Group consists of geochemists, geologists, and technicians working on a wide variety of projects for several programs and agencies, including Nuclear Waste Management (Waste Package-NNWSI, Spent Fuel Test, Geochemical Modeling-ONWI), Containment (of underground nuclear explosions), Basic Energy Sciences, the NRC, and various LLNL site investigations.

Geochemistry

The geochemists work primarily in low-temperature geochemistry performing rock/wasteform/water interaction experiments (to 350°C, 2 K, i.e., bar); equilibrium thermodynamic/kinetic reaction-path geochemical modeling (code development and application of EQ3/6); experimental measurements of chemical properties of aqueous electrolytes (solubility, density, activity and diffusion coefficients); and material characterization of solids.

Current material characterization facilities under Earth Sciences Department control include computerized quantitative x-ray diffraction (plus several types of powder cameras), a scanning electron microscope with energy-dispersive spectrometry (EDS) capability, sequential inductively coupled-plasma emission spectrometry, a fully automated electron microprobe with three wavelength spectrometers plus EDS, multi-detector alphaspectrometers, and research petrographic microscopes with cathodoluminescence and heating/freezing stage. We have added this year an ion microprobe for secondary-ion mass spectrometry (SIMS) and an infrared (IR) total carbon analyzer, and we have ordered an IR spectrometer. Through other LLNL departments the geochemists routinely do neutron activation and gamma spectrometry analyses, mass spectrometry, and auto- and induced-radiography. In addition, they have access to a transmission electron microscope and a scanning transmission electron microscope. Among the various LLNL analytical groups, state-of-the-art equipment is available for most analytical requirements.

During 1984 the geochemistry group performed several experiments to determine rock

(tuff)/water interaction using Dickson-type gold-bag rocking autoclaves, cold-seal bombs, and flow-through cells. We also conducted glass waste form leaching and durability studies done under both saturated/unsaturated and irradiated/nonirradiated conditions with and without the presence of other materials (such as tuff, stainless steel, etc.), and made single-mineral (quartz and feldspar) dissolution kinetics/solubility measurements. These studies involved not only the characterization and quantitative analyses of all aqueous and solid-phases, but also the geochemical modeling of the results using EQ3/6. In geochemical modeling code development we have added several capabilities to EQ3/6: a fixed-fugacity option to model systems with a constant vapor atmosphere; Pitzer's equations to model high-ionic-strength solutions; a graphics post-processor; and an economy (lower run time) calculational mode. Improvements have been made to the primary thermodynamic data base code (MCRT), and a precipitation kinetics option was added to the EQ6 code. We have measured the activity and diffusion coefficients of $MgCl_2$, $MnCl_2$, $CdCl_2$, $MnSO_4$, and $RbCl$, as well as the solubilities of the lanthanide nitrates in aqueous solutions. In addition to the programmatic work mentioned above the geochemists pursued independent research in many other areas. For example, we have studied recent and Pleistocene geochronology using uranium-series disequilibrium techniques; mineral spectroscopy and volatile species bound within minerals; point defects within minerals; hydrothermal transport and deposition of tin; and the application of geochemical modeling (EQ3/6) to nonnuclear waste migration, including coupling to simple hydrologic flow codes.

Geology

The geologists work primarily to characterize the geology of the NTS and the Livermore Valley. They study the effects of the geology of NTS on the containment of underground nuclear explosions and on the seismic hazard to and potential for local environmental contamination of the LLNL site. Group members are also involved in reservoir analyses, resource assessment of foreign nations, environmental assessment, and the technical review of seismo-tectonic studies related to siting of nuclear waste repositories.

During 1984 the geologists made statistical studies of borehole logs and lab measurements as indicators of clay and zeolite contents; quantitative determination of mineral content of geological samples by XRD; a study of the development of alluvial basins within the Basin and Range as revealed by a study of basin-fill; a study of borehole elongation as an indicator of tectonic stress orientation using downhole color movies; a comprehensive study of the stratigraphy, structure, and hydrology of the Livermore Valley; geologic influences on chlorinated-hydrocarbon distribution; and the applicability of directional drilling and hydraulic fracturing on the extraction of gas in tight sands. Independent research pursued by the geologists has included the use of quartz-grain-shape analysis as a means of identifying sources of alluvium; a study of freshwater ostracoda in Western Nevada; and a review of the use and protection of San Francisco Bay.

Examples of 1984 Research

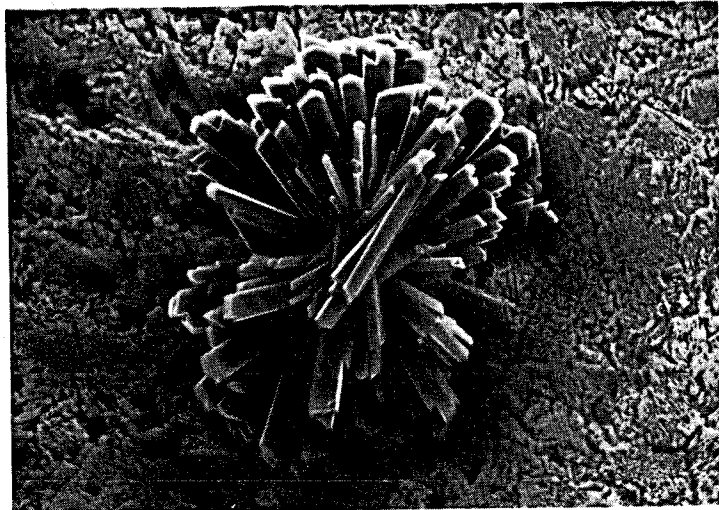
Hydrothermal Interaction Study

In support of the NNWSI Project, experiments were conducted to study the hydrothermal interaction of rock and water representative of a potential repository in tuff. Experiments were run at 150 and 250°C for 66 days using Dickson-type gold-bag rocking autoclaves modified to hold rock wafers. Fluid samples were taken periodically under *in situ* conditions of temperature and pressure for pH, cation (ICP-ES), and anion (IC) analyses. At the termination of each run the rock wafers were characterized by SEM and EMP analysis using both EDS and WDS. In both experiments aqueous silicon concentration was limited by cristobalite solubility. The aqueous sodium concentration rose slightly (150°C) or decreased very slightly (250°C), and magnesium was quickly removed in both cases, whereas the aqueous concentrations of potassium, calcium, and aluminum displayed more complex behavior, reflecting the effects of both dissolution of primary phases and precipitation of reaction products. At both temperatures the anion concentrations were essentially unchanged by reaction, with the exception

of alkalinity, which showed a rapid initial decrease. At the end of the runs the *in situ* pH calculated by EQ3/6 was slightly alkaline in the 150°C run, but more strongly alkaline at 250°C. At the lower temperature the amount of alteration products was very minor and was dominated by poorly crystallized, nonstoichiometric clays (illite/montmorillonite), whereas at 250°C the alteration products were much more extensive and well crystallized and were dominated by the zeolites dachiardite and mordenite (Fig. 9). Results of the 150°C experiment were compared with predictions based on the EQ3/6 geochemical modeling code. The final concentrations of all major cations in solution predicted by the model closely approached those actually observed in the experiment, although the model failed to account for all secondary phases observed.

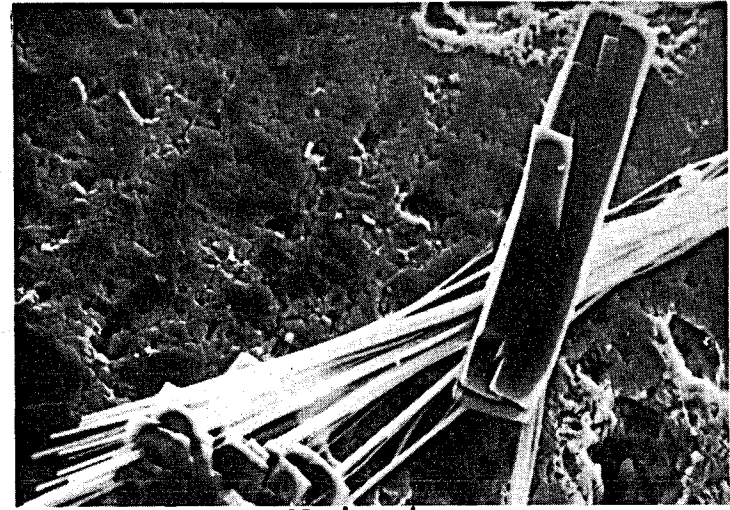
Extending the EQ3/6 Computer Codes to Geochemical Modeling of Brines

Recent modifications to the EQ3/6 geochemical modeling software package provide for the use of Pitzer's equations to calculate the activity coefficients of aqueous species and the activity of water. These changes extend the range of solute concentrations over which the codes can be used to dependably calculate equilibria in geochemical systems, and permit the inclusion of ion pairs, complexes, and undissociated acids and bases as explicit component species in the Pitzer model. Comparisons of calculations made by the EQ3NR and EQ6 computer codes with experimental data confirm that the modifications not only allow the codes to accurately evaluate activity coefficients in concentrated solutions, but also permit prediction of solubility limits of evaporite minerals in brines at 25°C and elevated temperatures (Fig. 10). Calculations for a few salts can be made at temperatures up to 300°C, but the temperature range for most electrolytes is constrained by the availability of requisite data to values <100°C. The implementation of Pitzer's equations in EQ3/6 allows these codes to be applied to problems involving calculation of geochemical equilibria in brines, such as evaluating the possible chemical environment for nuclear waste canisters located in a salt repository.



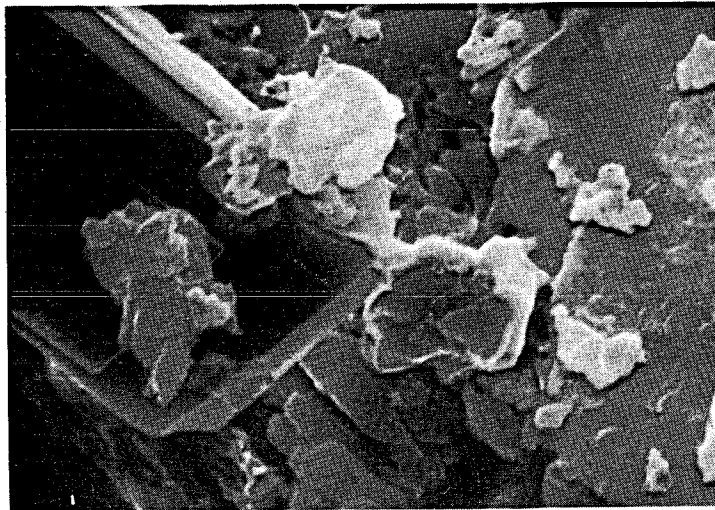
(a)

10 μ



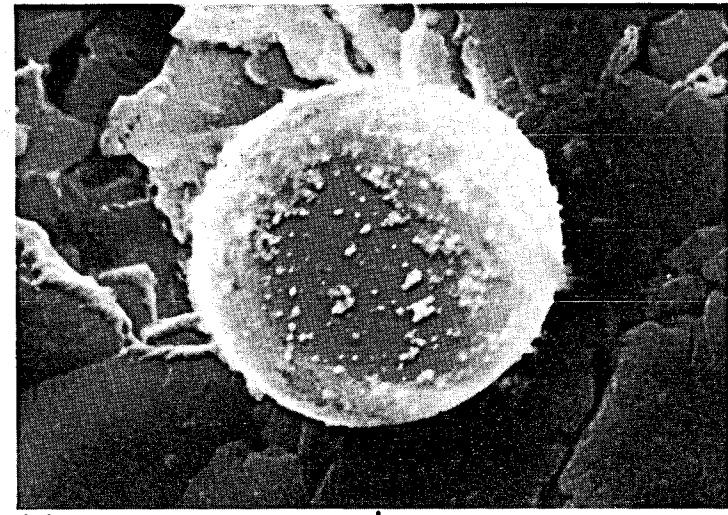
(b)

10 μ



(c)

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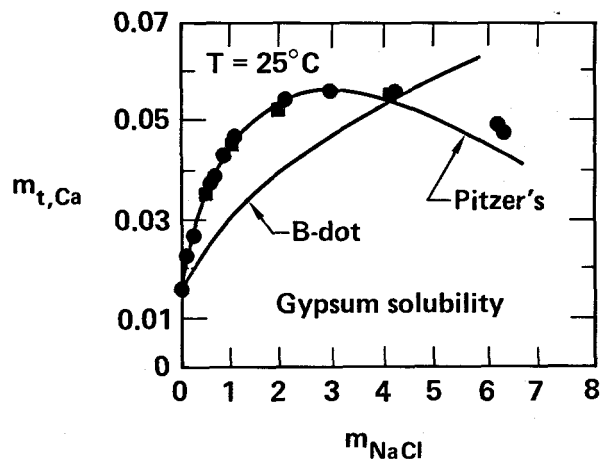


(d)

10 μ

Figure 9. (a) Dachiardite rosette produced in the 250°C experiment. (b) Coexisting prismatic dachiardite and mordenite penetrating a dachiardite rosette in the 250°C experiment. (c) Calcium-rich clay on dachiardite in the 250°C experiment. (d) Cristobalite produced in the 250°C experiment.

Figure 10. Modifications to the EQ3/6 geochemical modeling software package provide for the use of Pitzer's equations to predict the solubility limits of evaporite minerals in brine at 25°C.



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Research Group

Introduction

Formed to expand the basic research opportunities of the Earth Sciences Department and to facilitate the development of new initiatives not directly related to the major applied programs, the Research Group administers and participates in many activities. In the basic research area these include the Office of Basic Energy Sciences Geosciences Program, Institute for Geophysics and Planetary Physics, and the Energy Base Technology Program and Laboratory Institutional Research. In addition, the group is responsible for several small programs, including the Geothermal Injection Monitoring Project, the Site Seismic Safety Program, and an energy analysis project designed to monitor regional, national, and worldwide supplies and consumption of energy.

OBES Geosciences Program

The Geosciences Research Program is directed by the Department of Energy's Office of Energy Research, within the Office of Basic Energy Sciences, Division of Engineering, Mathematics, and Geosciences. Research supported by this program may be directed toward a specific energy technology, national security, conservation of the environment, or the safety objectives of the Department of Energy. The purpose of this program is to develop geoscience or geoscience-related information directly or indirectly applicable to one or more of these Department of Energy objectives, and to develop a broad, basic understanding of geologic materials and processes necessary for attaining long-term Department of Energy goals.

As an example of the work being supported under this program at LLNL, A. G. Duba (LLNL) and T. J. Shankland (Los Alamos National Laboratory) are measuring the thermoelectric effect in the mantle minerals olivine and pyroxene as a function of temperature, orientation, oxygen fugacity, and iron content. The purpose is to determine the effect of magnesium/silicon nonstoichiometry on mineral conductivity, and to apply the results to the inference of upper mantle temperatures from electrical data. The results to date indicate that the temperature in the earth is

$1600 \pm 150^\circ\text{C}$ at a depth of 200 km and increases to $1800 \pm 150^\circ\text{C}$ at a depth of 400 km. Detailed understanding of the temperature in the upper mantle is necessary to test alternative models for the nature of the rheological decoupling of the rigid lithospheric plate and the underlying asthenosphere.

The OBES program at LLNL also strongly supports the DOE Continental Scientific Drilling Program, which is focused on research drilling in thermal regimes. A brief summary of the recently initiated shallow drilling program at Long Valley Caldera, California, is highlighted later in this section.

Institute of Geophysics and Planetary Physics—Seismic Research Program

Lawrence Livermore National Laboratory currently interacts with other research institutes in the University of California system through the Institute of Geophysics and Planetary Physics (IGPP). Through LLNL's participation in IGPP we are providing support for two graduate students (one at U.C. Santa Cruz and the other at U.C. Santa Barbara), and partial support for a research seismologist at U.C. Santa Cruz. Furthermore, through IGPP, LLNL is participating in IRIS, the newly formed Incorporated Research Institution for Seismology, which is working on new, large-scale initiatives in seismology.

As an example of the work being supported, a graduate student from U.C. Santa Cruz has been working on coda-wave analysis for events in the Livermore area recorded on LLNL's local seismic network. (The coda wave is the final portion of the seismogram following the S-wave.) The high quality of LLNL's local network allows consistent comparisons of coda-waves on varied geological terrains. Coda waves are produced by scattering from heterogeneities in the path of propagation of the wave. The varying character of the coda waves reflects the varying physical properties underlying the seismograph stations. Through this analysis we hope to learn more about the complicated geology of the Livermore area, test theoretical models of coda-wave generation, and learn more about earthquake sources in the Livermore area by isolating path effects.

Energy Base Technology Program

The Energy Base Technology Program has been designed to provide a research and manpower base to support the existing energy programs as well as to encourage the development of new initiatives. As an example of the work in this program, we have been exploring the possibility of using image processing to infer the physical properties of rocks. In this approach, a digitized image of the surface of a rock is used to deduce various properties including porosity, specific surface area, and 2- and 3-point correlation functions. The statistical properties are then used to estimate physical properties such as electrical or thermal conductivity, elastic constants, and fluid permeability. To date, we have established the feasibility of measuring correlation functions by image processing, and have developed applications of these functions to procedures for estimating electrical and thermal conductivity. A new approach for bounding fluid permeability using spatial correlation functions has also been developed. Laboratory tests to compare properties inferred from image processing and experimentally derived values are presently being designed. The ultimate applications of the approach may include a logging tool for *in situ* measurement of properties too difficult or expensive to measure otherwise.

Site Seismic Safety Program

For approximately five years, Earth Sciences Department personnel have been involved in comprehensive geologic and seismologic studies of the laboratory site. The overall objective of the program is to evaluate the potential geologic hazards that could affect the safety of operations at the laboratory. As an example of the work done in support of this program, we have estimated the seismicity rate for East Bay faults. Estimates of the recurrence rates of seismic events of various sizes for given source regions are among the parameters used to probabilistically determine the hazard to a given facility as a result of strong ground motion. The statistics of the historical seismic record for the Hayward, Calaveras, Greenville, Las Positas, and Verona fault zones have been used to estimate the rate of earthquake occurrence and the relative distribution of small vs large earthquakes. These results, integrated with the results of geophysical exploration, trenching, and

drilling, suggest that the only significant seismic hazards are associated with strong motion resulting from faults located some distance from the laboratory.

Geothermal Injection Monitoring Project

The objective of the Geothermal Injection Monitoring Project (GIMP) is to evaluate the use of geophysical techniques to monitor the movement of brine injected into geothermal systems. The project has proceeded through three phases. In Phase I we evaluated the potential of geophysical methods for detecting the motion of injected fluids in geothermal areas, and identified approaches where additional development might enhance the usefulness of geophysical methods for this problem. In Phase II we pursued technical advances in four identified geophysical methods, primarily using field experiments funded in cooperation with other projects. These areas included the response of well bores to earth tides, cross-borehole electrical measurements, and detection of microseismicity and self-potential methods. We are presently in Phase III of the project, which will be focused on field studies at geothermal sites where injection will occur. We deployed a seismic net, and have collected baseline self-potential data before injection at the Mammoth-Pacific Geothermal Plant at Casa Diablo Hot Springs, Long Valley, California.

Research Drilling at Inyo Domes, Long Valley Caldera, California

A program of research drilling has begun at the Inyo Domes volcanic chain, which cuts north-south across the northwest rim of Long Valley Caldera (Fig. 11). The youngest features of this chain (four magmatic vents, at least six phreatic vents, and associated normal faults) are believed to be the surface expression of a dike or system of dikes that is at least 8 km long and was emplaced approximately 600 years ago. Both the drilling and supporting research are funded by the Office of Basic Energy Sciences of the U.S. Department of Energy. As an investigation of processes of heat and mass transfer in an anomalously hot region of the earth's crust, this effort is part of the national Continental Scientific Drilling Program (CSDP).

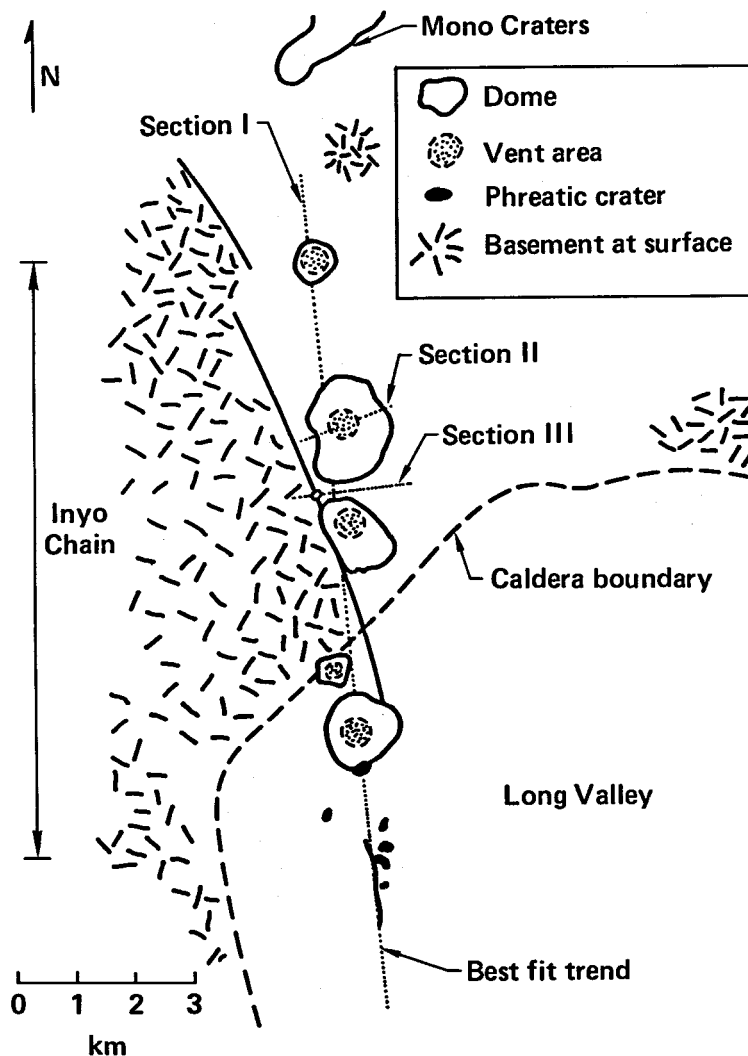


Figure 11. Generalized geologic map of the Inyo Chain and vicinity showing locations of cross sections. The three largest domes and the small dome in Sec. III are thought to have erupted during the most recent event.

Inyo drilling was initiated under a proposal for shallow drilling at Long Valley, Valles Caldera, and Salton Sea submitted to DOE in 1983 by four DOE labs. In 1984 a follow-up proposal was submitted by a consortium consisting of three national laboratories, the U.S. Geological Survey, and five universities.

The Inyo Chain is particularly well-suited for research drilling for a number of reasons. First, although dike propagation is thought to be the dominant mode of magma movement in the subvolcanic regime, rarely can the position of a young dike be as well constrained from surface evidence as at Inyo Domes. Second, this intrusion

is the most recent rhyolitic magmatic event in the western U.S. It should not be thermally equilibrated nor should the glass of the intrusion be hydrated. Third, because the Inyo chain cuts across the structural boundary of the caldera, the dike is emplaced in two contrasting environments pertinent to consideration of continental volcanism. One is a thick, porous, permeable, and water-saturated volcanic pile represented by the caldera fill. The other is silicic crystalline basement, represented by Sierran granitic rocks. Finally, the dike is the most recent leak from the evolving Long Valley Caldera magma system and an accessible analog to intrusions that may be forming

now at greater depth beneath the seismically and tectonically active southwest caldera moat and the resurgent dome.

The scientific objectives for drilling the Inyo system are to characterize and compare the thermal, chemical, and mechanical behavior of magma in the contrasting environments of caldera fill and crystalline basement. To meet these objectives three holes have been drilled to date. During October 1983 a vertical 150-m hole was cored through Obsidian Dome, largest of the young magmatic vents. During September and October 1984 two holes were drilled: a 600-m slant-core hole intersecting the conduit that fed Obsidian Dome (Fig. 12), and an 830-m slant-core hole intersecting the Inyo Dike between Obsidian Dome and the Glass Creek Flow (Fig. 13). Results indi-

cate that the north end of the 600-year-old dike chain is underlain by a rhyolite dike that reached the surface at Obsidian Dome and within 650 m of the surface beneath Glass Creek. The dike is 8 m thick below Glass Creek but broadens to 70 m at a depth of 500 m, where it forms the conduit that fed Obsidian Dome. Analysis of the samples from the dike and conduit, thermal modeling of the intrusion complex, and structural analysis of the intrusion mechanisms will be the focus of the scientific activities at the participating institutions over the next year. A 1-km drill hole designed to intersect the dike within the caldera is tentatively planned for 1986. Seismic and other geophysical surveys in support of the drilling program are also being designed.

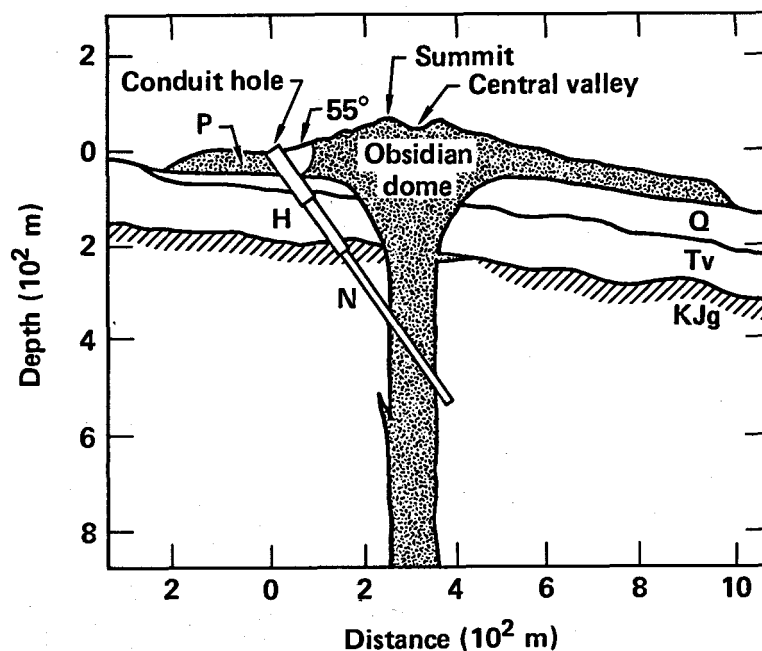


Figure 12. Cross section II drawn before the drilling showing plans for the conduit hole. Hole sizes are $P = 123$ mm, $H = 96$ mm, and $N = 76$ mm. Conduit position was inferred from topography on the dome, and conduit size was inferred from fossil analogs. Drilling confirmed the portrayed geometry with the exception that the conduit was somewhat narrower and the basement rocks (KJg) somewhat deeper than expected. Q is Inyo tephra, colluvium, and Bishop tuff; T_v is andesitic flows and cinders; KJg is predominantly granodiorite and quartz monzonite.

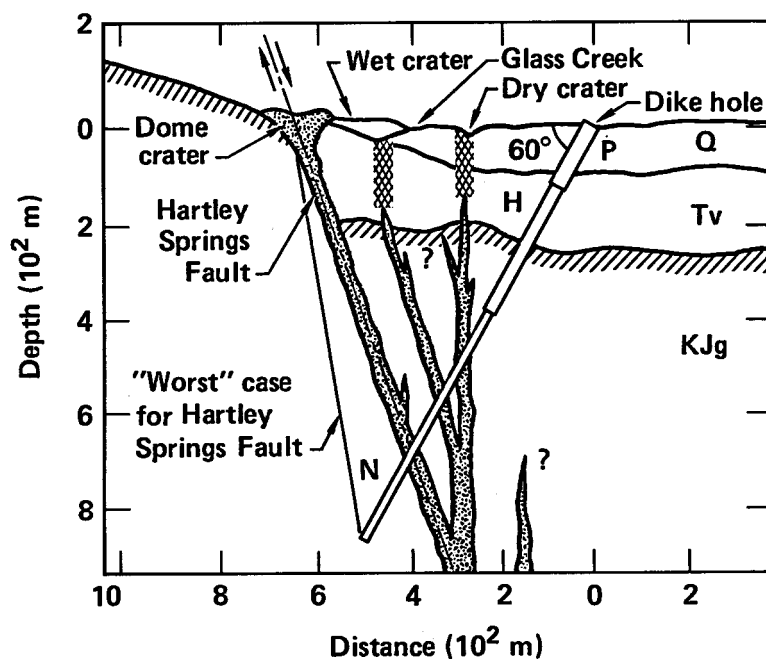


Figure 13. Cross section III showing plans for the dike hole again drawn prior to the drilling. Hole encountered the intrusion beneath Dry Crater in the position portrayed. Drilling stopped before any additional intrusions were intersected.

Research Group Publications

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