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Annual Report 1987

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Clyde J. Sisemore

Clyde J. Sisemore, a member of the Containment Group in the Earth Sciences Department, died July 25, 1988, of complications from heart bypass surgery. He was born on March 22, 1934, near Fayetteville, Arkansas. He earned a B.S. in physics at Fresno State and an M.S. in physics at the University of California, Berkeley.

He began his career at the Laboratory in 1955, working on the Plowshare Program until it ended in the early 1970s. In this program, Clyde worked on *in-situ* solution mining of copper ores. In cooperation with the Kennecott Mining Company, this work established the feasibility of recovering copper from ore broken underground by nuclear or conventional explosives. He served as one of the original physicists who worked in the Laboratory's oil shale program. He played a key role in planning and coordinating joint field experiments with industry. The most noteworthy of these was the $100 million in-situ experiment by the Rio Blanco Oil Shale Company in which the Laboratory provided technical support in planning, retort modeling, and data acquisition and interpretation. In recent years Clyde had been a member of the Nuclear Test Containment Group and also did work for the Seismic Treaty Verification Group.

Clyde was among the originators of SLIFER, one of the first techniques for making hydrodynamic yield measurements of nuclear tests. These measurements have become the preferred U. S. monitoring approach for improved verification of the Threshold Test Ban Treaty.

Clyde was a respected, thorough scientist, helpful to many, and a loving family man. He is missed.

Introduction

The Earth Sciences Department at Lawrence Livermore National Laboratory conducts work in support of the Laboratory's energy, defense, and research programs. The Department is organized into ten groups. Five of these – Nuclear Waste Management, Fossil Energy, Containment, Verification, and Research – represent major programmatic activities within the Department. Five others – Experimental Geophysics, Geomechanics, Geology/Geological Engineering, Geochemistry, and Seismology/Applied Geophysics – are major disciplinary areas that support these and other laboratory programs. This report summarizes work carried out in 1987 by each group and contains a bibliography of their 1987 publications.

The Earth Sciences Department conducts work in support of three major laboratory mission areas – energy, defense, and basic research. The Nuclear Waste Management Program is the largest single program within the Department, representing slightly less than 40% of our efforts. The major activity of that program is to design and evaluate a waste package for encapsulating high-level nuclear waste for permanent geologic storage in a tuff repository. The Fossil Energy Program, representing 5% of our efforts, supports a variety of energy projects focused largely on the issue of alternative sources of liquid fuels. In the defense area three programs – Containment, Treaty Verification, and Shock Physics – represent about 35% of the Department's work. The primary objective of the Containment Program is to ensure the containment of radioactive debris from the Laboratory's underground nuclear tests at the Nevada Test Site. The Verification Program supports a variety of tasks largely focused on developing better methods for verifying compliance with test ban treaties and supporting Department of Energy personnel as they help formulate arms control agreements, negotiate treaties, and evaluate compliance. Basic research activities currently represent about 10% of the Department's work, roughly split between the Office of Basic Energy Sciences (OBES) Program and the Laboratory's Institutional Research and Development Program (IR&D). An additional 10% of the Department's work is devoted to a wide array of smaller projects, including Environmental Protection and Z Program special projects.

To carry out these programs, the Department is organized into ten groups – half are program groups and half are disciplinary groups. The program groups – Nuclear Waste Management, Fossil Energy, Containment, Verification, and Research – are responsible for the oversight and management of the major programs. The disciplinary groups – Geochemistry, Geology/Geological Engineering, Experimental Geophysics, Seismology/Applied Geophysics, and Geomechanics – are the resource from which programs draw their expertise. Discipline group members often divide their work among several programs. Some disciplinary work is done for Laboratory programs or divisions outside Earth Sciences.

All of the programs supported by the Department are inherently multidisciplinary in nature. The Department itself comprises more than 100 professional scientific personnel spanning a variety of subdisciplines: geology, seismology, physics, geophysics, geochemistry, geohydrology, engineering geology, mining engineering chemistry, chemical engineering, and mechanical engineering. Resident technical support groups add significant additional technical expertise, including Containment Engineering, Computations, Electronic Engineering, Mechanical Engineering, Chemistry and Materials Science, and Technical Information. In total 180 professional scientists and engineers are housed in the Earth Sciences Department complex, making it one of the largest geoscience research groups in the nation.

The Department organization structure has evolved over the years to meet the changing needs of the programs. Two changes were recently made in response to current and anticipated future needs of the Department. Two new disciplinary groups were formed – a Shock Physics group headed by Lew Glenn, and a Flow and Transport group headed by Richard Knapp. The scope direction and capabilities of these groups will be highlighted in next year's report.

This is a report of research accomplished by staff members of the Earth Sciences Department during calendar year 1987. It contains a description of the organizational groups in the Department, including 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 provided brief summaries of research projects completed by group members as well as a complete bibliography of publications by group members during the year.

Geology/Geological Engineering

The Geology/Geological Engineering Group applies its expertise in a synergistic way to programs and projects both within and outside the Earth Sciences Department. The group's expertise embraces rock mechanics; soil mechanics; hydrology; engineering geophysics; and structural, environmental, and economic geology. We develop and perform *in situ* and laboratory tests. We provide analysis and numerical simulation to support experiment planning; data analysis and interpretation; and hydrologic, mechancal, and thermal analyses. Our data acquisition and management capabilities are important aspects of the Department's technology base through work in database management, data statistics, geologic exploration and mapping, geotechnical instrumentation, hydrologic instrumentation, remote sensing, site characterization, technical reviews, and well logging.

Civilian Radioactive Waste Management

We support the Nevada Nuclear Waste Storage Investigations (NNWSI) Project by providing technical and administrative leadership for large-scale *in situ* tests of the near-field waste package environment in partially saturated, welded volcanic tuff. These tests examine the hydrologic and thermomechanical responses of fractured, porous rock to an accelerated thermal load cycle conceptually similar to that expected from an emplaced waste package. Our task integrates computational and experimental activities in geohydrology, rock mechanics, and geophysics. Results from these tests will support performance assessment and design activities for the high-level nuclear waste repository proposed for Yucca Mountain, Nevada.

Our major contributions in technical expertise support the NNWSI in the Prototype Engineered Barrier Design Tests (PEBDT) for the Exploratory Shaft Testing. The prototype tests are designed to evaluate the technical feasibility of various measurement techniques used to monitor the hydrologic and thermomechanical response of the rock mass during a heating and cooling cycle. One test involves injecting compressed air into preselected sections of a heater emplacement borehole. We will measure permeability before heating the rock, then again after completion of the heating cycle to assess the thermal effects on the permeability of the rock. The borehole probe includes a packer assembly comprising three inflatable packers. Test zone pressures and temperatures are monitored by pressure transducers and thermocouples.

We are studying the feasibility of modifying existing geotechnical instruments for use in the Waste Package Environment Test (WPET). The effect of high temperatures on instrumentation during tests is of special concern. Another instrument evaluation includes the analysis of results of laboratory tests of a borehole jack in an aluminum block. These tests were conducted to address questions about the phenomenology of borehole dilatometer measurements of rock mass deformability.

Our group continues to support NNWSI in the preparation and coordination of the site characterization plan for the proposed Yucca Mountain nuclear waste repository site. This major Department of Energy (DOE) document is required for release to the Nuclear Regulatory Commission (NRC), the state of Nevada, and the general public as a step in the selection of Yucca Mountain as the first U.S. repository site for high-level radioactive waste.

Repository Technology Program

Based on our expertise in rock mechanics and hydrology, we were invited to participate in the design and performance of several experiments at the Underground Research Laboratory (URL) in Manitoba, Canada. We have the lead role among U.S. participants in developing new techniques for measuring fluid flow and mechanical behavior in several experiments dealing with nuclear waste repository sealing systems and engineered barriers.

In a detailed review of state-of-the-art geotechnical instrumentation, we identified three areas where improved instrumentation and data analysis are needed for carrying out the experiments: earth pressure measurement, moisture sensing, and groundwater tracer detection. Earth pressures are always difficult to measure, particularly at elevated temperatures. An experimental and calculational effort to improve the interpretation of data from existing mechanical devices is under way. To monitor moisture changes in sealing materials, we are working with the Engineering Research Division of LLNL to develop a new technique based on measuring changes in microwave resonant frequencies. For determining groundwater tracer velocity, we are collaborating with the Environmental Sciences Division to develop fiber optic sensor systems that can be embedded in the sealing materials. These systems will eliminate the need to retrieve groundwater samples, and thereby allow continuous monitoring.

GENASYS (Geotechnical Engineering Analysis System) is a two- and three-dimensional hybrid boundary-element finite-element code being developed for this program. When completed, it will compute the coupled deformation and fluid-flow response of fractured nonporous rock masses subject to excavation. We are developing the two- and three-dimensional boundary element part of the code. An important aspect of its development and validation will be its use in simulating the excavation response experiments that are being conducted at the URL. In addition to and in support of this code development work, theoretical models and experimental methods are being developed to improve our ability to predict the coupled response of fractured rock formations.

We have used the first version of the GENASYS code to predict the stresses and displacements induced by the excavation of Instrument Room 209 at the URL. In this experiment, which is a trial run for the main excavation response experiment, the response of the rock mass to the excavation of a tunnel in a sequence of nineteen excavation steps was measured by an array of instruments that include borehole extensometers and stressmeters. The excavation sequence (Fig. 1) consists of a pilot hole excavated in the first ten steps, then enlarged in nine additional slash steps. The deformed cross sections at the end of excavating the pilot hole shown in Fig. 2 illustrate the lack of symmetry in the three-dimensional deformation of the rock mass.

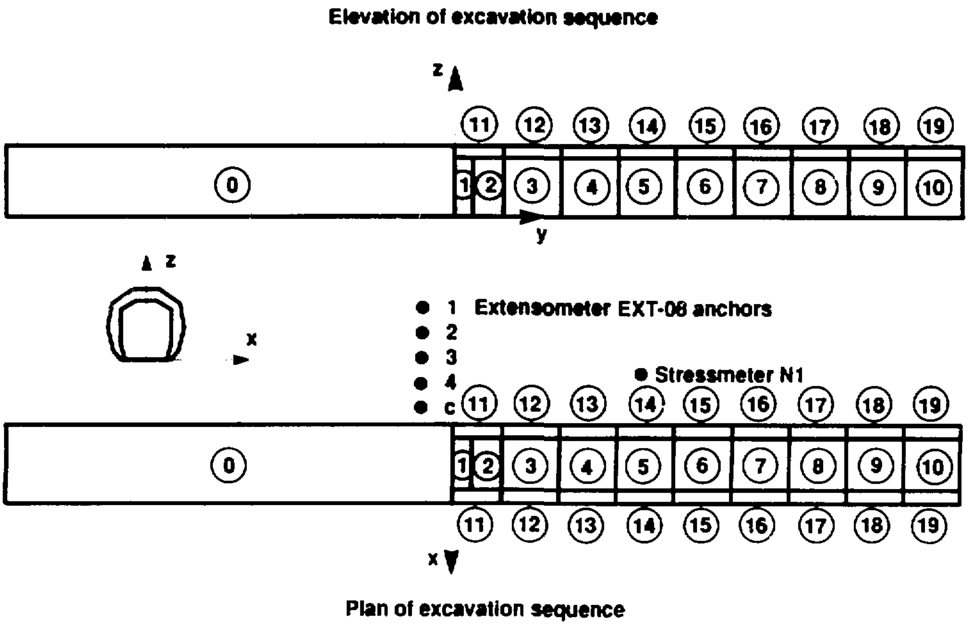

Figure 1. The nineteen excavation steps needed to construct Instrument Room 209 at the Underground Research Laboratory (URL). The pilot hole was excavated in the first ten steps, then enlarged in nine additional steps. The approximate location of one extensometer (EXT-08) and one stressmeter (N1) are shown.

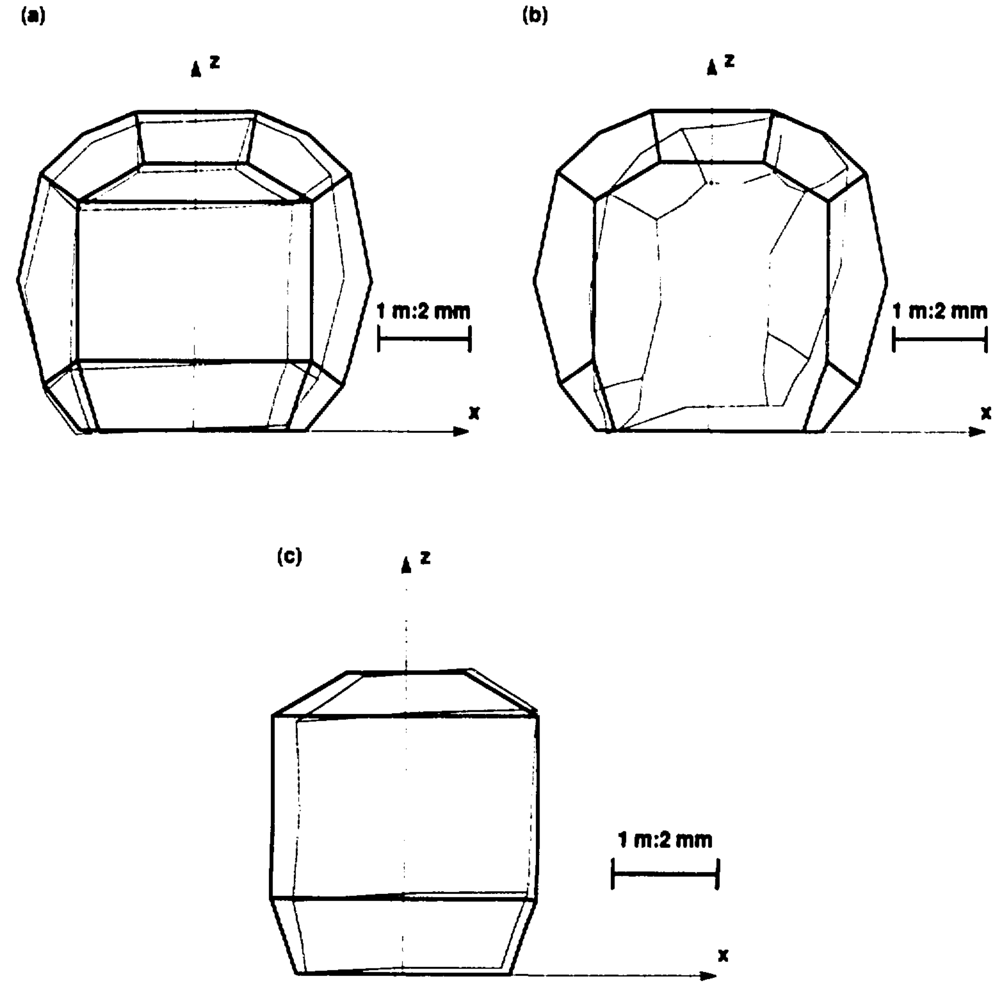

Figure 2. Cross-section geometry and deformed cross sections when the pilot hole has been completely excavated through step 10. (a) Left face, $y = -21.75$ m, (b) initial excavation face, $y = 0$ m, (c) right face, $y = 24.9$ m. Displacements shown are magnified 500 times.

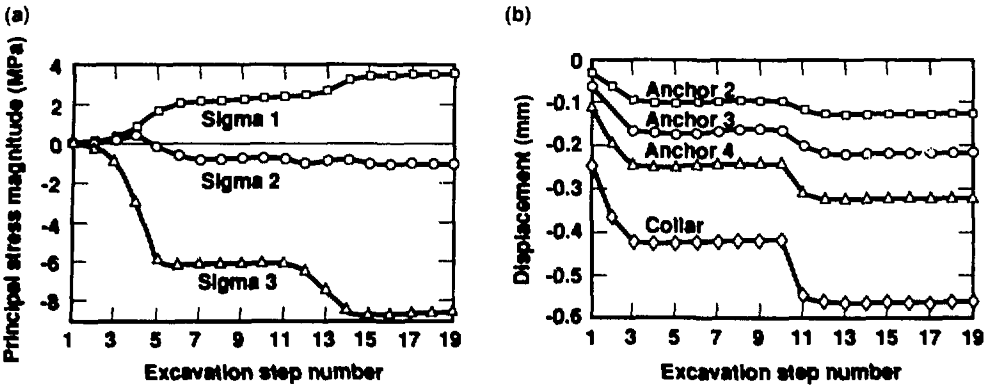

Figure 3. (a) Principal values of stress change at stressmeter S1; (b) change in displacement between anchors of extensometer EXT-08 relative to the deepest anchor 1.

Figure 3 shows the computed changes in the magnitudes of the principal stresses and extensometer anchor displacements relative to those of the deepest anchor that would be measured by this stressmeter and extensometer. These quantities are measured from the initial state of stress and deformation induced by the excavation of the initial access tunnel (excavation step 0 in Fig. 1). The principal stresses and relative displacements of the extensometer anchors change rapidly during the first few excavation steps of both the pilot hole and the additional slash steps, and subsequently reach asymptotic values that correspond to a uniform hole of infinite length as the three-dimensional stress disturbance at the excavation face moves away from the points of measurement.

Our calculations assume linear elastic rock deformation and primarily account for the three-dimensional geometry of the excavation and the highly anisotropic *in situ* stress state that preclude two-dimensional idealizations. To model this excavation sequence with GENASYS, we discretized the surface of the tunnel using 50 to 100 curved quadratic boundary elements and 150 to 300 boundary nodes. The computational time for a run ranged from 30 to 60 min of Cray time, with input/output operations accounting for a significant fraction of this time due to the out-of-core solution of the matrix equations. Boundary element computations of this kind using GENASYS are accurate and cost effective, with the entire sequence computed for less than $8000.

Containment Program

We are responsible for the Containment Program Data Base, ensuring the data are processed, of high quality, archived, and prepared for presentation in a timely fashion to meet Nuclear Test Program schedules. The database activities include processing of log and sample data as well as inclusion of event-related and geologic data. An ongoing task this year has been to convert these data bases and the processing and modeling codes to a new VAX system.

The geologists, along with the geophysicists in the Containment Program, produce site characterization reports, which are thorough descriptions of drill hole locations to be used for underground nuclear tests. Geologic and geophysical data are interpreted to provide information on medium characteristics, samples, geophysical logs, lithology, and geology. These reports are utilized by the Containment Program in their evaluation of proposed nuclear tests and as input to the Containment prospecti.

Three members of our group serve as containment scientists. These roles require evaluation of the experiment, emplacement, site description, relevant experience, and phenomenology. The containment scientist writes the prospectus, describes the event and containment activities to the Containment Evaluation Panel, and serves on the Event Management Team until the event is detonated.

Military Applications

Our primary contribution to the Military Applications Evaluation and Planning Program has been to aid in the understanding of the survivability and effectiveness of various warhead types as earth penetrator weapons (EPW). In particular, we have been involved in the characterization of earth materials encountered during impact tests conducted into frozen soil in Alaska and into sandy soils and concrete at the Tonopah Test Range (TTR). We carried out field studies for both the Alaska and TTR tests; for the Alaska tests, we collected frozen soil samples for mechanical testing. The geologic data are incorporated into predictive calculational models in order to facilitate comparisons to real targets. In turn, the calculations will be used to choose the most acceptable EPW candidate from stockpile weapons or from proposed designs for a robust penetrator.

Our group has developed a comprehensive plan to experimentally investigate shock-wave effects at depth in layered geology. Along with the Experimental Geophysics and Geomechanics Groups, we have designed a series of innovative laboratory experiments involving chemical explosives in large, composite blocks of rock that will simulate certain shock-propagation phenomena, including reflection, refraction, and energy absorption caused by layering. This information, combined with our proposed add-on measurements to large-scale explosive tests in the field, will help verify calculational models of ground shock response for Hard Target Kill.

Environmental Protection

To assist the Environmental Restoration Division of the Environmental Protection Department, we have continued our direction of field studies at the Laboratory and Site 300. These studies have involved drilling monitoring wells and sampling soil and rock strata for volatile organic (VOC) and high-explosives (HE) compounds. Analytical data were evaluated to develop plume maps and explanations of changes in VOC concentrations with time. The HE data were analyzed mainly with respect to depths of penetration of HE compounds into soils beneath abandoned wastewater lagoon sites. On the Laboratory site, the two-dimensional transport code, SUTRA, from the United States Geological Survey (USGS) has been used to better understand the extent and behavior of contaminant transport by groundwater.

We have contributed to these field studies by using a microcomputer to generate well logs, draw geologic maps and contours, make isopach maps, and solve hydrogeologic problems. Our state-of-the-art system is capable of reading well information from a data base to generate cross sections and fence diagrams.

In addition to investigating the extent and nature of contaminated groundwater at the Laboratory site, we have the responsibility to design, plan, and implement appropriate remedial actions to clean up these groundwater problems while meeting the substance and form of requirements from the numerous involved regulatory agencies. In July 1987 the Laboratory site was placed on the National Priority List (Superfund) for these activities; we immediately became accountable to the Environmental Protection Agency (EPA) as well as the Regional Water Quality Control Board, the State Department of Health Services, and the City of Livermore. We are continuously negotiating with these agencies to ensure compliance with Comprehensive Environmental Response Compensation and Liability Act/ Superfund Amendment Re-Authorization Act (CERCLA/SARA) requirements as we move forward in the cleanup process. The preparation of the Remedial Investigation/ Feasibility Study required by the EPA before actual cleanup begins will take approximately two years.

Nuclear Regulatory Commission

At the request of the NRC, we provided technical review and commentary on topical reports prepared by the DOE and DOE contractors regarding aspects of the geology of proposed nuclear waste repository sites in bedded salt at Deaf Smith County, Texas; in basalt at Hanford, Washington; and in tuff at Yucca Mountain, Nevada.

Unconventional Gas Recovery Program

In support of the Unconventional Gas Recovery Program, we studied the feasibility of determining *in situ* deformation moduli from hydraulic fracturing pressure records. Because a hydraulic fracture responds to the *in situ* properties of a large volume of rock, at least as large as itself, fracturing can be an attractive means of determining the *in situ* deformation moduli of a rock mass at different length scales. With this motivation, extended analytical results were derived for estimating the *in situ* crack-opening modulus from bottom hole pressure records for *in situ* conditions that result in the propagation of constant-height hydraulic fractures. We developed and generalized a theoretical formulation that unifies and extends existing Perkins–Kern–Nordgren (PKN) and Christianovitch–Geertsma–De Klerk–Daneshy (CGDD) constant-height fracture models to obtain a hybrid CGDD-PKN model that applies to constant-height fractures of arbitrary length/height aspect ratio. These results are useful for interpreting fracturing data and for designing fractures for crack-opening modulus measurements.

Sensitivity analysis of the uncertainty in the crack-opening modulus measured from bottom hole pressure records shows that the crack-opening modulus computed from the initial CGDD-type fracture extension phase will be much less sensitive to the uncertainty in fracture height than that computed from the final PKN-type fracture extension phase. If the crack-opening modulus is to be computed from the usually observed final PKN-type fracture extension period, then the fracture height must be known with much less uncertainty than the uncertainty in the crack-opening modulus that is to be resolved through such measurements.

We are conducting laboratory experiments to understand hydraulic fracture behavior near geologic interfaces and thereby develop improved diagnostics for stimulation of gas sand reserviors. In the first year of this three-year effort, we have investigated various means of detecting and controlling fluid-driven fractures in gypsum cement blocks containing sandstone lens structures. We have also developed new equipment for applying stresses to the blocks to simulate *in situ* conditions near an underground sand lens. We have discovered that the most effective detection scheme appears to be an externally mounted ultrasonic transmitter used in conjunction with an array of inexpensive piezoelectric film receivers embedded in the block. A distinct signal change is noted as a crack passes between the source and receiver, thus locating the front in both time and space. This system will be used to track a fracture near an interface and correlate its behavior with diagnostic characteristics in the fluid-injection pressure-time record.

Z-Program Applied Technology and International Assessments

We provide studies of the oil and gas development in Brazil with emphasis on future potential in these areas. We also analyze Soviet geology for applications related to treaty verification issues. Both these studies contribute to U.S. and world security. Technical support is also provided for other special projects with geology and geological engineering elements.

Howard University

In cooperation with Howard University, the Earth Sciences Department and the Historic Black College Program sponsor a summer field geology course at the Nevada Test Site (NTS) (Fig. 4). Applied geology and its problems and techniques are emphasized in recognition of growing numbers of environmental problems geologists will be required to confront in the future. Many unique facilities (i.e., boreholes, tunnels, and trenches) are available at NTS and can be used to provide training in various techniques and procedures of applied geology. The course also provides a background in traditional field geology techniques. Instructors include professionals from Howard University, USGS, DOE, and LLNL Earth Sciences Department.

Many of the students have continued on to advanced degrees or expressed an interest in doing so upon graduation. Two of the students have returned as student assistants in the course. Another student currently has a one-year technical appointment in the Earth Sciences Department.

Figure 4. Students and faculty from the first cosponsored Lawrence Livermore National Laboratory/Howard University summer field geology course. From left to right: Oliver Jones, Kevin Bacon, Brian Price, Dr. Fred Wilson (HU), and Dr. Larry McKague (LLNL).

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Experimental Geophysics

The Experimental Geophysics Group conducts research in rock and mineral properties, high-pressure physics using the diamond-anvil cell, and crystal growth. In 1987 we measured the physical properties of materials ranging from hydrogen to single crystal olivine over an extremely wide range of pressures and temperatures. This work, conducted in support of the Laboratory's energy, defense, and research programs, deepened our understanding of the physics of the earth and planets as well as the physics of phase transformations at high pressures.

Rock Properties

Shock-Wave Studies

At the Giant Magnet Experimental Facility, we digitally recorded explosion-induced motion in geologic materials. We can simultaneously measure particle velocity and piezoresistance gage responses to determine the multicomponent stress-strain history in the test material. This information provides a means to validate computer models used in simulation of nuclear underground testing, chemical explosion testing, dynamic structural response, and earth penetration response. The facility can accommodate geologic samples as large as 1.5 m on a side and, with the use of multiple-turn gages, it has been possible to obtain particle-velocity time histories at strains from 10^{-1} to as low as 5×10^{-7}, or at stresses from a few tens of kbars to less than a bar.

The piezoresistance measurements provide data from triple-material foil gages and from ytterbium foil gages for strains below 10^{-3} or at stresses below about 1 kbar. Our analysis shows that the triple-material gage containing foils of ytterbium, manganin, and constantan provide three independent resistivity measurements for the gage oriented in a perpendicular direction relative to the radial propagating shock front. Our analysis of the ytterbium foil gages, which were tested in both perpendicular (normal) and parallel (tangential) directions relative to the radial shock front, shows that the resistivity responses from these two orientations are independent measurements, with both depending upon (1) the radial stress history and (2) the two tangential strain histories. This analysis indicates that the material properties of the foil, the dimensions of the foil, and the material surrounding the foil greatly influence the total resistivity response of foil gages in a multi-component stress-strain field. These piezoresistance gages provide a breakthrough in the ability to measure stress-strain time history and validate computer codes used for ground-motion calculations.

Physical Properties for the Salton Sea Scientific Drilling Project

For the Salton Sea Scientific Drilling Project (SSSDP), we measured ultrasonic *P*- and *S*-wave velocities, electrical resistivity, and brine permeability. Two cores of siltstone from 919-m and 1158-m depths have been studied at confining pressure, temperature, and pore pressure that closely simulated *in situ* conditions in the borehole. We also obtained x-ray tomographs, ultrasonic tomographs, and impedance images of these samples. Our results indicated that the ultrasonic wave velocities measured in the laboratory were comparable to those obtained by sonic logging. These cores were found to have strong anisotropy in ultrasonic velocities; at *in situ* conditions the *P*-wave velocity measured along bedding was smaller than that measured perpendicular to bedding. This was probably caused by the combined effects of pressure and temperature on velocity of a layered medium. This ultrasonic velocity anisotropy, if proven to generally exist in the Salton Sea rocks, is very important for the exploration and understanding of geophysics in a geothermal field.

Thermal-Stress Microfracturing

Thermal microfracturing occurs in rock loaded by thermal stresses produced either by natural processes or engineering applications such as nuclear waste disposal. Active and passive acoustic methods show promise for monitoring changes induced in a rock mass by thermal loads. By monitoring acoustic emissions at high temperature and pressure, we have demonstrated that relatively more emissions occur at lower pressure than can be explained by crack formation. Our findings suggest that fundamental changes in the fracture process occur at pressures important to engineering applications.

Measuring Joint Topography

Accurate modeling of fluid flow through joints in rocks has consequences for a number of important applications, from resource recovery to nuclear waste isolation; however, the physics of joint behavior and of the flow of fluids between rough surfaces is poorly understood. To increase our understanding, we have designed an experiment to simulate joint behavior in the laboratory. By making quantitative measurements of joint topography for a tensile surface in gabbro, then combining that data with permeability and joint closure measurements, we have been able to show that the cubic law for fluid flow in a single fracture holds for smaller apertures than predicted by numerical modeling of the flow field.

X-Ray and Optical Studies in the Diamond Anvil Cell

Diamond anvil cell studies concentrated on x-ray and optical measurements in the 100-GPa range. Structural and volume change data for some rare-earth elements and actinide elements were collected up to 130 GPa (1.3 Mbar). We used synchrotron x-ray sources at Brookhaven National Light Source and Stanford Synchrotron Research Laboratory to collect x-ray data at and above 100 GPa pressure. An x-ray beam from a synchrotron source collimated to 10 mm or less has enough intensity to permit data collection in an hour or two at these pressures. By reducing the area of the sample to be x-rayed, the pressure gradient (which is 5–6 GPa over 60 mm area) could be brought down to 1.0 GPa. We reported that plutonium goes through a structural change at high pressure and room temperature. Similar structural changes were also noted in δ-plutonium. We discovered a new high-pressure phase in neodymium. This triple-hexagonal close-packed phase, missing in the rare-earth-element high-pressure phase-transition sequence, was later confirmed in gadolinium and samarium.

We have advanced the pressure limits of the diamond-anvil cell for containment of soft samples to 2 Mbar. We have successfully contained samples and have made *in situ* optical measurements of xenon and hydrogen to this pressure. Our experimental results for these materials illustrate that the insulator-to-metal transitions theoretically predicted to occur at or below 2 Mbar do not occur and must exist at significantly higher pressures than previously expected. In the case of xenon, we have measured the electronic band-gap to be ≥ 1.9 eV at 2 Mbar, indicating that the transition may not occur below 3 Mbar. We have observed no optical absorption features below the diamond absorption edge (2.5 eV) in hydrogen up to 2 Mbar, indicating that the insulator-to-metal transition in this material will occur at even higher pressures. We have also studied the high pressure behavior of bromine, whose high-pressure electronic behavior is thought to be an analog for hydrogen. We have observed the insulator-to-metal transition in bromine at about 1 Mbar.

We have studied electrical, optical, and structural properties of fayalite (Fe_2SiO_4) to maximum pressures between 1 and 2.25 Mbar at room temperature. Results of electrical resistance and optical absorption measurements made up to 0.9 Mbar extrapolated to metallic values above 1 Mbar. However, measurements of infrared reflectivity to 2.25 Mbar indicated that the transition to a metallic state did not occur. Subsequent *in situ* and recovery x-ray measurements indicated that fayalite transforms irreversibly to an amorphous state at about 0.4 Mbar.

Crystal Growth/Electrical Conductivity

We received the thermal image furnace for our crystal growth laboratory in October 1987. In early December, we grew our first olivine with a nominal iron content of 15 wt%. Thermal stresses, generated by the large temperature gradient inherent in the thermal image furnace, cause our crystals to develop cracks parallel to the growth axis. We are attempting to solve this gradient problem by developing a resistance furnace to heat the sample after it leaves the melt zone. Further studies to fully characterize the olivine crystals, including electrical conductivity measurements, are underway. We have also started to grow diopside and melilite for on-going diffusion experiments in the Earth Sciences Department.

The complex impedance of a core of black shale from 5.4 km deep in the Münsterland 1 borehole near Münster, West Germany, indicates a conductivity of about 1 S/m, independent of frequency over the range 10^{-3} to 10^{5} Hz. This high conductivity, which is equivalent to that measured for either molten basalt or olivine at about 1500°C, is attributed to carbon at grain boundaries. The carbon is the residue of pyrolysis reactions that proceeded during diagnesis of organic-rich sediments. Such black shales could be responsible for some crustal conductivity anomalies, which could be associated with overlying gas or oil. It is also possible that some carbon-rich rocks are subducted to greater depths and could contribute to production of upper mantle conductivity anomalies.

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Containment

The primary goal of the Containment Group is to ensure the containment of radioactive debris from LLNL's underground nuclear tests at the Nevada Test Site. The main objective of the group is to develop sound technical bases for containment-related methodology. The containment design of a proposed test takes into account many factors, including the geologic setting, the physics design of the experiment, the emplacement and stemming of the experiment, and the previous experience with similar experiments.

In September 1987 the Containment Group cosponsored the Fourth Symposium on Containment of Underground Nuclear Explosions, which was held at the U.S. Air Force Academy in Colorado Springs, Colorado. At this symposium, members of the Containment Group presented 15 papers on topics covering line-of-sight design, geology, material properties, stress measurement, stress calculations, geophysics, medium properties, cavity pressure, collapse phenomena, and late-time gas flow. Some of the advances that we presented at the conference are summarized below.

Calculations

We studied geologic structures in which a relatively weak working-point tuff medium is located between two hard-rock layers. If the hard-rock layer is close to the cavity, it can retard cavity growth and increase cavity pressure to the point of exceeding the residual stress field. In one case, two-dimensional TENSOR calculations showed that the residual stress in the tuff is about the same level as the cavity pressure. This leads to the speculation that horizontal seepage could proceed quickly into the weak tuff. To further study the seepage possibility, two-dimensional calculations were run with the CRAM code developed by S-Cubed in La Jolla, California. This code uses a new dynamic-fracture model that calculates the opening, propagation, and closing of cavity-gas-filled hydrofractures during dynamic ground motions.

A conservative assumption is that the fluid pressure in the entire crack network is identical to cavity pressure. The results of the conservative dynamic fracture model in CRAM show cavity gas penetrating the residual stress field horizontally.

In situ rock strength is a key parameter in containment calculations. The projectile method appears promising for determining rock strength in our large-diameter (2- to 4-m) hole environment. We are developing a gas-gun launcher system that will be capable of measuring both depth of penetration and deceleration of a reusable projectile in these holes.

We compared penetration of a 13-kg projectile fired at about 30 m/s from a prototype launcher to penetration of an 84-g projectile fired at about 500 m/s from a seismic gun. The first targets were 60-cm cubes of gypsum cement, mixed to provide a range of densities (1.64 to 2.0 g/cc) and strengths (3 to 17 MPa). We found that penetration depth is proportional to projectile kinetic energy for projectiles with the same nose size and shape, impacting targets of approximately constant strength. The ratio of kinetic energy to penetration depth is approximately proportional to target strength. Tests in tuff with a wide range of strengths at NTS give a similar linear relationship between the ratio of kinetic energy to penetration and target strength, as well as a linear relationship between deceleration and strength (Fig. 5). Thus, penetration can indeed be used as a measure of strength.

Stemming and Plugs

The stemming design of an emplacement hole typically includes six sanded-gypsum-concrete plugs that perform as gas impedance barriers or structural members or both. The condition of the rock in the vicinity of the plug is important in the performance of the plug. The *in situ* acoustic velocity of the rock has been examined as a tool to help choose plug locations.

Velocities measured in the walls of large-diameter boreholes with the dry hole acoustic logger (DHAL) are typically lower than velocities across similar geologic media measured farther from the borehole wall using other techniques (Vibroseis). This velocity difference is attributed to a disturbed zone around the borehole wall that may be due to drilling or to weak rock in the presence of overburden stresses. Modeling suggests that lower velocities should be observed next to the borehole wall, and that shear failure of the medium is necessary to reduce the velocity. Data indicate that the borehole walls for many holes appear to have failed sufficiently to relieve tangential stresses over large distances along the depth of the hole. From this analysis, it is prudent to consider the possibility that the damaged annulus of the hole is a potential pathway for radioactive gas. We conclude that, where exact plug locations are not dominated by other factors, plugs should be placed in regions where the velocity measurements indicate minimal annulus damage.

Phenomena

Gas samplers at the Nevada Test Site have detected radioactive noble gas following several events detonated beneath Pahute Mesa. This has been attributed to atmospheric pressure cycling ("breathing") assisting diffusion in enabling gaseous radioactive fission debris to reach the surface. The geology of an event site, in particular the depth of the Rainier Mesa Member of the Timber Mountain Tuffs, appears to play a role in the amount and timing of this phenomenon.

By comparing fluctuations in atmospheric pressure and subsurface pressure (measured in postshot holes of opportunity), we have been able to calculate the bulk diffusivity of chimney regions to quantify the diffusion characteristics of tuff and alluvium. The diffusivities calculated to date range from about 130 to 31,000 m^2/hr. These diffusivities are only one parameter in a gas transport model that is under development. Before gas transport predictions can be reliably made from transport models, other parameters such as fracture number, spacing, and aperture must be known *in situ*. We are presently examining methods to determine the other parameters.

We have made advances in several other measurement techniques. Shear velocities of geologic material are important parameters in calculations. Relative shear-wave velocities can be calculated from signals recorded by the two-receiver DHAL. An energy packet within the DHAL signals has been identified as the Rayleigh wave that travels along the wall of the empty borehole. The velocity of the Rayleigh energy is related to the shear wave velocity. The

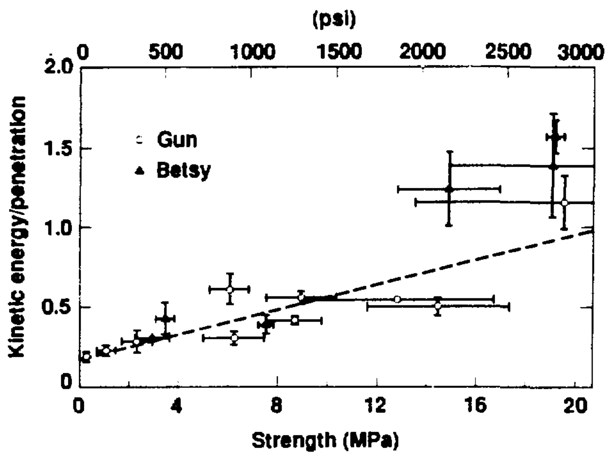
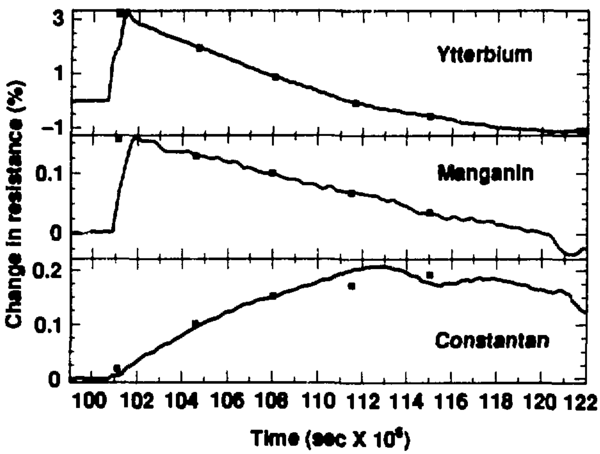


Figure 5. Strength vs ratio of kinetic energy to penetration depth (Newtons x 10^{-5}) for 13-kg projectiles (gun) and 84-g projectiles (Betsy).

signals from the two DHAL receivers are filtered, windowed, and cross-correlated to obtain the best estimate of the time delay between the arrival of this Rayleigh energy at each of the receivers. From this time delay, the Rayleigh wave velocity is calculated. With the borehole diameter and signal wavelengths, Vs is calculated.

Measurements of shot-indicated stress as a function of time and position provide both an empirical basis for phenomenological concepts of containment as well as data to validate predictive calculational analysis. We studied a triple-material piezo-resistance gage for multicomponent stress. The three piezo-resistance materials used in the gage are ytterbium, manganin, and constantan. The output from this gage is a history of the resistivity change for each material in the gage. The three diagonal components of the stress (strain) tensor can be inferred from the resistivity measurements. We compared the gage resistivity measurements with the calculated gage response for spherical shock loading in polymethylmethacrylate (PMMA) (Fig. 6). The close agreement of the calculated and measured resistivity changes shows that the performance of the triple-material gage can be used to infer the stress history of shock-loaded materials.



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Geomechanics

The Geomechanics Group is composed of engineers and scientists with expertise in the mechanics of geologic materials. Most of the group's activity is related to developing and applying sophisticated computer models to the analysis of complex problems of shock, fracture, and flow in the solid earth. The phenomena we study generally involve one or more couplings between thermal, mechanical, and hydraulic effects. The group provides support to LLNL energy projects, such as the isolation of nuclear waste or the recovery of deep natural gas, and to defense programs, such as the containment of underground nuclear tests or the ground effects of earth penetrator weapons. Four projects highlight the achievements of the group in 1987.

Multiphase Dynamics of Geologic Media

The physics of wave propagation in porous rocks and soils is highly dependent upon the degree of fluid saturation in the pores. Waves attenuate more rapidly in gas-filled porous materials than in liquid-saturated materials because of pore crushing and collapse. Soil liquefaction may occur when pore-pressure buildup disrupts the frictional equilibrium of normal and shear stresses. The response of geological materials as affected by the degree of liquid saturation has a direct impact on LLNL's programmatic goals in defense-related areas such as containment, treaty verification, earth-penetrator weapons, and hard targets.

A new, comprehensive model was developed to describe the dynamic response of three-phase media to shock. It explicitly treats the flow of the fluids (air, water) independently of the solid matrix. This model has been incorporated in the TENSOR ground-motion code and verified against one-dimensional shock-tube calculations for saturated soils (there are no independent results for partially saturated soils). Figures 7 and 8 illustrate the importance of the independent handling of solid and water, showing the solid and water-pressure profiles in the one-dimensional shock tube after rebound of the shock at the tube's end. An analog situation in nature would be shock reflection at a hard-rock interface of low permeability, overlain by pervious softer rocks or soils. Because the water pressure is high ahead of the principal solid shock, due to the leading returning water shock wave, there is a region of very low effective solid normal stress ahead of the solid shock. Thus, the *solid shock will be traveling into a region of* lowered effective solid strength, thereby increasing the extent of damage to the solid matrix, as contrasted with what it would be in a dry material.

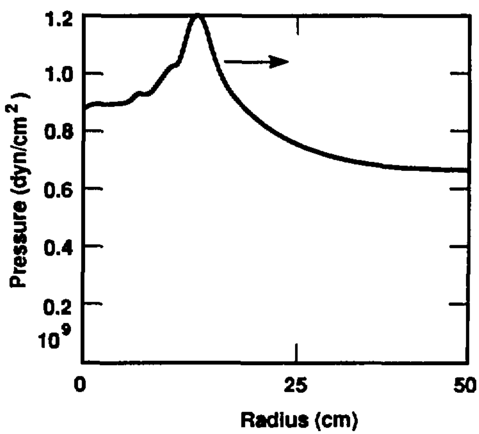

Figure 7. Liquid pressure after rebound.

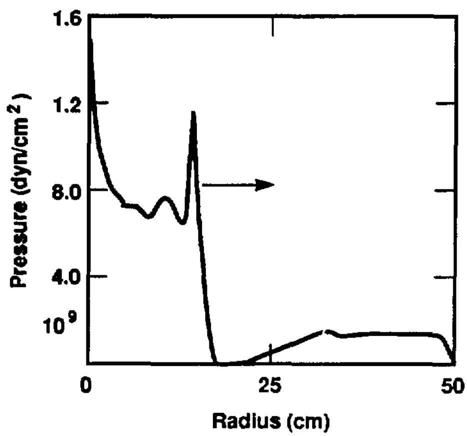

Figure 8. Solid effective pressure after rebound.

New Insight in Cratering Phenomenology

The phenomenology of explosive cratering in hard rocks is of interest in the energy field, defense field, and planetary science. Traditionally, the analysis of explosive events has been performed by using dynamic continuum codes, mostly based on finite difference approximations. These codes have been very useful in predicting ground shock effects at depth; however, they are not adequate for representing the full-cratering process. Figure 9 is a case in point. This continuum computation of a particular underground explosion shows a very large (>60 m) mounding of the surface, and sharp displacement discontinuities over a zone extending from the cavity to the surface. It is clear that extensive rock breakage will take place in the medium, in the mound, and along the displacement discontinuity surfaces, prior to material being ejected. From there, a large amount of block motion will take place in the ejecta, with attendant dilation due to block motion; the above physics is beyond the reach of continuum codes. To gain more realistic insight into such cratering phenomena we have turned to a different modeling technology known as discrete block models.

Over the past several years, a few numerical models have been developed specifically aimed at simulating the motion of discrete macroscopic, inelastic, frictional particles. One of these, the LLNL DIBS (Discrete Interacting Block System) model is a two-dimensional polygonal-particle model, which tracks the motion of each individual particle (or element) in a system of many as it interacts with other particles and boundaries under applied loads and gravity. Elements have arbitrary polygonal shapes and are themselves rigid; however, their contacts, which are corner-on-side, have both stiffness and damping in the normal and tangential directions. They also possess frictional and cohesive strengths. These features can simulate realistic nonlinear and nonelastic interactions in rock masses composed of rock blocks separated by joints and faults.

The calculation starts with a given geometric configuration and a set of initial velocities or applied forces. The forces acting on all particles due to that instantaneous configuration (and applied loads and gravity) are determined; then, an explicit finite-difference integration of the equations of motion of all particles is carried out for one small time-increment, to determine new positions and velocities for all of the particles. The particles are moved, time and velocities are updated, and the procedure repeated. The method has been verified by comparison with analytic predictions and with laboratory tests of the motion of individual blocks and assemblies of particles.

The SULKY nuclear event was the object of the first of three calculations; it was a 90-ton nuclear test at depth of burial of 27 m. The DIBS simulation is shown in Fig. 10. The initial force time-history was chosen heuristically to match the known spall velocity of 26 m/sec. The peak pressure was 31.4 MPa, declining to zero in steps, over 65 msec. It was applied to the walls of a 10-m diameter cavity, the size of which was estimated from 1-D hydrodynamic calculations of the real event. The DIBS/SULKY simulation captured the approximate height of the rubble and the creation of a "retarc." It also showed the pronounced effect of rock mass dilation along the shear surfaces on the velocity field and hence on the ejecta pattern. A second calculation (Fig. 11) showed the expected result for a SULKY yield buried at only 15 m; and a third calculation showed very little disturbance at the ground surface for a 54-m depth of burial. The DIBS calculated the expected spall velocities of the second and third explosions within 2% and 7% respectively.

Discrete block modeling is not a mature technology in spite of the interesting results obtained, as above. Realistic ground motion models must provide scenarios for fragmentation that takes place between the continuum phase and discontinuum phase. Also, the discrete models must be developed to provide realistic three-dimensional calculations of rotations and bulking.

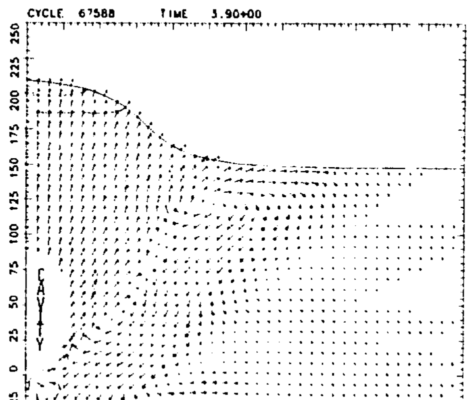

Figure 9. Displacement field in a continuum calculation of a particular underground explosion.

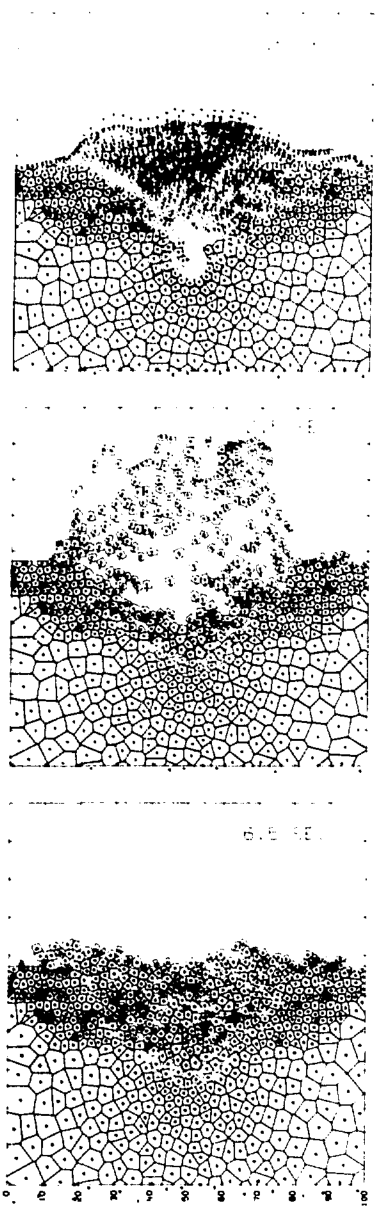

Figure 10. Cratering simulation of the SULKY event (90 tons buried at 27 m).

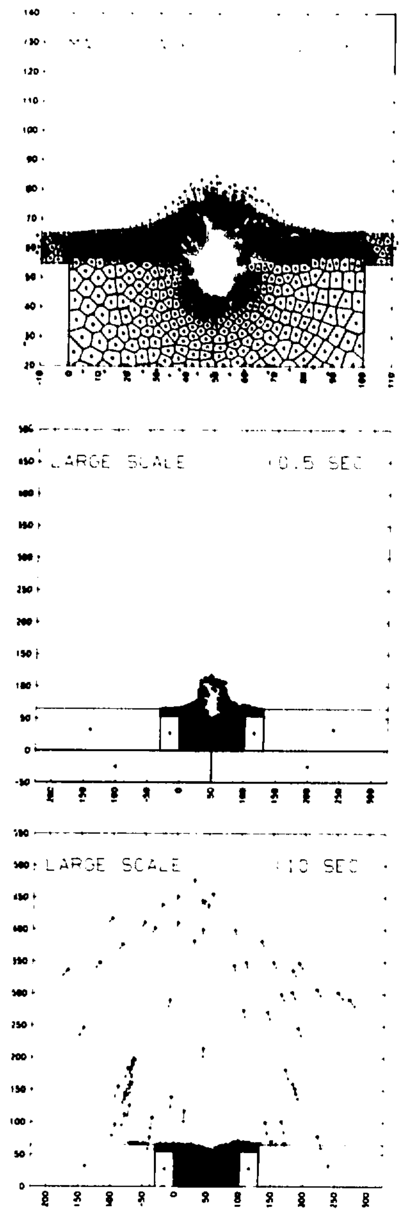

Figure 11. Cratering simulation of a 90-ton nuclear explosion buried at 15 m.

Geologic Factors Adverse to Nuclear Containment

Decisions made as to the expected safe containment of nuclear explosions at a given site are based upon previous experience and analysis of the new site. Once the site geology has been defined, this analysis is performed within the geomechanics group using ground-motion models such as the TENSOR or DYNA codes. Experimentally measured or otherwise estimated geologic material properties are used in parametric analyses of the effects of the given explosion. The expectation of containment of the radioactive products is based on predicting that a zone of residual tangential stresses will develop around a nuclear cavity upon rebound of the ground, after passage of the initial shock wave, and that these tangential stresses will be higher than the cavity gas pressure.

Some geologic combinations of layering, layer hardness, and material saturation have been determined to hamper the formation of this residual stress field. These insights were gained through the extensive calculational database developed over the years, and some measure of site data. Two situations are selected to illustrate geologies potentially detrimental to containment: a shot point in a weak layer located between two strong, hard layers (Fig. 12), and a shot point in a hard, saturated layer overlain by a soft pervious material (Fig. 13).

The figures show the extent to which a region of tangential stress develops with values lower than cavity pressure; this area is shown as dark shaded. In Fig. 12, the strong rock layers prevent cavity growth in the upper and lower directions resulting in elevated cavity pressure. The weaker material located between the hard layers characteristically supports a low residual hoop stress. The figure shows an area connected to the cavity that has residual hoop stress less than the cavity pressure.

In Fig. 13, the interaction of the outgoing shock wave with the porous layer causes a rarefaction wave to return downward into the cavity region. The wave reduces the residual hoop stress around the cavity. In addition, the strong rock surrounding the cavity influences the cavity growth to be less and the cavity pressure to be higher. The combination of effects results in cavity pressure greater than the residual hoop stress above and at the level of the cavity.

Such situations are judged conducive to gas escape and such sites may be avoided. These numerical models of nuclear test effects continue to be a key part of containment estimation.

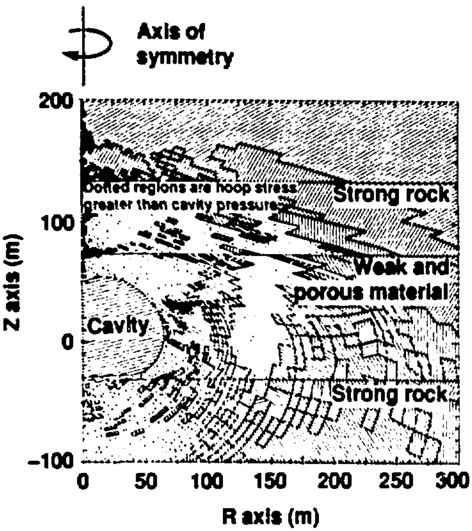

Figure 12. Nuclear event in a weak layer located between two strong layers.

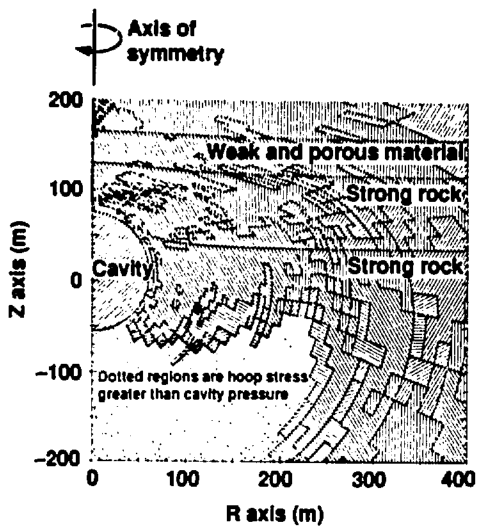

Figure 13. Nuclear event in a hard, saturated layer overlain by a pervious material.

Micromechanical Models of Brittle Material Response

Brittle materials loaded under quasi-static or dynamic conditions develop internal microcracking, which changes their properties and can lead to their failure. Today most brittle failure models are phenomenological in nature and use a macroscopic empirical approach to characterize material behavior. An alternative modeling approach has been pursued, which is more atuned to the internal deformation and failure processes taking place in these materials. Salient features of the new microcrack-dependent material response are:

- Stochastic microcrack density function that identifies various species of microcrack by a set of physical attributes such as microcrack opening, microcrack size, microcrack orientation, and their associated rates of change;
- A deformation functional that represents mathematically both the continuous and discontinuous contributions to microcrack-dependent deformations between two atoms in a material body;
- A thermodynamic internal energy functional that represents mathematically the energetics of microcrack creation, microcrack area change, and microcrack surface-strain energy.

This model has been used to interpret experimental data of microcrack density evolution in polymers as shown in Fig. 14. The model has also simulated microcrack localization and failure of a brittle material under quasi-static tensile testing. The most recent application has been for dynamic loading due to an explosion in a cylindrical borehole (Figs. 15–17). As the shock from the explosion propagates outward from the borehole, a decrease in microcrack density is predicted along a radius (Fig. 15). Figure 16 shows a comparison of the particle velocities for a microcrack-dependent material and an elastic material. The model for microcrack-dependent material predicts a larger radial velocity behind the shock front, because the creation of microcracks significantly decreases the effective material strength and reduces the hoop (tangential) stress component. Figure 17 shows a comparison of the hoop stresses vs radius for microcrack-dependent and elastic materials. Due to circumferential deformation from microcracks, the hoop stress for the microcracked material is much less than that for the elastic material. This dense evolution of microcracks behind a shock front is responsible for fragmentation failure in brittle materials. In general, the evolution of microcrack density during the deformation of brittle materials can induce large changes in the values of intrinsic material properties. For example, increases in the density of microcracks change the porosity and the permeability that influence the transport of fluids through porous rocks.

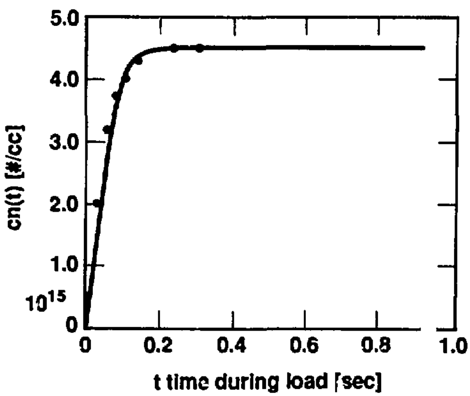

Figure 14. Microcrack density for 2.5 kg load history.

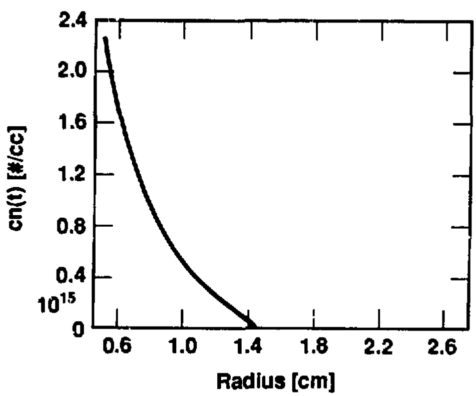

Figure 15. Microcrack density vs radius for microcracked material.

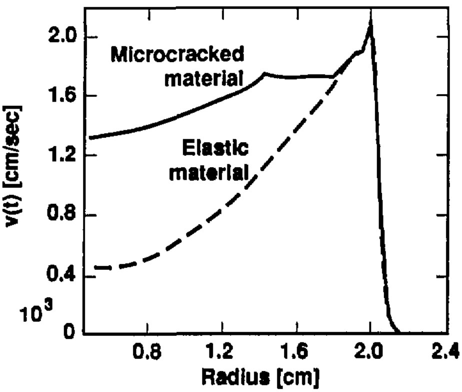

Figure 16. Radial velocity vs radius for microcracked materials and elastic materials.

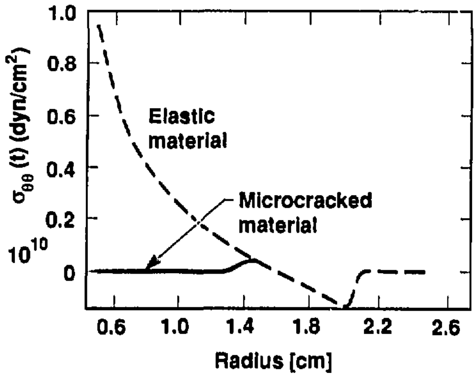

Figure 17. Tangential stress vs radius for microcracked materials and elastic materials.

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Verification

The Verification Group manages and carries out projects that use LLNL's seismic, technological, and computational expertise; geologic and seismic data bases; and classified national defense and intelligence information to develop better methods for verifying compliance with test ban treaties, interpreting intelligence data, and supporting DOE personnel as they help formulate arms control agreements, negotiate treaties, and evaluate compliance. During 1987 we directed projects in the following areas:

- **Regional seismic systems.**
- **Regional arrays and signal processing.**
- **Regional discrimination.**
- **Evasion and counterevasion.**
- **Test ban issues.**
- **Verification technologies.**

Regional Seismic Systems

As a major contribution several years ago to the development of in-country seismic monitoring technology, Sandia National Laboratories and LLNL, at the direction of the DOE, set up the Regional Seismic Test Network (RSTN), which comprises five seismic stations in the United States and Canada. This network was designed to model operational considerations that might be encountered in realistic monitoring situations. In addition, we installed a temporary array in Kansas, where the platform geology is similar to that in wide areas of the Soviet Union. During 1987, we performed location, site selection, and wave propagation studies using data from those sources.

Location Studies

As part of our research to better detect and characterize events, we are developing more accurate location techniques. We have carried out research on means to minimize regional location errors using data from the RSTN by (1) enhancing the recording signals through filtering, (2) identifying more types of seismic signals to give a redundancy for averaging errors, and (3) determining velocity variations for different travel paths. This effort has enabled us to locate smaller magnitude events with better accuracy. Location accuracy has been improved to about 50 km.

Site Selection Studies

A viable in-country seismic network for monitoring test ban treaties depends upon our ability to select suitable sites for seismic stations. High-frequency signals hold promise in detecting decoupled shots. Effective high-frequency stations (>10 Hz) rely on the premise that *quiet* sites with very low seismic noise can be found throughout the Soviet Union.

Our site selection study within the midwestern United States addresses these issues. The midwestern sites are not *quiet* sites, but they are representative of agricultural regions and indicate the sensitivity of high frequencies to cultural noise.

Our study implies that site selection procedures designed for short periods are inadequate for high frequencies. Above 10 Hz, strong spectral lines from mechanical sources and diurnal variations dominate the seismic noise; this cultural noise would obscure spectral reinforcement that often characterizes large chemical explosions and reduce the promise of high frequencies as a discriminant of decoupled explosions.

To eliminate the offending sources requires a large increase in their distance from a prospective seismic station. For example, the minimum distance from an active quarry must increase from 5 km to between 40 and 90 km. Table 1 compares our recommended minimum distances to those from the RSTN siting criteria and to earlier guidelines for short periods.

Table 1. Recommended minimum distances from noise sources

Sources of Disturbances		Minimum Distances: Carder (1963)[1] (km)	NVO-235-1 (km)	Revised (km)
Oceans	a	300		500
	b	1000		1000
Inland seas, bays, and large lakes	a	150	50-100	150
	b	500		500
High waterfalls, cataracts, or excessive flow over large dams	c	40	3-5	40-100*
	d	60		
Transcontinental oil or gas pipelines	c	20	3-5	20-35
	d	100		
Small lakes	c	20		20
	d	50		50
Reciprocating power plant machinery, rock crushers, etc	c	15	3-5	40-90
	d	25		
Non-reciprocating power plants, balanced industrial machinery	c	2	1-10	25
	d	4		
Low waterfalls, rapids on large rivers	c	5	3-5	10
	d	15		
Railways, if frequent operation	c	6	10-15	50-100
	d	15		
Airports and airways (heavy traffic)		6	10-15	20??
Small villages (water pumps)		-	1-3	25
Busy highway or mechanized farms		1	5-10	10-20
Graded county roads, high buildings		300 m	1-3	2-6
Low buildings, high trees		100 m		500 m
High fence, low trees, large rocks		50 m		100 m

[1]Carder, D. S., "The Requirements of a High-Sensitivity Seismograph Station," VESIAC Report 4410-63-X, October 1963.
a - with coastal mountain systems as western North America.
b - with broad central and coastal plains as eastern North America.
c - source and seismometer on widely different formations, or with intervening mountain ranges or alluvial valleys.
d - source and seismometer on same formation and with no intervening mountain ranges or alluvial valleys.
* - from NORESS information.

These recommendations must also apply to the final installation: power poles, fences, and surface structures intercept wind; while fans, power generation equipment, and similar mechanical equipment often increase the background noise. Only by emphasizing remote station sites can the prerequisite *quiet* sites be located and exploited for seismic verification using high frequencies.

One means of minimizing background noise levels is to emplace the seismometers below the surface in boreholes. At depth, the effect of seismic wind noise is reduced and penetration into unweathered rock allows better coupling to competent bedrock. Data from our field deployment near Red Lake, Ontario, and its comparison with RSON (an RSTN location near Red Lake) point out that interference

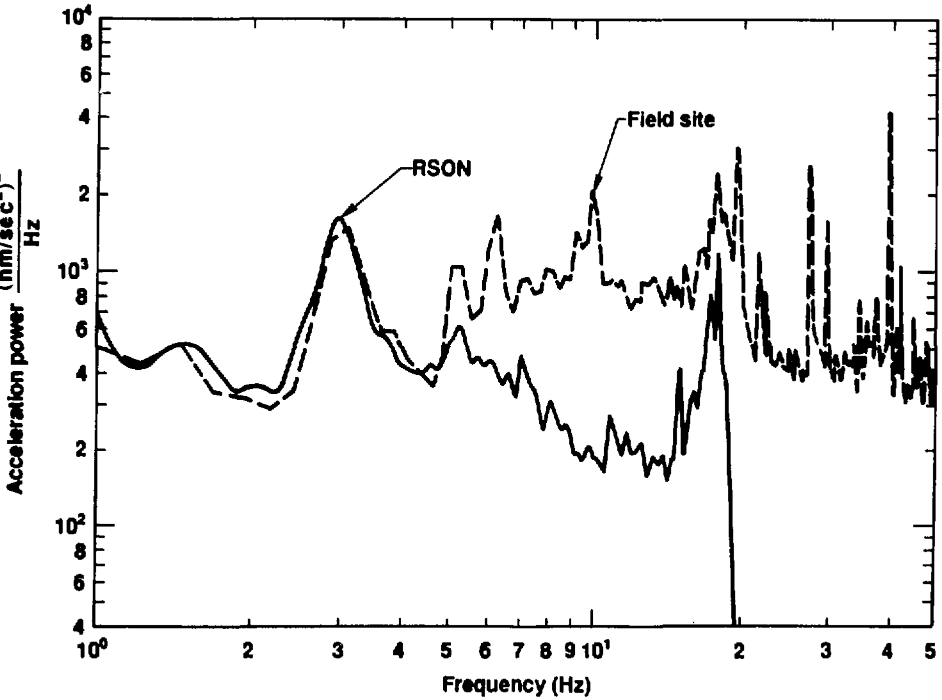

Figure 18. Comparison of mean acceleration spectra from RSON (solid line) and high-frequency site (dotted line) between 0900 and 0930 CDT on July 24, 1985. Below 5 Hz the spectra exactly match, while a dip occurs at 13 Hz—a null from standing wave interference for a seismometer located 100 m below the surface.

of the upgoing seismic wave and its reflection from the free surface decreases the amplitude of both noise and signals at specific frequencies (broad spectral nulls or holes). This affects *both* the body wave signals and the noise, and complicates the estimation of source parameters (e.g., corner frequency and high-frequency asymptote) and decay of high-frequency noise. For valid interpretation of borehole data, the effect of spectral nulls must be removed during analysis.

Figure 18 compares the noise spectra at RSON to the spectra from the high-frequency field site. Both sites see the same background noise at low frequencies: between 5 and 15 Hz the spectra diverge with the borehole seismometer, RSON, as the quietest site by 6 dB. As the spectra approach 18 Hz, they are again converging.

The dip in noise power at 13 Hz may actually represent a side effect of seismometers emplaced within a 100-m borehole at RSON. Seismic waves vertically incident on a free surface have a null point at depth of 1/4 wavelength, and additional null points for the standing wave are located every additional 1/2 wavelength in depth.

For this structure, the fundamental frequency for the first null occurs at 13.5 Hz, which agrees with the maximum divergence in Fig. 18. Between the first null (13.5 Hz) and the second null (40 Hz) is a point of reinforcement at 27 Hz, which should give amplitudes equivalent to the free surface; this could explain the convergence of the two noise spectra as the frequency approaches 18 Hz. The signal spectra should also have the same sequence of nulls and reinforcements in its spectra; thus, the decrease

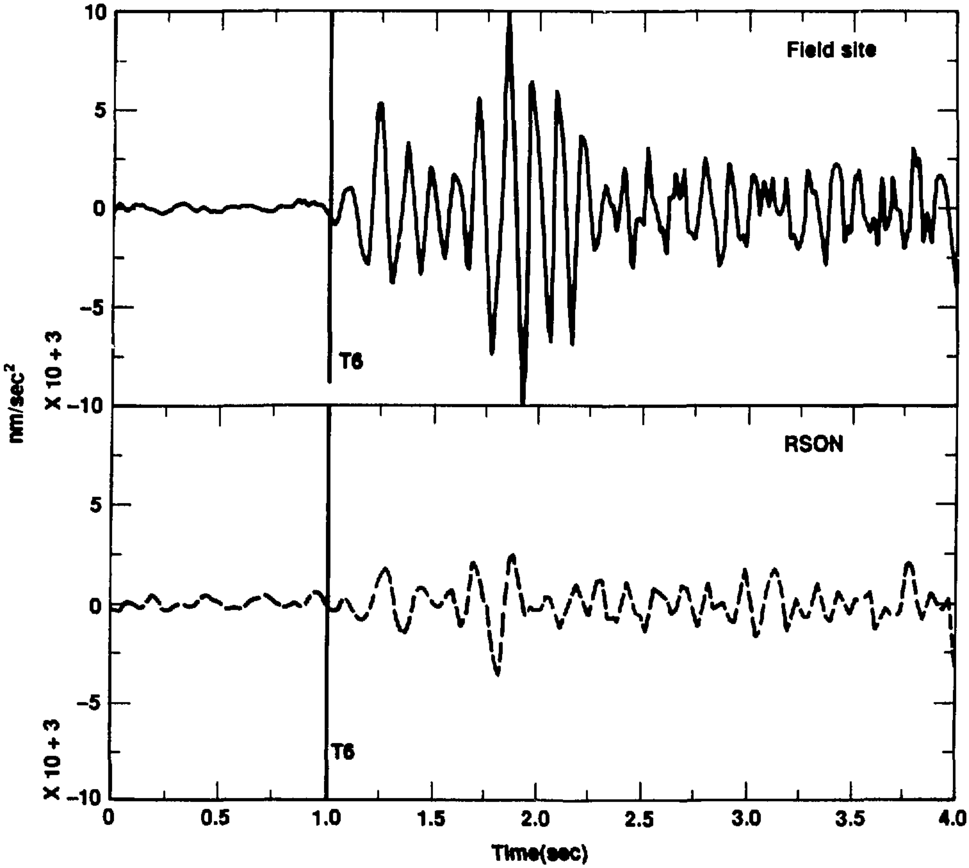

Figure 19. Comparison of regional P_n phase at RSON and high-frequency site in equivalent passbands. A 1- to 17-Hz passband allows direct comparison between the waveforms for an explosion of 380 km on August 6, 1985. The separation between the stations is 6 km. The field site shows much greater amplitudes and signal-to-noise ratio than RSON. The cause may be standing wave interference from emplacement within a 100-m borehole, or perhaps local geologic heterogeneities. A lower-frequency teleseismic event, which occurred four days earlier, shows excellent agreement betweeen waveforms recorded at the two sites.

in noise at the null does not improve the signal-to-noise ratio (SNR) for detection, but may merely produce a more complex spectra.

For teleseismic events at low frequencies (near 1 Hz), the waveforms match one another. For P_n from a regional explosion at 380 km (Fig. 19), the amplitudes from the borehole seismometer at RSON are a factor of three smaller at the dominant frequency (8 Hz) than at the surface site. A broad spectral null near this frequency agrees with the theory for an incident angle near 45° from vertical. Our SNR should remain constant; however, our surface field site has a much greater SNR than RSON for this regional phase. Different frequencies for spectral nulls from P_n and noise could partially account for the poorer SNR at RSON. If the null for P_n occurs at a lower frequency than the noise, the SNR would decrease. Alternately, local heterogeneities along the path focus and de-focus the regional phase and produce high amplitudes for P_n at specific sites.

Distinguishing between these two mechanisms is important for site selection and installation of seismometers. Spectral nulls from borehole emplacement of the seismometer represent a disadvantage compared with surface installation, but this disregards isolation from wind noise, which can be achieved within a borehole.

Wave Propagation Studies

In a network installed in the Soviet Union for treaty verification, there will be an initial period of testing and calibration. Included in this testing will be a study of the geologic structure around each station from an analysis of the received seismic signals. This information will be important to in-country monitoring because it enables us to make allowance for wave propagation in order to analyze seismograms for source characteristics. We are undertaking such a study on the dispersion of the R_g and trapped SH waves at the temporary array installation in Kansas.

At the Kansas array, we collected a large number of seismograms of quarry explosions at distances ranging from 100 to 150 km. These show pronounced surface waves, which may be used to calibrate the structure along the path from the source to the array. Since the geology is reasonably uniform in this platform area, calibration of short regional paths provides a calibration of the array site itself.

Surface waves give a relatively quick method of estimating shallow structure around the station. Structure is inferred from the dispersion of the surface waves, which is a property of channelled waves. The propagation velocity of such waves changes with frequency, generally increasing as frequency decreases.

Dispersion occurs because the medium velocity typically increases with increasing depth. Surface waves occupy a range of depths. Lower frequency waves have longer wavelengths and typically sample the earth to greater depths than do higher frequency waves, thus encountering higher velocity material; consequently, they travel faster. Higher frequency waves, with shorter wavelengths, are confined to shallow surface layers with lower velocity material; consequently, they travel slower.

Measured dispersion curves can be used to infer the average velocity structure along the path from the source to the station. This estimate sheds light on the geologic structure around and under the station. A knowledge of the geology provides solutions to interpretation problems, such as the causes of complexity in signals and the causes of systematic bearing errors.

Figure 20 shows one of scores of R_g surface waves recorded by the Kansas array; it shows the signal filtered into different frequency bands to demonstrate the dispersion phenomenon more clearly. The signal in this example comes from a coal mine about 120 km southeast of the array. Figure 21 presents the dispersion curve measured for this wave.

To turn the measured dispersion curves into an estimate of structure involves a series of modeling steps in which structures are hypothesized, theoretical dispersion curves are computed, then they are compared against the measured quantity. The models are adjusted to bring the measured and theoretical curves into agreement.

DSVS/SEC

As part of DOE's project to design, fabricate, and deploy a Deployable Seismic Verification System (DSVS), we are assembling a System Evaluation Center (SEC) to determine the suitability of the data for treaty monitoring requirements. We feel that in order to adequately check and verify the system, the data will have to be processed in a treaty monitoring environment.

The DSVS SEC consists of an integrated data-analysis package of routines developed at the Laboratory in the Treaty Verification research program. These routines include SAC, a data analysis and display code; XAP, a signal-processing routine; and MAP, an interactive mapping and plotting program. The software is implemented on a UNIX-based computer system with a local area network. Our eventual goal is to develop an environment in which both automated and interactive processing methods can be used to efficiently develop and test DSVS data and network processing strategies that can be used to verify the operation and capability of DSVS.

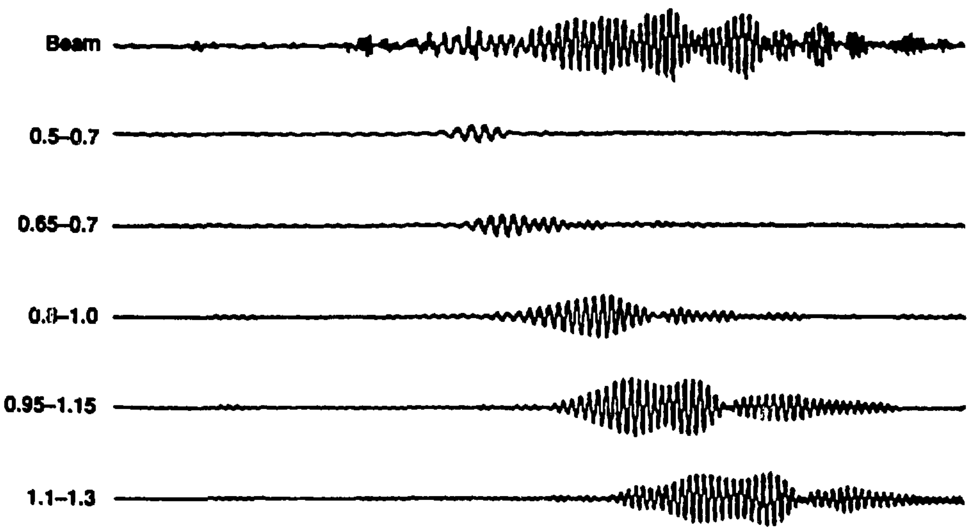

Figure 20. Seismic signal from a coal mine explosion as recorded by the Kansas array and as passed through band-pass filters: 0.5–0.7, 0.65–0.85, 0.8–1.0, 0.95–1.15, and 1.1–1.3 Hz.

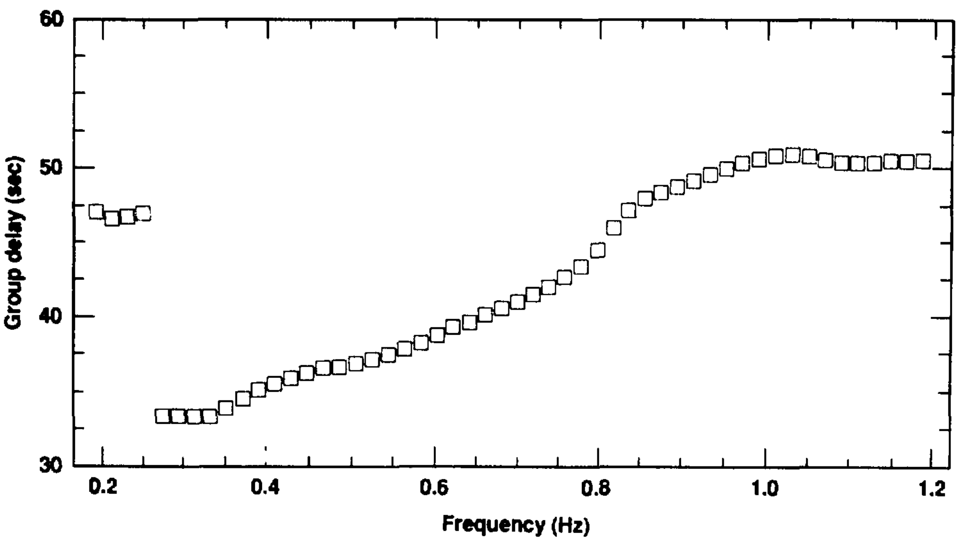

Figure 21. R_g dispersion curve for signal shown in Fig. 20.

Regional Arrays and Signal Processing

Regional arrays (sets of interrelated seismometers deployed in areas of about 10 km^2 or less) offer significant monitoring advantages over a single station deployed at the same site. The arrays can detect smaller signals, identify seismic waves on the basis of their propagation velocity across the array, and carry out preliminary locations of the source of the waves, and they are more robust when faced with certain types of spoofing. However, these advantages are not acquired without cost. The arrays are more complex systems, and the multiple signals they generate require more extensive processing. The fact that they occupy more territory than a single station may cause them to be viewed as being more intrusive.

Our efforts in the array and signal processing area during 1987 were designed to investigate the relative capabilities of arrays and single stations, to compare the array capabilities with those of other technologies such as high-frequency monitoring, and to develop efficient algorithms for carrying out detection, location, and identification functions using array data.

During 1987, we continued our comparisons of performance of three-component systems and arrays given various SNRs. In addition, we continued to develop and/or test algorithms for use on array data, some of which involved the application of expert systems.

Event detection and location under high-noise conditions are crucial, often overlooked problems in the treaty verification context. Most seismological research is conducted under conditions of relatively high SNR, i.e., low noise, for the compelling reason that good results are easy to obtain. However, the high SNR condition is not an appropriate assumption for an actual monitoring exercise. Under any conceivable treaty, the monitored nation will have access to the data from a monitoring network in real time, just as the nation doing the monitoring will. Should the monitored nation wish to perform a clandestine test, it may choose the time of the test, selecting a favorable opportunity for evasion. It would certainly elect to conduct the test under conditions of high natural (or unnatural, deliberately arranged) background noise.

Against this backdrop, a question arises about the limitations that high-noise conditions would impose on detection and location. Since arrays and three-component stations are, to some extent, competing candidates for use as elements of a monitoring network, we need to know how well each would perform under severe noise conditions. When considering the composition of a monitoring network, we need to know where arrays are really needed and where we can get by with three-component stations.

Unfortunately, the performance of an array or a three-component station for location is dependent *not only on the data collected by the instrument*, but how the data are processed. To measure the exact performance, we must specify the exact signal or data processing method (algorithm) that will be followed. For example, we conducted a comparison of array and three-component station location performance by simulation, based on a choice of algorithms that we considered to be good. The difficulty with this approach is that the results depend on the choice of algorithm. The results may be disputed on the basis of choice of algorithm, because there are as many algorithms as there are people engaged in algorithm research.

Fortunately, there is a way out of this impasse. Recent developments in sonar signal-processing theory offer the possibility of estimating the performance of the best possible method, even if that method is unknown. Formerly, it was possible to do this only for high SNR, but now it is possible at low SNR.

We are now in the process of adapting these methods for estimating location performance to the seismic verification problem. We have begun with the simplest case, that of perfectly coherent signals and incoherent noise, which produces estimates that are relatively easy to obtain, but are too optimistic. They are appropriate for certain fairly restrictive cases (limited array aperture, low-frequency signals). Figure 22 shows the results comparing array direction estimation performance and three-component station performance with these restrictions. We are now in the process of extending the work to more realistic conditions of poor signal coherence and spatially correlated noise. With these improvements, we expect to obtain information on optimal array designs and comparison with single three-component stations, particularly regarding maximum usable aperture and number of array elements.

Signal imperfections due to seismic heterogeneities can at times cause serious problems in the location of seismic events using conventional methods.

The purpose of our study was to determine ways of solving the seismic heterogeneity problem. By adopting and extending the MUSIC (MUltiple SIgnal Classification) algorithm to seismic array data and to three-component signals, we have made some progress on this problem.

We have completed two important substudies using the MUSIC algorithm for the seismic event location problem and using the NORESS seismic array data (Fig. 23). The first substudy focused on calibrating the array with real signals. In many frequency-wavenumber methods, direction and velocity estimation is obtained by assuming perfect planewave signals. When signal imperfections distort the properties of a plane wavefield, the assumption of perfect signals can be a source of error in the estimation process. However, the array calibration strategy of MUSIC is an effective way to accurately locate seismic sources in spite of signal refraction, scattering, and weak multipath. The algorithm involves computing and storing the eigenvectors for events whose locations have been determined by some other means. When the location of a new, unknown event is to be determined, a matching operation is performed by projecting the eigenvectors of the stored events with those of the new, unknown event. The best match between the new event and the known events determines the location of the new event.

The second substudy was concerned with designing high-resolution arrays when there is a rapid loss of spatial coherence. The array calibration was performed by assuming perfect planewave propagation. A bearing estimation study with various configurations of the NORESS array and with events from strongly heterogeneous sites (Fig. 23) indicates that with the MUSIC algorithm the bias of the direction estimate was reduced by an average of ~4° in ten of the twelve events by adopting a smaller aperture subarray (Fig. 24). Improvement in bearing estimation in MUSIC with a reduced aperture might be attributed to increased spatial coherency in the array. For methods with less resolution, the improved signal coherency in the smaller array is possibly being offset by severe loss of resolution and the presence of weak secondary sources.

We have also extended the MUSIC algorithm to single three-component stations in order to determine the bearing of the important regional phase, L_g. Our future work will address the extension of MUSIC to an array of three-component stations.

Using expert systems methodology, we are continuing to develop a computer capability for rapid inspection and analysis of seismic records, such as might be obtained from a seismic network involving arrays in the Soviet Union.

As additional aids for seismic interpretation, we

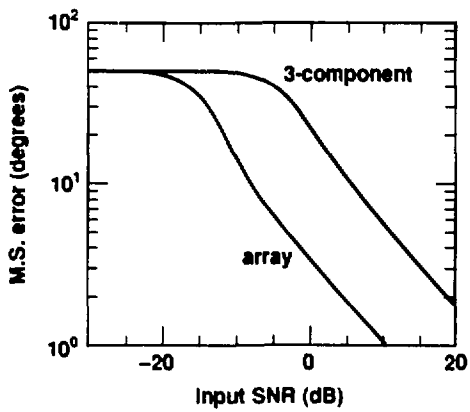

Figure 22. Array and three-component station mean-square direction estimation error for 2- to 5-Hz signals and a 13 element NORESS subarray with 1.5-km aperture. The array has a smaller error and 13-dB advantage in SNR.

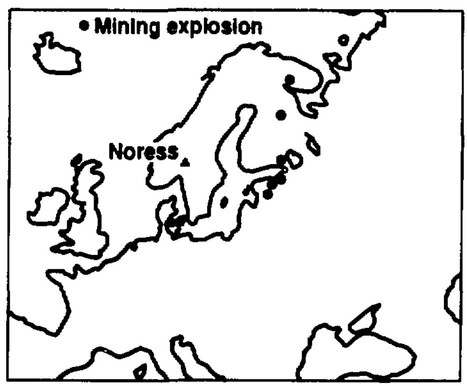

Figure 23. The NORESS array is located near Oslo, Norway. The events were located about 1000 km east of the array.

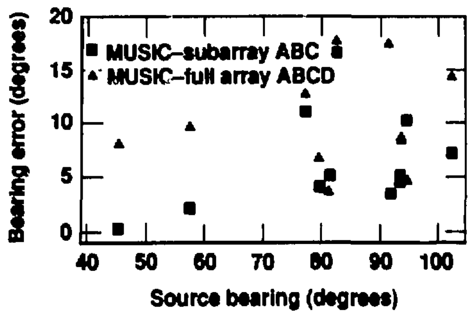

Figure 24. Bias in the bearing estimation (y-axis) vs location of the known events (x-axis). Comparison of MUSIC performance on the two arrays, ABC and ABCD.

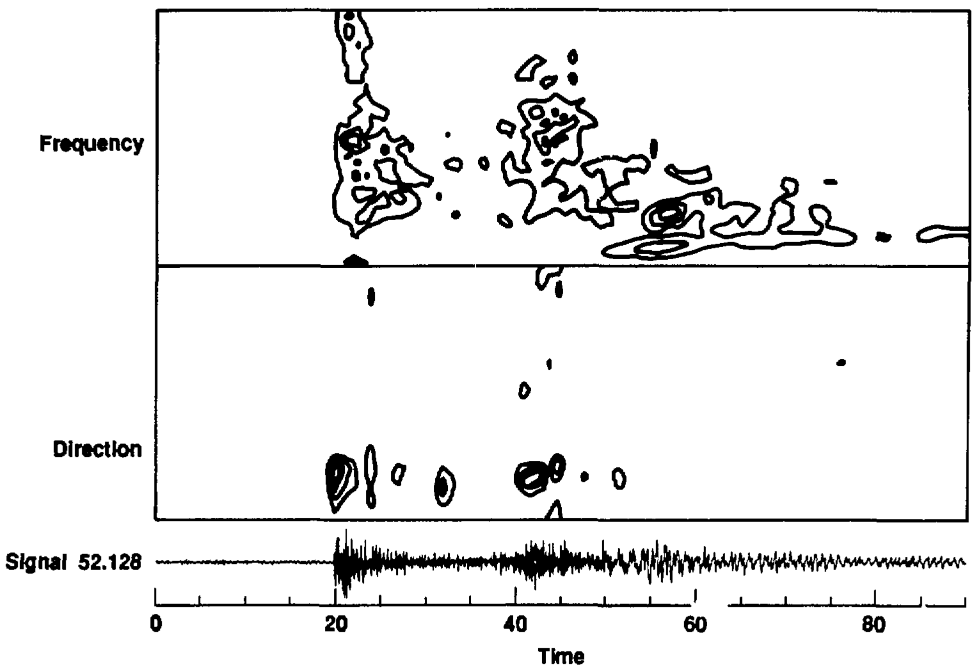

Figure 25. Polarization, rectilinearity, and total power distribution for a seismic signal from a quarry blast as recorded at the Kansas array.

have increased the number of distribution plots available to the seismic analysts at the Laboratory. These now include (1) power as a function of time and frequency; (2) power as a function of time and bearing; (3) array coherence as a function of time and frequency for a specific velocity and bearing; and (4) polarization, rectilinearity, ellipticity, and total power of a multichannel signal (usually three-component) as a function of time and frequency. These distributions are implemented as stack signals in the computer program XAP, and can be manipulated just as any other signal. Therefore, the analyst can generate new distributions from those listed above by suitable operations.

An example of the usefulness of distributions is shown in Fig. 25. This is a mining explosion recorded by the Kansas array at a distance of about 150 km. The bottom trace is the signal recorded at a single station of the array. The contour map directly above it displays the distribution of power in the waveform as a function of direction and time at a particular frequency (4 Hz). It shows clearly that the first two major waves in this event are arriving from about 60° east of north. The fact that they arrive from the same direction is consistent with both waves originating with the same event: they are said to associate. The top contour map displays the distribution of signal power as a function of frequency and time. The third major wave arriving at about 47 seconds is identifiable as a surface wave because of its low frequency and the fact that its frequency increases somewhat with advancing time (normal dispersion; in fact two modes are clear in the distribution). The first wave is identifiable as a *P* wave because of its higher frequency content. On the basis of context (ordering or precedence) the second is the associated *S* wave.

The characteristics of the waves as well as their approximate times of arrival are made explicit in distributions. This is a great benefit to seismologists, who must otherwise infer important interpretation characteristics indirectly from the waveforms. We have demonstrated the feasibility of computing these and other distributions in real time for the NORESS data stream, and have developed an interactive graphical tool for examining direction and velocity distributions, which is color coded (for different frequency bands) to increase the amount of information available visually for interpretation.

Regional Discrimination

Although most verification analysts recognize the importance of having in-country seismic stations at regional distances from all source locations, little has been done to systematically evaluate the discrimination performance of such regional seismic stations. In part, this is owing to the recognition that the results are highly dependent on the geophysical properties of the region. In part, the lack of such studies is owing to the lack of a suitable database. In 1987 we continued the systematic study of the extensive database of explosions and western U. S. earthquakes that we began to compile in 1985. We have extended the study of the discriminant based upon relative differences in the body- and surface-wave magnitudes generated by explosions and earthquakes, have considered discriminants based upon spectral content (including some high-frequency studies), and have done some initial work on the use of multivariate statistical techniques for discriminaton.

In our previous work (see the *1986 Earth Sciences Annual Report*), we compared surface-wave vs body-wave discrimination results obtained using published regional western U.S. magnitude definitions with those obtained using a new definition that did not include the period of the waves being measured.

Using the new definition, we significantly lowered the misclassification rates (of explosions as earthquakes and of earthquakes as explosions). Much of our work in 1987 went beyond the standard magnitude discriminant studies and focused on new and modified discriminants. One of these is a modified spectral ratio discriminant that takes the spectral ratio in the 0.5–1 Hz band to that in the 2–4 Hz band for P_n, P_g, and L_g for Nevada Test Site (NTS) explosions and earthquakes located near NTS. Selecting earthquakes near NTS minimized the need for accurate path corrections.

In our study we found that similar measurements were less than satisfying; consequently, we modified the discriminant by extending the band to higher frequencies utilizing our broadband capabilities. We also wanted to see if simple distance corrections could be applied to make the technique work for a wide distribution of regional events. In a pilot study we tested the technique on 74 western U.S. earthquakes and 78 NTS explosions.

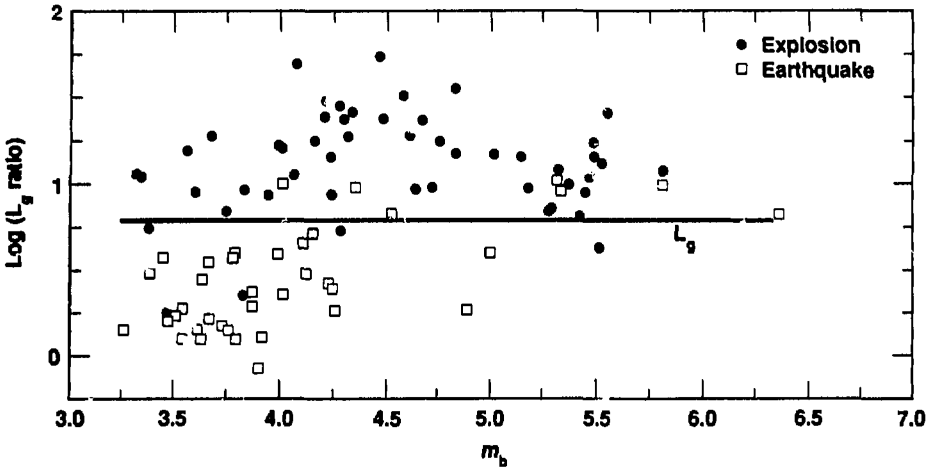

Figure 26. Good separation of earthquakes and explosions is observed for m_b<4.5 for all phases.

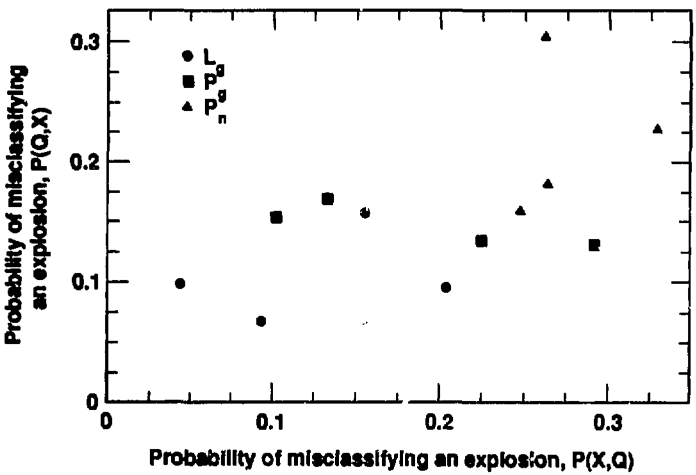

Figure 27. L_g performs the best, followed by P_g and P_n.

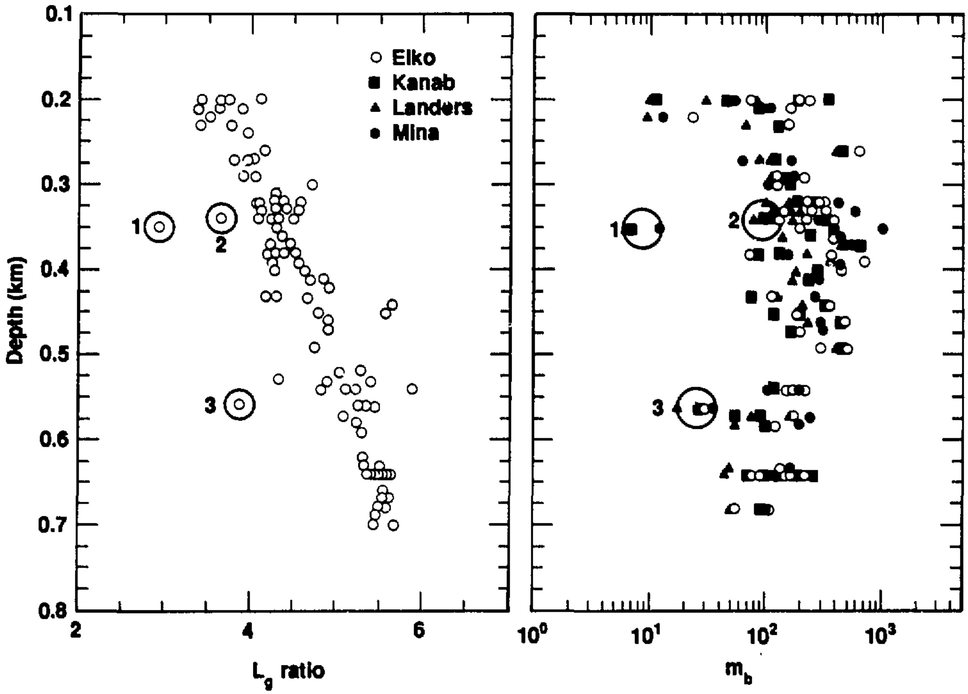

Figure 28. Overburied explosions show low spectral ratios and may be misclassified.

After applying simple distance corrections, we found the ratio of (1–2)/(6–8) Hz energy worked very well for P_n, P_g, and L_g down to small magnitudes (m_b~3; Fig. 26). L_g performs best, followed by P_g and P_n (Fig. 27); single-station misclassification probabilities ranged from 6–20% for L_g.

We noticed that a few explosions were consistently misclassified and discovered these were overburied. The left panel of Fig. 28 shows m_b vs depth, where three overburied explosions are highlighted and the rest of the points are close to standard containment depths. The right panel highlights the L_g spectral ratio for these same three events; they are rich in high frequencies relative to normally buried explosions. Unless adequate recording bandwidths are available, it may be possible to spoof the spectral ratio technique by overburying the explosion.

Figure 26 shows that the L_g spectral ratio for explosions appears to increase to about m_b ~4.5, then decreases. A similar pattern is observed for P_g and P_n. In contrast, the L_g spectral ratio for earthquakes appears to increase and then level off above m_b~4.5. Because of NTS containment procedures, it is difficult to determine if the explosion pattern is a depth effect or a source scaling effect.

Figure 29 shows fits to the L_g spectral ratios for commonly used earthquake and explosion source models. The latter models have depth-dependent effects built into the time function and cavity radius terms. The fit to the earthquake ratios is quite good for events with reasonable stress drops; however, the source model fails to predict the decrease in ratio for $m_b \geq 4.5$ using a realistic NTS structural model. Thus, the existing explosion source models may not be accurate at high frequencies, or other

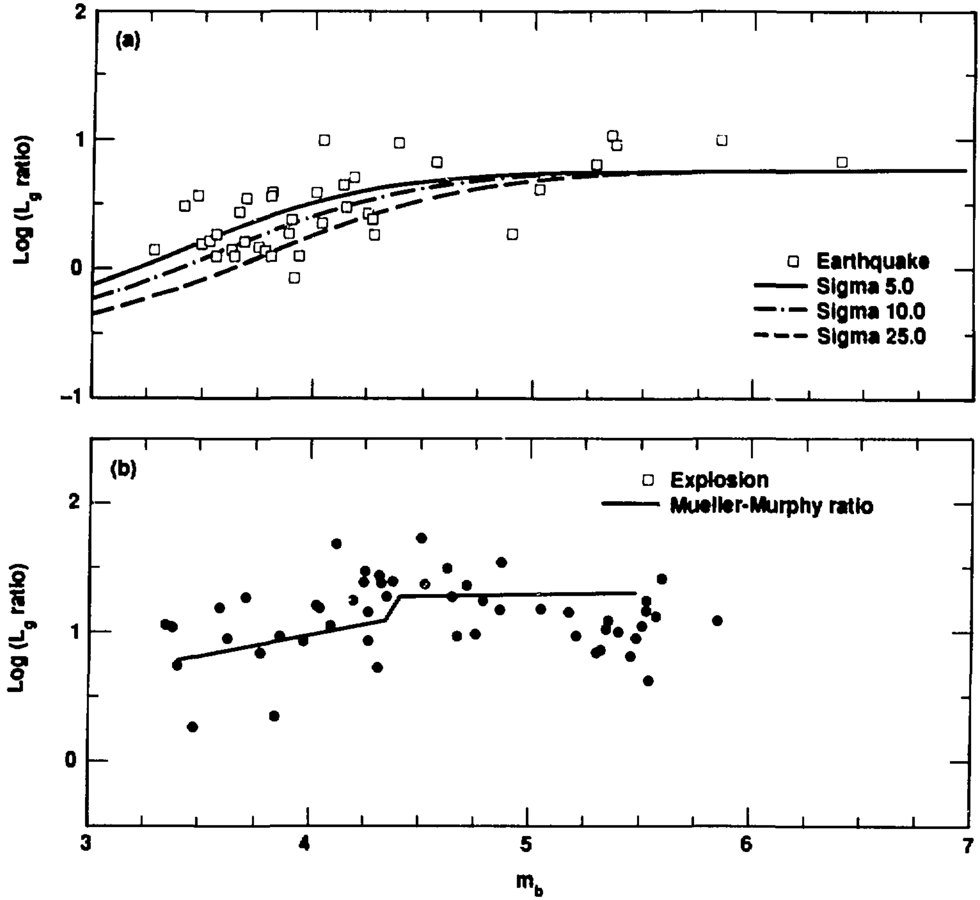

Figure 29. (a) Fits of Brune dislocation source model for stress drops of 5, 10, and 25 bars; and (b) Mueller-Murphy explosion source model to L_g spectral ratio (1–2)/(6–8) Hz vs m_b. The "spectral crossover" is difficult to explain using existing explosion source models.

factors may be contributing to the observations such as depth dependence of regional phase excitation or effects due to strain dependent attenuation.

Future work addressing these observations will involve calculation of regional synthetic seismograms with explosion source models that include effects of strain-dependent attenuation.

Evasion and Counterevasion

As part of our examination of evasion techniques, we have investigated the phenomenology associated with the generation of seismic waves by explosions. These studies have taken two forms: (1) a re-examination of the Salmon/Sterling data, and (2) the continuation of a comprehensive laboratory study of near-source explosion phenomenology.

The results of our re-examination of the Salmon/Sterling experimental data are significant with regard to seismic monitoring of a potential low-yield threshold or comprehensive nuclear test ban. Original analysis of data obtained in the Salmon and Sterling experiments indicated a corner frequency for Sterling near 10 Hz, a factor of 4 less than predicted by the simplest decoupling theory. The fact that Sterling apparently did not behave in accordance with theory had been disturbing. Our comprehensive analysis of the experimental records, based on direct spectral analysis of the free-field data, indicates that the Sterling experiment is in near perfect agreement with theory.

The Salmon/Sterling series was designed to provide experimental confirmation of the cavity decoupling concept for underground nuclear explosions. Salmon was a tamped (fully coupled) explosion with a yield of 5.3 kt, shot at a depth of 830 m in the Tatum salt dome (near Hattiesburg, Mississippi) on October 22, 1964. The explosion created a nearly spherical cavity, slightly larger than 17 m in radius. It cracked the surrounding salt to an observed radius near 150 m. Estimates of the "elastic radius" range from 174 to ~600 m.

On December 3, 1966, the Sterling experiment occurred inside the Salmon cavity. The device yield was 0.38 kt, producing an equilibrium pressure-to-overburden ratio of ~1. The rule-of-thumb value for decoupling is <0.5. By this criterion, the walls of the cavity were slightly overdriven. If the response were completely elastic, then the spectrum of the reduced velocity potential would display a corner (eigen) frequency, $f_c = c/2\pi R$, where c is the longitudinal wave speed in the surrounding medium and R is the cavity radius. For the Sterling parameters, $f_c \cong 42$ Hz. Analysis of the data, however, showed that the corner appeared at about 10 Hz. This implied that Sterling was only partially decoupled and that there was a considerable inelastic zone surrounding the cavity.

We recomputed the reduced displacement potential (RDP) using only the digitized output from the free-field Sterling gages and found that the previous analysis was in error. The reason for this discrepancy was traced to the method by which the original determination was made. Instead of using the near-field data from Sterling, near-field spectral data from the tamped shot that created the cavity (Salmon) were convolved with the Sterling-to-Salmon spectral ratio obtained from more distant seismic stations. The SNR of the seismic Salmon data was found to approach unity near 10 Hz (where the noise is due to the instrumentation not the earth), thus limiting the use of the spectral ratio method to this value as an upper bound.

The results are in very good agreement with elastic theory and imply that the decoupling factor of 70 observed in the seismic data for Sterling corresponds to *full* decoupling.

Test Ban Issues

In 1987 we supported DOE on test ban issues in specific ways: representation and participation in several interagency and international activities and further application of an analytic framework to the decision-making process of dealing with test ban issues.

We continued to furnish a technical representative for the DOE/ISA (for the ninth year) on the U.S. Delegation to the Ad Hoc Group of Scientific Experts (GSE), which meets twice a year in Geneva. The GSE has a mandate from the U.N. Conference on Disarmament (CD) to design a modern system for international exchange of seismic data and to design and carrry out experiments to test various aspects of the design concept. The main purpose of the system would be to aid countries in monitoring compliance with a Comprehensive Test Ban Treaty (CTBT), if and when one were agreed to.

The Group achieved consensus on a new organization of five study groups and experiment coordinators to further the work. The study group convenors will be responsible for drafting material for the next report to the CD. The experiment coordinators will be responsible for drafting material for coordinating the design and execution of experiments. Our representative has been designated as the U.S. Coordinator at National Data Centers for the U.S. Delegation.

As a byproduct of the GSE activity, we have participated in informal cooperative research studies with scientists from West Germany and Sweden.

We furnished technical representatives for DOE on U.S. Delegations to the Nuclear Test Experts Meetings (NTEM) and the Nuclear Test Talks

(NTT) in Geneva, both of which were bilateral discussions with the Soviet Union related to the Threshold Test Ban Treaty (TTBT).

We played a significant role for the DOE's participation in a comprehensive study of yield estimation by multiple methods for an interagency group: the Arms Control and Verification Committee (ACVC). As part of the ACVC work, we investigated methods of combining data in order to achieve better seismic yield estimates.

By combining measurements of multiple seismic phases (m_b, m_{bPn}, m_{bLg}), we have found that the uncertainty of seismic yield estimate is reduced. This methodology can be used to improve seismic yield estimates of events at Soviet test sites.

Our work was sparked by a study done by Ralph Alewine of Defense Advanced Research Projects Agency (DARPA), who combined three teleseismic phases for NTS events and found a significant reeduction in the uncertainty of the seismic yield estimate.

We used data from 50 NTS events, all of which occurred in saturated rock. We combined a teleseismic measurement for the body-wave phase (m_b) from Peter Marshall of the Atomic Weapon Research Establishment (AWRE) and two regional phase measurements from the LLNL NTS Network (LNN) seismic stations, m_{bPn} and m_{bLg}. We combined these seismic phase measurements as a weighted average, accounting for any correlations between the individual estimates. Although the different seismic estimates did show some correlation, the uncertainty in the combined yield estimate is still significantly lower than for any individual estimates but not as low as Alewine's results using teleseismic phases.

Using an objective procedure to combine the individual seismic measurements for events at the Shagan River Test Site (m_b, m_{bLg}, and M_0), we obtained a combined yield estimate. This uncertainty in the combined yield estimate for events at the Shagan River Site is also lower than the uncertainty in any individual phase estimates at NTS.

Analytic Framework for Evaluating Treaty Issues

We have formulated an analytic framework incorporating decision-analysis methods in order to study such test ban issues as quotas, TTBT, and low-yield threshold test ban.

Quotas on Nuclear Testing

We have recently completed a paper on quota restrictions in nuclear testing. Many recent studies have focused on treaty provisions involving reductions in threshold yield levels. In our study we extend these analyses by focusing on treaty provisions involving both quotas and yield reductions.

Verifying quotas is potentially complicated because they combine troublesome aspects of other test-limiting treaties. To determine compliance with yield restrictions, verification systems must be capable of accurately estimating the yield of tests. This is problematical, even at the relatively high 150-kt threshold under the current TTBT. However, under a quota restriction, allowed tests would also have to be scrutinized to assure there were no concurrent tests, just as is required with the current Peaceful Nuclear Explosions Treaty (PNET). Finally, counting the number of tests and assuring that none are conducted above the quota restriction or in unauthorized locations is similar to verifying a CTBT.

Our paper reviews options for quotas coupled with restrictions on the yield of allowed tests. We discuss the factors that influence the choice of quota and yield levels and the monitoring challenges for treaties involving quotas. We also discuss representative treaty options and verification systems, and identify inferior verification options based on a simple analysis. We conclude with guidelines for further analysis of viable treaties and verfication systems.

Threshold Test Ban Treaty

We are currently developing an analytic framework for evaluating compliance with the TTBT. The framework integrates analytic techniques to answer two key questions: (1) are the Soviets complying with the threshold, and (2) how should the U.S. respond to evidence of violations?

A decision maker's concerns are broader than "Do the data indicate a violation?" For the issue of evaluating Soviet compliance, several factors must be considered. These include:

- What do seismic and other data tell us?
- How accurate is our monitoring?
- Are violations militarily significant?
- What are Soviet motivations for complying with or violating the treaty?

Issues to be considered when deciding how to respond to the evidence include:

- Should we take strong action?
- What are the implications of incorrect actions?
- What are the Soviets expecting us to do?

The analytic framework should incorporate decision makers' judgement in each of these areas.

There are two outstanding issues related to the question of analyzing TTBT monitoring data and responding to evidence of violations. First, procedures and approaches must be developed to integrate information from diverse sources to arrive at consistent estimates of test yields. Most of the earlier studies have relied only on evidence from a single source of information (e.g., teleseismic *P*-wave magnitudes). Second, compliance evaluation approaches must be extended to consider explicitly the wide range of decision makers' concerns mentioned above, including the deterrence effects of effective monitoring and U.S. and Soviet cost/benefit considerations. These approaches should significantly extend the applicability and usefulness of current approaches, including those based only on statistical error considerations.

Our goal is to develop a compliance evaluation framework to meet these needs. The framework includes provisions for making explicit judgements about uncertainty in monitoring data, significance of violations, Soviet motivations to violate, U.S. values of possible outcomes, and Soviet values and expectations.

In a related task we are assembling existing data on Soviet testing, designing the process of calibrating the monitoring network, and developing procedures for combining monitoring data from all sources. The data and analysis from this task will be input to the compliance evaluation framework discussed above.

Low-Yield Threshold Test Ban Decision Framework

We are developing an analytic framework for evaluating low-yield threshold test ban decisions. The analysis focuses on the coupled yield threshold decision and verification system decision. The framework incorporates decisions, uncertainties, and values; it explicitly models the interaction between U.S. and Soviet decisions.

We are currently focusing on two components of the framework. An evidence-response model includes procedures for interpreting monitoring evidence and responding to evidence of violations. The approach is the same as for the compliance evaluation framework discussed above. A value model explicitly takes into account the military value of testing, benefits of arms control, and the disbenefits of violations and false alarms. When finished, these components will complete the framework.

Most of our recent efforts have focused on the issue of the value of testing as a function of yield. Judgements about relative values of testing and yield limits are crucial to a variety of treaty decisions, including responding to evidence of violations, negotiating a low-yield threshold test ban treaty, and choosing verification measures at given thresholds.

We have developed an assessment procedure that helps quantify experts' knowledge of the value of testing. We are currently talking to experts, both within the Laboratory and outside, about this issue.

Verification Technologies

The Verification Group manages and participates in projects designed to enhance existing monitoring technologies and develop advanced concepts.

In 1987 we continued our program of monitoring extremely low-frequency (ELF) electromagnetic (EM) emissions (1–30 Hz) from underground nuclear tests. We have been searching for ELF electromagnetic emissions from NTS underground nuclear tests to see if a signature can be found to augment our capabilities for treaty verification.

We are looking at the ELF band because only those frequencies are expected to maintain a measurable strength at distances greater than a few hundred kilometers from ground zero. In addition, any low-frequency EM energy that is coupled into the wave-guide defined by the earth's surface and the ionosphere may create a resonance, called a Schumann resonance, that may be detected worldwide at ELF frequencies.

Schumann resonance signals are detected using north-and-east-directed magnetometers in the horizontal plane (horizontal B field) and a simple antenna that detects the vertical electrical field. Worldwide thunderstorm activity provides a constant background of nonstationery ELF Schumann resonance signals that, for our purposes, are considered to be background noise.

We monitored four underground tests and obtained mixed results. For some events, signals were detected, mostly at close stations, which may indicate that underground nuclear tests produce EM signals that excite the earth-ionosphere (Schumann) cavity. Unfortunately, signals are not always detected, and, in addition, spurious signals explained only by other mechanisms confuse the picture.

As part of our advanced concepts effort, we are investigating methods to improve close-in seismic yield estimates by using downhole airgun seismic calibrations. Close-in seismic estimates of nuclear test yields from surface ground-motion measurements are frequently in error by factors of 2 or more, particularly at lower test yields. One major factor that causes errors in these yield estimates is the unknown seismic characteristics of geology in the region of the emplacement hole. We are attempting to improve the accuracy of close-in seismic yield estimates by experimentally determining seismic properties of the emplacement hole region with a small downhole airgun source.

Seismometers mounted at the surface are used to measure the travel time and relative amplitude attenuation of the airgun impulse originating near the working point of the emplacement hole. Accelerometers are later mounted at the seismometer locations to record the ground movement during the actual test event. The accelerometer recordings can then be corrected to account for the influence of the local geology along the seismic propagation path by using the airgun calibration results to thereby improve the final yield estimate.

This empirical approach requires an accumulation of statistically meaningful samples of airgun calibration with the associated nuclear event recordings. Provided that consistent relationships can be determined from the data, this approach has the potential advantage of improving close-in seismic yield estimates.

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Nuclear Waste Management

The Nuclear Waste Management Group's primary mission is to manage projects sponsored by the DOE Office of Civilian Radioactive Waste Management (OCRWM) through the Nevada Nuclear Waste Storage Investigations (NNWSI), Salt Repository Project (SRP), Repository Technology Program (RTP), and Basalt Waste Isolation Program (BWIP) offices. The technical activities are carried out jointly with other groups in the Earth Sciences Department, with other divisions and departments at LLNL, and with contractors. The OCRWM program at LLNL comprises three major activities plus support to the DOE in additional areas. These activities are the design and evaluation of a waste package for encapsulating high-level nuclear waste for permanent geological storage in a tuff repository; the improvement, use, and maintenance of the geochemical code, EQ3/6; and the Spent Fuel Test—Climax (SFT–C).

Waste Package Research and Development

The largest activity in the Nuclear Waste Management Group is the development of a waste package for a repository in tuff. This activity is divided into a number of smaller ones: characterization of the environment in which the package will function; testing of both glass and spent-fuel waste forms; testing of metallic materials for the waste package containers; evaluation and testing of other materials that might affect the waste package environment and performance; integrated testing of multiple components; the design of the waste packages and specification of the processes for their fabrication, closure, and inspection; field testing to support predictions of performance of emplaced waste packages; and deterministic and probabilistic assessment of the performance of the waste package over the extended time scale (thousands of years) of the repository function.

In December 1987, Congress designated Yucca Mountain near the Nevada Test Site as the single site that will be characterized for the nation's first nuclear waste repository. Because LLNL is responsible for design of the waste package for the Yucca Mountain repository, our studies have become a major focal point in this scientific field. Some highlights of 1987 in this waste package work follow.

Dissolution Experiments

Dissolution experiments for the silicate mineral cristobalite were completed as part of the characterization of the environment in which the waste package will be stored. This work used natural and synthetic material in flow-through cells. The dissolution rate was determined over a wide range of temperatures and pH levels. The results expand significantly the data available for this silicate mineral and provide an independent check of dissolution kinetic rate laws used in the EQ3/6 code.

Waste Package Environment

Another study in environmental characterization — extracting water from unsaturated rock — has been accomplished through the use of a semipermeable-membrane high-pressure technique. This method displaces water in rock pores with a noble gas at high pressure. The rock sample, which is in hydrologic contact with the semipermeable membrane, is dehydrated in the process. The displaced water is collected when it passes through the membrane. This technique has the potential of allowing us to analyze dissolved species in pore water trapped in rock. The technique is an extension of a widely used method for analyzing water in soils.

Computer Simulations

We have developed the capability to perform computer simulations of the hydrological and thermal processes that are expected to occur around a waste package. These calculations show the movement and drying of the water in the host rock due to the heat given off by the waste packages. Because these simulations extend over several thousand years, extensive modifications to the original code were necessary to improve its efficiency for our particular set of problems. Other enhancements to our physics models further improve the usefulness of the code for application to conditions at Yucca Mountain. These enhancements will aid in the modeling of future laboratory and field experiments as well as in furthering the understanding of the long-term hydrological environment around a waste package.

Gas Phase Transport

Preliminary numerical work was completed on an analysis of gas phase advective transport of ^{14}C at Yucca Mountain. The mass fraction of ^{14}C in the flowing gas phase is controlled by radioactive decay. Retardation is greatest at low temperatures, high liquid pH, and high liquid saturations. Accurate prediction of ^{14}C transit times requires knowledge of the timing of carbon release from waste containers, knowledge of the hydrologic conditions, and good chemistry. Although there is considerable uncertainty in these variables, an example calculation suggests transit times to the accessible environment on the order of the half-life of ^{14}C, which is 5,720 years.

Hydraulic Properties of Topopah Spring Tuff

A series of laboratory experiments have been performed on samples of Topopah Spring tuff to determine their characteristic hydraulic properties. This ongoing work is designed (1) to determine the empirical relationships between capillary tension and moisture content and relative and absolute (saturated) permeabilities, and (2) to ascertain the nature of fracture healing that may occur at increased temperatures. Bulk, saturated permeability decreases of approximately one order of magnitude have been observed when natural fractures are present. These occurred at temperatures in the range 50–100°C over time spans on the order of a couple of hours. Current work is aimed at determining whether the same processes happen within man-made, "saw-cut" fractures.

Ion Microscope Upgrade

The Cameca ion microscope was upgraded with the installation of a new resistive anode encoder. This development will allow the quantitative mapping of elemental concentrations in materials and provide depth profiles with resolution of less than one micron. This facility is currently being used to determine radionuclide transport properties in tuff.

Field Experiments in Tuff

We demonstrated in a field experiment in G-Tunnel at NTS that drying and wetting phenomena in porous, fractured tuff are strongly affected by the presence of naturally occurring fractures in the rock. The experiment used an electrical heater to induce drying, and wetting occurred after the heater was turned off. Spatial distributions of moisture content in the rock were mapped using a high-frequency electromagnetic geotomography technique. This successful experiment is leading to more complex experiments in the exploratory shaft facility at Yucca Mountain.

Geochemical Modeling Using EQ3/6

The regulations established by the Nuclear Regulatory Commission for storing high-level waste set unprecedented technical performance objectives, involving time periods of 1000 to 10,000 years. Extrapolations to these times can only be done by computer modeling, and these models must be based on an understanding of the fundamental scientific processes involved. A significant achievement in addressing design requirements implicit to 10,000-year performance was the modeling of complex geochemical interactions using the EQ3/6 geochemical code. In 1987 EQ3/6 was revised to provide faster operations and the ability to model solid solutions for a number of systems including carbonates, clays, and feldspars. Improvements in the EQ3/6 database added the capabilities of using the commercial software package (INGRES) to structure input of new data, to effectively handle large volumes of data (1400 species), and to provide the framework for including large volumes of data from the Nuclear Energy Agency (NEA) and International Union of Pure Applied Chemistry (IUPAC). A beta test version was released with all changes subsequent to 1985, including dissolution kinetics, precipitation kinetics, high-ionic-strength solutions, and a fixed-fugacity option for gases.

Using the improved code and database, we modeled the dissolution of spent reactor fuel and nuclear waste glass. These simulations involved up to 39 elements, 594 aqueous species, and 586 solids. Common applications of EQ3/6 or other geochemical

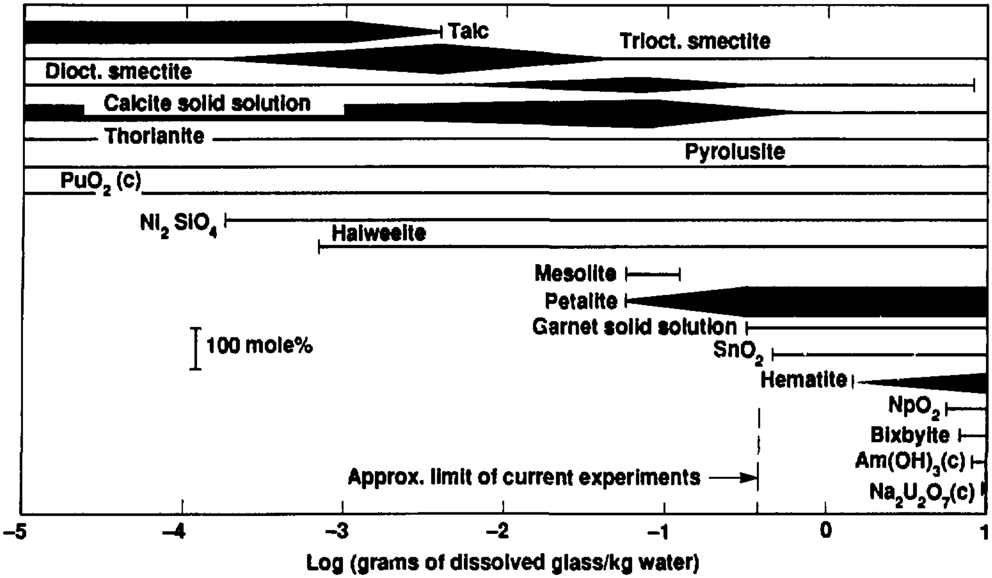

Figure 30. Mole percent precipitates in DWPF glass at 90°C.

codes involve fewer than a dozen elements and far fewer aqueous and solid species. Thus, the publication of these calculations represents a significant demonstration of our ability to model the highly complex interactions among rock, water, waste, and container material in the natural environment.

Figure 30 illustrates a sequence of solid precipitates that are calculated to form as waste glass dissolves. Current laboratory experiments have dissolved, at most, about 0.4 g of glass into a kilogram of water and have taken up to a year. This simulation extends to dissolution of 10 g of glass per kilogram of water, representing much longer experiments than would be practical to perform. Figure 31 shows how the calculated concentrations of elements in solution vary as glass dissolves and the solution equilibrates with precipitated phases. The concentration of radionuclides in solution is the parameter to be controlled in the repository.

Working closely with the Technology Transfer Program, we have distributed the code to several hundred users including universities, foreign countries, other national laboratories, and research groups as well as commercial users.

Spent Fuel Test—Climax

The SFT–C tested storage of spent-fuel reactor assemblies in the Climax granitic stock at the north end of NTS. The test was designed and constructed from 1979 to 1980, was operated with fuel in place from 1980 to 1983, was monitored and decommissioned through 1984, was analyzed in 1985, and final reports were written in 1986. In 1987 all reports on the SFT–C were completed and printed, providing full documentation of the only test storage of high-level waste material in granitic rock to the present.

The results of the SFT–C are documented in more than 50 reports on subjects as varied as the test design and construction, data acquisition systems, thermal studies, thermomechanical studies, test geology and geomechanics, radiation dose documentation and calculations, and transport and handling systems. Although work on the SFT–C has been completed at LLNL, we continue to receive requests for technical information both from within the U.S. and from organizations in other countries.

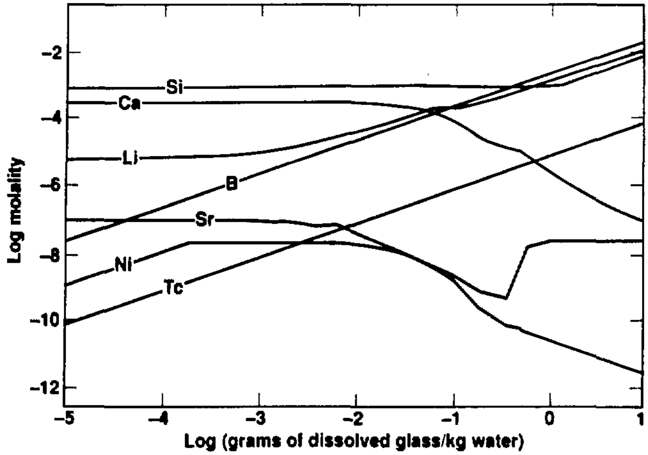

Figure 31. Variations in the calculated concentrations of elements in solution as glass dissolves and the solution equilibrates.

Canadian Cooperative Technology

For the past several years, the Waste Management Group has been involved in a cooperative program with the Canadian Nuclear Waste Program to transfer technology developed at the SFT–C and other LLNL expertise to the Atomic Energy of Canada Limited (AECL) Underground Research Laboratory (URL) near Pinewa, Manitoba. In 1987 this work continued to concentrate on instrumentation and modeling of coupled geomechanical and hydrologic processes. Work was initiated in these processes; much of the cooperative work is now directed towards planning field tests that will be conducted in the URL. Additional details are provided in the description of the Geology/Geological Engineering Group's activities.

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Geochemistry

The Geochemistry Group comprises geochemists, petrologists, and physical chemists working on a variety of earth science projects. The geochemists and physical chemists work primarily in low-temperature geochemistry performing experiments to determine the solubility and dissolution kinetics of minerals and to study waste-form/rock/water interactions as a function of temperature and pressure. In addition, they are currently working to develop and apply equilibrium thermodynamic/kinetic reaction-path geochemical modeling (EQ3/6) and to study the distribution of radioisotopes between fluids and solids in natural waters. They are also measuring the chemical properties of aqueous electrolytes (density, activity, and diffusion coefficients) and studying the distribution and chemical reactivity of dissolved inorganic species in surficial and ground waters. The petrologists are developing microanalytical techniques—primarily infrared—to study the composition of fluid inclusions; studying the isotope systematics and determining the age of basalts from the Rio Grande Rift, granulites from Sri Lanka, and ophiolites from the Sierra Nevadas; studying crustal metasomatism; studying heat production by natural radioisotopes in the lower crust of the earth; and performing material characterizations of a variety of solids.

1987 Accomplishments

During 1987 the geochemists conducted experiments to study the durability of glass waste forms and spent fuel, as well as the interaction between various waste forms and canister materials under both saturated and unsaturated conditions. We studied the stability of natural volcanic glass to hydrothermal alteration (zeolitization) and the ability of zeolites to resist crystallization to more stable phases (analcime) using samples taken adjacent to a potential nuclear waste repository in tuff. In support of database development for the EQ3/6 geochemical modeling code, we determined the solubility of quartz as a function of ionic strength (NaCl concentration) and temperature over the interval from 150 to 350°C. In addition, we determined the dissolution kinetics of muscovite as a function of time and pH at 70°C, and began a similar study to determine the dissolution kinetics of cristobalite. We began the process of acquiring or synthesizing and completely characterizing pure mineral standards to be used for measuring the basic thermodynamic properties needed to accurately model their geochemical behavior.

In EQ3/6 code development we upgraded the option for using Pitzer's equations to calculate activity coefficients in high-ionic-strength solutions, we improved the ability to model mineral solid solutions, and we began to develop a capability to model the dissolution of clay minerals.

We began the development of a new technique to measure the gas contents of fluid inclusions using Fourier transform infrared spectroscopy. During this past year we have nearly completed the installation of completely automated x-ray diffraction and x-ray fluorescence analytical laboratories. Activity coefficient measurements were completed for NaCl–$MgCl_2$ mixtures and for $La(NO_3)_3$, $Pr(NO_3)_3$, $NiCl_2$, and $ZnCl_2$. Mutual diffusion coefficient studies were completed for NaCl–KCl solutions. We studied the speciation and high-temperature behavior of trace volatiles (H_2, H_2O, CO_2, etc.) in silicates. We continued studies of the petrologic, chemical, and isotopic nature of the deep continental crust in Sri Lanka; determined the age and studied the Sm–Nd, Sr, and Pb systematics of Rio Grande Rift basalts; and determined the age and the Sm–Nd, Sr, and Pb systematics of ophiolites from the Sierran foothills.

As one example of the research we are conducting, Fig. 32 shows the results of our measurement of the rate of muscovite dissolution as a function of bulk solution pH at 70°C. We find that over almost the entire pH range the dissolution rate is a function of pH. Also, there are at least two different mechanisms involved in the dissolution process, one in acid solutions that involves an activated complex containing H^+ on the surface of the mineral and one in basic solutions that involves OH^-. Furthermore, our data suggest that the only other estimate available of muscovite dissolution rate is too high because of experimental complications from grain size and chemical affinity effects.

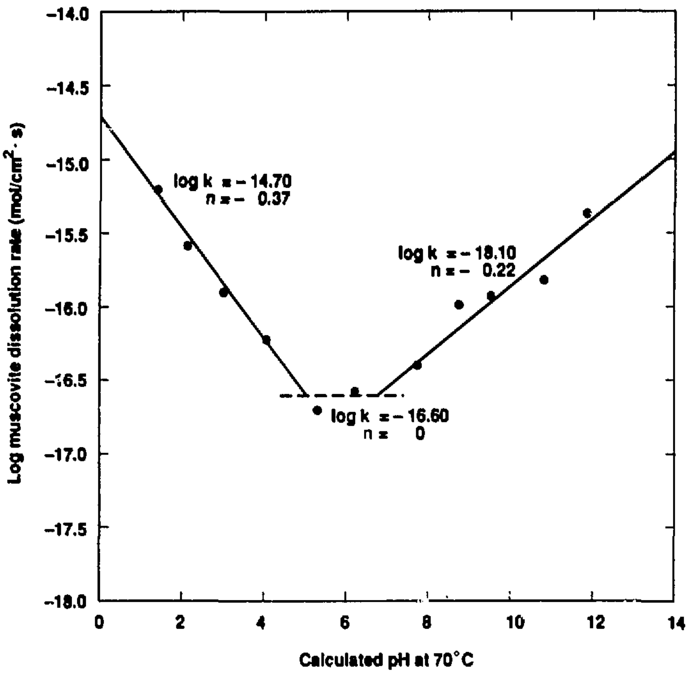

Figure 32. Muscovite dissolution rate vs pH at 70°C.

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Fossil Energy

The Fossil Energy Group supports several energy projects in the Earth Sciences Department. These projects range from research in oil shale to studies of the granular flow of solids and production of gas from unconventional gas reservoirs. Three programs were particularly noteworthy in 1987: the granular flow of solid material, petroleum geochemistry, and a new program—mild coal gasification.

Granular Flow of Solids

The objective of this project is to develop a fundamental understanding of, and the ability to predict, the flow behavior of granular solids. Advancement of the science of granular flow has broad scientific and industrial applications ranging from understanding landslides to the development of technologies for a variety of new synthetic fuels, including coal gasification and liquefaction, oil shale retorting, and tar sand processing.

We are using new mathematical models that calculate the motion of large numbers of interacting granules to directly simulate flows of real granular solids. These molecular-dynamics-like calculations are providing new insight into the microstructural details of flow behavior and are also being used to determine relationships between macroscopic quantities such as stress, strain rate, density, and mean kinetic energy of granules. The calculations agree with laboratory measurements where such data are available, and they agree with theories when comparable simplifying assumptions are made in the model (such as assuming frictionless and nearly elastic particles).

Comparisons with annular shear cell tests confirm that the model calculations capture the essential features of rapid shear flows of granular solids. Direct comparisons with laboratory tests of gravity flow through arrays of horizontal rods and with flows in inclined channels have provided further corroboration (and calibration) of our numerical simulation models. The simulations are providing guidance for the development of new statistical mechanical theories to describe such calculated features as anisotropic velocity and stress distributions within the flowing granular materials. During the coming year we plan to expand our study of boundary interactions and also initiate an extension of our modeling to include the effects of an interstial fluid.

Compositional Kinetic Model of Petroleum Formation

The objective of this project is to derive and verify quantitative chemical kinetic models of petroleum generation and expulsion from its source rock. We are conducting parallel studies in oil generation kinetics, oil cracking kinetics, phase-equilibrium calculations, and geological modeling to achieve that objective.

It is now well recognized that the chemical kinetics of oil generation derived from laboratory experiments covering a time frame of minutes to weeks extrapolate qualitatively to geological time of millions of years, but there are still major questions about how to derive kinetics for quantitative use in oil exploration. Related questions concern how sensitive the chemical kinetics must be determined for each source rock. Last year we developed and reported a relatively simple technique for measuring oil generation kinetics from micropyrolysis. We have made additional measurements during 1987, examining four lacustrine and eight marine source rocks and demonstrating that there are significant variations in the predicted oil generation temperatures of kerogens of the same general type. We also showed that other, more complicated experimental procedures are adversely affected by mass transport processes, which cause significant errors in the kinetic parameters. We have partially completed a comparison of various experimental procedures to determine the simplest, most reliable procedure for measuring oil generation kinetics.

The ultimate economic interest is in how much oil migrates to traps, so generation kinetics must be coupled to thermodynamic and transport properties to predict the timing of expulsion from the source rock. Depending on how efficient the expulsion is in various circumstances, variable amounts of oil may be cracked to gas before being expelled; this in turn affects the driving force for oil expulsion.

Moreover, understanding the mass transport contributions to various laboratory experiments is essential to properly interpret them. To address these issues, we are using more rigorous phase equilibrium calculations and have incorporated the Peng-Robinson formalism into our detailed pyrolysis model. We have just started a comparison of model calculations with a variety of published experimental results. We have also begun reexamining published literature to improve our oil cracking kinetics.

Because there is no rigorous theoretical proof that a quantitative extrapolation of chemical kinetics to a geological timescale is valid, it must be demonstrated empirically by deriving thermal histories of thermal sediments from geological models and then comparing the resulting predictions with geochemical evidence. Therefore, the verification of the chemical kinetic models depends on a good understanding of both the geologic thermal history as well as how oil migration influences the geochemical evidence. We have improved our geological modeling capability by writing a computer program for backstripping and steady-state thermal modeling of a sedimentary column. Application to the Uinta Basin showed that the simple geological model we used a few years ago is within the uncertainty of more sophisticated geological models. We have also analyzed several samples from that basin to improve the certainty of our previous demonstration that laboratory chemical kinetics extrapolate well to a geologic time scale.

Mild Coal Gasification

Background and Objectives

Bituminous coal, heated in the absence of oxygen, will pyrolyze to produce approximately 25% of liquid product that can be upgraded to liquid fuel. The other products from this "mild gasification" process are 15% medium-Btu gas and 60% char. The gas would be burned on-site for process heat and the char could replace coal in power plants, or be upgraded to higher-value products like coke. The DOE, through the Morgantown Energy Technology Center (METC), has a program to develop mild gasification technology using a combination of industrial and scientific contractors. We have been part of this program since March 1987, in large part because of our experience in the closely related area of oil shale retorting.

Our primary objective is to identify and develop a process that is reliable, efficient, and economic. The data, correlations, and operating experience we produce are to be used by industry to design, build, and operate demonstration or commercial-scale plants. Technology transfer to industry, particularly the METC contractors, is an important aspect of our project.

Progress

We have reviewed many mild gasification processes. High volatile bituminous coals are targeted for mild gasification because they produce the highest liquid yields. During pyrolysis these coals soften, swell, and become sticky, causing severe problems with many processing approaches. We have recommended three processes as being the best candidates for further development, and we will be developing one of these processes—the externally heated screw pyrolyzer—to determine its ultimate commercial potential. Both single-screw and twin-screw methods are possible. The coal is heated by contact with the hot barrel and screw walls. The oil vapor and gas are removed through vents that lead to a condenser.

The principal disadvantage of a single-screw method is that deposits may accumulate in the channels, clogging them. We are assembling a single-screw pyrolyzer with which to assess the severity of this problem. Fully intermeshing twin screws are self wiping and do not have this deposit problem, but they are expensive. We measured heat transfer rates to coal in a rented twin screw. From these data, we can more accurately estimate the size and cost of the twin-screw process.

Technology transfer has also been a main thrust of the Fossil Energy Group. We have shared our findings, served on an advisory panel, and provided technical advice and interpretation on experiments and plans to an industrial DOE contractor in this program.

Future Work

Several specific tasks are planned for the rest of FY 1988. We will complete assembly of the single-screw pyrolyzer and run it to evaluate the severity of deposit formation and other potential operating problems. Industry representatives will be invited to observe these tests. We will refine our throughput and cost correlations for the twin screw. Based on these results, we will focus our development efforts on either a single- or a twin-screw pyrolyzer.

During FY 1989, we will either modify the single screw or purchase and install a twin screw so that well-instrumented, material-balanced runs can be made. The results and attending correlations, as well as our operating experience, will allow more confident process scale-up by industry. In addition, during FY 1989 we plan to put considerable effort into bench-scale research to improve the liquid yield and the liquid quality.

Longer term work will include developing one or both of the other two processes we recommended. These processes use hot solid particles to heat the coal, which offers special advantages but is more complex.

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Seismology/Applied Geophysics

The Seismology/Applied Geophysics (SAG) Group uses its talents to support many programs and projects throughout the Laboratory, including the Seismic Monitoring Project, the Nuclear Test Containment Program, the Nuclear Waste Management Program, the Unconventional Gas Program, the LLNL Site Seismic Program, and the Basic Energy Sciences Program. The SAG Group emphasizes a multidisciplinary approach to problems. Expertise in the group covers a very broad spectrum; its strengths lie in the areas of seismic research; seismic instrument development; borehole geophysics; geostatistics; logging tool design; structural geology; and seismic processing, analysis, and interpretation. In addition, group members provide management for several LLNL programs including Seismic Monitoring, the LLNL Site Seismic Program, and the LLNL Seismic Observatory.

Seismology and Geophysics to Characterize Processes and Structures

We are conducting a number of studies to develop and utilize geophysical techniques to characterize subsurface processes and structures. These studies are carried out for the Office of Basic Energy Sciences, the Geothermal Program, and the Institution of Geophysics and Planetary Physics.

We have observed how seismic waves are modified as they propagate through the Earth. By means of artificial explosions as seismic sources to produce seismic velocity and attentuation images of the Medicine Lake volcano, we have related these images to processes occurring to the local geothermal systems. Steve Taylor and Jay Zucca have participated in field programs to utilize the later parts of natural seismic signals to look for scattered and reflected energy from anomalous zones in the crust of Long Valley.

Some of our studies measure earthquake mechanisms to understand processes occurring in the Earth. Howard Patton is studying the mechanisms of large Basin and Range earthquakes to infer the state of stress in the Earth's crust. Using data from Coalinga, CA, Steve Jarpe has examined the value of seismograms from small earthquakes for predicting the amplitude of ground motions from major earthquakes. Jarpe, Larrying Hutchings, and Paul Kasameyer have installed high-resolution seismic networks and arrays near the Salton Sea in California, to look for signals caused by geothermal production and injection.

Our group has been involved in two projects to understand thermal processes with the Earth. Kasameyer and Robin Newmark are completing a study of the near-surface thermal gradients associated with a portion of the Salton Sea geothermal field. Jerry Sweeney has used geologic data to estimate thermal histories for a number of sedimentary basins in order to provide input to models of petroleum maturation used to predict the depths at which oil might be found.

Our group has also used innovative methods to study geologic structures. Nai-hsien Mao has completed a geostatistical study in which he produced the best estimate of the shape of the basement surface beneath Yucca Flat using three disparate datasets: well logs, gravity, and seismic-reflection surveys.

Seismic and Other Research for Treaty Verification

We carry out many research projects for the Nuclear Test portion of the Treaty Verfication Program. These projects involve characterization and analysis of the nature of seismic sources, propagation paths, or noise characteristics of recording sites, and the application of the insights learned to issues related to treaty verification. Many of these studies are discussed in the Verification section of this report (pp. 26–43).

We have studied many aspects of the nature of the seismic source. Discrimination between explosions and earthquakes is one important area being studied. Our efforts include the use of our extensive database to evaluate a number of traditional discriminants based on data from regional networks, and the analysis of newer discrimination techniques involving higher frequencies. Patton has applied the Nuttli method to explosions in the database to assess yield estimation capabilities. In order to assess the effectiveness of cavity-decoupling, Marvin Denny has re-examined seismic data from a pair of explosions in a salt dome.

By studying the effects of propagation, and structure and local noise on seismograms, we improve our ability to record and interpret seismic data accurately. Jarpe and Keith Nakanishi are studying the ways in which regional structures influence the origin of the apparent direction of seismic energy. Taylor has used post-*P* energy to determine the crustal structure beneath regional recording stations, and Smith has evaluated the propagation of high-frequency energy over particular paths. Local site and system noise has been evaluated for the RSTN sites by Taylor and Nakanishi, and at a site-selection experiment in Kansas by Smith. In addition, Terri Hauk has participated in signal-processing research for regional arrays.

Our research for the Treaty Verification Program has also included experimental studies of the above-ground propagation of low-frequency electrical signals away from underground nuclear tests. Fred Followill has participated in the initial evaluation of this approach, and Sweeney is leading a data collection effort to determine the size of these signals at different distances from the explosion.

Borehole and *In Situ* Measurements

The SAG Group has carried out a variety of research activities in the development and interpretation of borehole and *in situ* measurement methods for the Nuclear Test Containment, Nuclear Waste Isolation, and Unconventional Gas Programs. Mao has developed a concept for a logging tool that measures velocity differences for shear waves polarized in different directions, and uses the results to infer the state of stress near a borehole. In response to the Containment Program's need to characterize the material surrounding an emplacement hole, Newmark has developed a data processing method to determine shear-wave velocities and Poisson's ratio from full wave sonic logs recorded in large, dry holes, and has participated in *in situ* penetrator studies to estimate the shear strength of rocks. Mao has evaluated application of geostatistical methods to measurements of properties around a buried waste canister.

Programmatic Support

The SAG Group provides a broad range of programmatic support to efforts of the Earth Sciences Department. Our support covers areas from equipment maintenance and data recording to managing large elements of programs and participating in support of international negotiations.

We are responsible for a large number of seismic data recording and analysis methods. The Seismic Observatory, directed by Norm Burr, is responsible for developing, maintaining, and fielding equipment for recording seismic data; for design, development, maintenance, and operation of a computer system and associated software to be used for the cataloguing, processing, and interpretation of the data; and for networking computers within the Earth Sciences Department. The Observatory maintains a four-station, broadband digital seismic system that surrounds the Nevada Test Site. Bob Rohrer routinely records signals from NTS events and provides yield information.

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Research

The primary mission of the Research Group is to expand the basic research opportunities available to scientists in the Earth Sciences Department. Current activities are distributed across two major programs: Office of Basic Energy Sciences Geosciences Program (OBES) and the Laboratory Institutional Research and Development Program (IR&D). In addition, the Institute of Geophysics and Planetary Physics (IGPP) provides a vehicle for interactions and collaborations with other research institutions in the University of California system. In this report we highlight examples of research activities in each of these programs.

IR&D - Fluid Flow and Transport Modeling

Many LLNL and DOE programs apply porous media flow and transport models to problems in nuclear waste isolation, enhanced hydrocarbon recovery, geothermal energy, subsurface radon migration, and groundwater contamination. In many instances, the successful development of such models will require significant advancements in our conceptual understanding of the relevant physical processes as well as the continued development of numerical techniques and modeling philosophies to solve the corresponding mathematical statements. Anticipated applications involve complex, interacting phenomena that occur in a variety of subsurface environments, including uniform, heterogeneous, and fractured porous media. Flow of multiphase liquid and gases, transport of various reactive chemical species in these phases, and transport of energy are among the phenomena of interest.

The ability to simulate relatively simple flow and transport processes in heterogeneous porous media has existed for years. However, the nature and complexity of many problems recently encountered strain our understanding of the physical behavior of these systems as well as the data and numerical techniques required in simulating them. Consequently, improved conceptual and mathematical models must be developed. Numerical methods must be refined and improved not only to treat the new and diverse equation structures but also to develop more efficient and practical tools capable of addressing a broad range of large, complex problems. Moreover, improved mathematical models and simulators will ultimately require carefully designed and conducted experiments in order to calibrate their constitutive equations and to provide a basis for model validation. In the past year significant accomplishments were made in the following areas of our project: (1) the development of a theory describing the movement of a liquid front in an unsaturated, fractured porous system; (2) the development of a very flexible, configurable finite-element code for modeling a broad range of flow and transport processes in porous media; (3) the modification and implementation of existing geochemical codes to include one-dimensional transport processes, including advection, diffusion, and dispersion, and (4) the initial development of a particle-based simulator to handle general reactive transport problems in porous media.

Enhancements made to LLNL's version of the TOUGH hydrothermal flow code originally developed by Preuss at Lawrence Berkeley Laboratory, as well as the development of pre- and post-processors, have facilitated significant achievements in several modeling studies, including several conducted for the Nevada Nuclear Waste Storage Investigations (NNWSI) Project. For the IR&D project, we conducted a modeling study of partially saturated flow in a fractured rock mass subjected to an episodic infiltration event. The system was idealized as being a semi-infinite set of parallel, vertical fractures. Flow in the fracture is dominated by gravity, while flow in the matrix blocks is dominated by capillary imbibition. Figure 33 is the liquid saturation distribution around a 50–μm fracture two days into the infiltration event. A parameter sensitivity study identified fundamental functional relationships between the fracture and matrix properties. A critical observation was that for noninterfering fractures, the fracture penetration depth h varies as $t^{1/2}$ for t sufficiently large.

Many existing codes, including TOUGH, are hardwired to address a broad range of flow phenomena, many of which may not be relevant to a particular model application; the result is wasted computational effort. Moreover, modifying hardwired codes to address additional flow phenomena is typically time-consuming. We have designed our new configurable, general finite-element code to facilitate configuring the model to account only for flow phenomena that are relevant to the particular application. This flexibility is implemented in our simulator by having the code able to take, as input, the governing equations for the problem. Through a simple list-oriented simulator language, the code converts the equations into the appropriate calls to the user-supplied constitutive subroutines necessary to generate the coefficient matrix used by the numerical solution method. These user-supplied routines can be written in Fortran or C. A "tool-box" of model-generic subroutines is available for the generic functions such as I/O and finite-element coefficient generation. The file format for the I/O data is hierarchically arranged for fast searching during postprocessing and is consistent with the list structure of our high-level simulation language.

The first phase of code development was to develop the basic generic portions of the code, such as the high-level language translator, finite-element operator functions, numerical solution, I/O functions, and a postprocessor. This phase is now essentially completed. The next phase is to configure the code to specific problems and to perform code verification on these problems. We have begun code verification on the comparatively simple problems of (1) flow in saturated porous media and (2) the diffusive release of a radioactive material in water. The latter problem is important to the study of the underground storage of radioactive materials.

In addition to the simple reactive chemical transport implemented in LLNL's version of the TOUGH code, we have made significant progress in modifying and developing codes capable of predicting changes in fluid composition and mineral zonation as a fluid flows through and reacts with a porous media. Reactions of interest are irreversible dissolution and precipitation, equilibrium precipitation, adsorption, ion/isotope exchange, and radioactive decay. Transport processes include advection, diffusion, and dispersion. Accomplishments include: (1) modifying an existing reactive transport simulator; (2) modifying LLNL's EQ6 code to simulate high-Peclet-number reactive transport; (3) developing general criteria for evaluating the validity of the local equilibrium assumption; and (4) initiating the development of a more general, particle-based reactive transport simulator.

A general, one-dimensional reactive transport code MCCTM developed by Lichtner was identified and implemented on LLNL's computers. During implementation it was found that the code was unable to handle certain types of reactions and became very inefficient when reaction fronts were encountered. The code has been modified to handle more general reactions and to be more computationally efficient. Although computational problems still remain in treating reaction fronts, it has proven to be a useful tool for scoping calculations on simplified systems.

With its EQ6 code, LLNL has been a leader in reaction path modeling of spatially static water-rock interaction. We have successfully modified EQ6 to simulate one-dimensional, high Peclet number reactive transport in a Langrangian reference frame. The modifications to EQ6 include the application of stationary-state theory. Reaction fronts that develop in natural systems move at a slow rate relative to transport and reaction rates. The fronts are considered to be stationary until inlet solution composition, fluid velocity, or reaction rates change upstream or until one of the reactant minerals completely dissolves. In this situation, steady-state concentration profiles develop upstream from a reaction

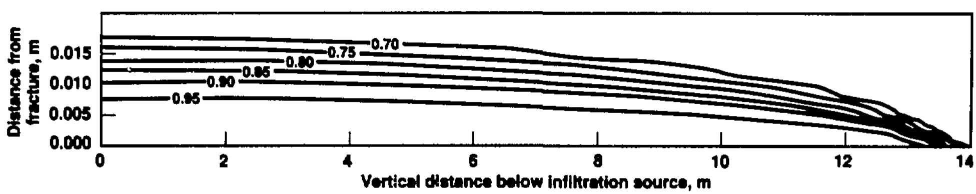

Figure 33. Liquid saturation distribution around a 50-µm fracture two days into the infiltration event. The figure is rotated 90° counterclockwise, and the horizontal distances are exaggerated by a factor of 100.

front, and precipitation and dissolution rates can be linearly extrapolated for the duration of the stationary state. Typically, stationary states endure for 104 years, permitting a model time step of comparable magnitude, which greatly accelerates computations.

Computations are further accelerated if a condition of overall local equilibrium (LEQ) can be assumed. LEQ is a good approximation if an initial disequilibrium condition relaxes to an equilibrium state over a distance and time period that is less than the spatial and temporal scales-of-interest. Spatial scales range from subcrystal to 10^0 *m* for laboratory investigations and from subcrystal to 10^3 *m* for field investigations. The computational time step and grid block size define the scales-of-interest in the computer model. An equation for the time and length scales is derived and analytically solved for a single component (silica), monomineralic (quartz), one-dimensional system. The time and distance required for an impulse of fluid, initially undersaturated with respect to quartz, to relax to equilibrium is calculated for a wide range of conditions. LEQ appears to be a good approximation for high-temperature systems. Low-temperature systems must be carefully examined before LEQ can be confidently applied.

We are also in the process of developing a particle-based simulator for general reactive transport problems in porous media. This simulator will be an extension of an earlier particle-tracking solute transport code used to study the dispersive nature of contaminant plumes driven by a spatially heterogeneous flow field. A conservative, particle-based transport model conceptually represents the mass of one or more aqueous chemical components as a large collection of particles, much in the same way as in particle-based plasma dynamics simulators. The particles are moved in space over discrete increments of time by advective, diffusive, and dispersive forces. A reactive transport simulator will, in addition, selectively remove or add particles after each time step to accommodate the loss or gain of component mass due to chemical reactions. Particle-based transport models can be extremely efficient in large, three-dimensional problems, particularly those involving multiple components, as other simulators, based on finite elements or finite differences, are often restricted to two-dimensions because of computational limitations. The particle-based algorithm is also well suited to parallel computer architectures, allowing for increased computational efficiency.

OBES – Continental Scientific Drilling Program: Inyo Drilling Project

Objectives and Approach

The general goal of research drilling in the Inyo Domes volcanic chain of eastern California was to improve our understanding of the thermal, chemical, and mechanical behavior of magma during its ascent toward the surface. The approach was to sample, by wireline diamond coring techniques, the subsurface portions of an igneous system that is so young as to be essentially unchanged by geologic events subsequent to its emplacement. In particular, this approach permits us to determine the distribution of retained magmatic volatiles before these components are redistributed by hydration and alteration, and to establish the relationship between eruptive and intrusive events before delicate tephra layers and structures are removed by erosion. Under favorable conditions, such an approach would permit measurement of the distribution of magmatic heat in an actively cooling intrusion. The sampling of intrusive structures by coring also provides information about subsurface features, such as fragile vent breccias, that would not survive exposure of such systems by erosion.

The Inyo chain was chosen for a drilling investigation because (1) it is the youngest of the rhyolitic volcanoes in the contiguous United States and hence the youngest of easily accessible rhyolitic systems, (2) its surface-accessible portions had been well characterized, and (3) a well-defined concept had been developed concerning its subsurface configuration. That concept, which was based on evidence that the linear array of vents had been active contemporaneously 600 years ago, was that the eruptions and accompanying surface formation were the surface manifestation of the emplacement at shallow depth of a rhyolite dike. It was suggested that such intrusive feeders were the general case for rhyolite volcanoes, because of the mechanical facility of intruding magma as a fracture-filling sheet rather than as a finger. The geometry of the hypothesized target lent itself to testing by drilling. Moreover, because the hypothesized dike crossed the structural boundary of the Long Valley caldera, the opportunity existed to compare the behavior of the same magma in the contrasting geologic environments of caldera fill and Sierran basement. A program of drilling (Fig. 34) was laid out that would sample the far-vent (Inyo-1) and near-vent (Inyo-2) sections of the largest of the lava extrusions, vented (Inyo-2, conduit) and unvented (Inyo-3) portions of the dike outside the caldera, and the dike inside the caldera (Inyo-4). Specific objectives were to compare the structure, chemical zonation, crystallinity, and volatile content of these igneous units in relation to the large variety of conditions in which they were emplaced, and to determine the relationship of eruption products to individual intrusive units and events.

Findings

Figures 35 and 36 display the general results of the four core holes. Subsurface structures encountered in the Obsidian Dome area were remarkably close to predrilling predictions, although there were surprises in the distribution of porosity, volatiles, and crystallinity, and in the existence of strong chemical gradients within units. In contrast, results at South Inyo Crater differed dramatically from a predrilling model that took theory, careful surface observations, and the previous drilling results into account.

The Obsidian Dome rhyolite lava flow was found to be about 50 m thick at both sample points, with a microcrystalline interior, 20-m-thick glassy carapace, and 10-m-thick glassy base. Obsidian is restricted to the distal portion of the flow; the entire near-vent section contains significant primary porosity (vesicles). Volatile contents throughout the sections are consistent with degassing to atmospheric pressure. The flow was fed through a conduit that is 30 m wide at 400–500-m depth. This feeder developed within a zone of tephra-related vent breccia and smaller intrusions that is 50-m wide. The conduit appears to be an enlarged portion of a simple dike that is 6-m wide at 600-m depth, 1 km south of the Obsidian Dome vent. In contrast to the lava flow, the intrusive portion of the system is wholly crystalline except for < 10-cm-thick glassy margins on the section through the unvented portion of the dike. The flow was found to have a mafic-downward zonation, from rhyolite to rhyodacite, that matches a radial-outward zonation in the conduit. The unvented portion of the dike is chemically more uniform and matches a portion of the tephra eruption; hence it is believed to have been emplaced early in the eruptive episode, during the explosive phase. No thermal anomaly clearly attributable to the intrusion was found.

Inyo-3 had encountered a sizable rhyolitic dike beneath an area of small phreatic craters and no discernible surface deformation. In contrast, the portion of the Inyo chain within Long Valley caldera that was active 600 years ago is characterized by much larger phreatic craters and spectacular surface fractures. Hence, it was postulated that Inyo-4 would intersect a silicic dike much larger than the one intersected by Inyo-3. Although Inyo-4 closely followed the planned trajectory across the Inyo trend and directly under the largest of the phreatic craters, it encountered no young silicic intrusion. Instead, it encountered a 16-m-wide breccia zone, the center of which is rich in pillow-like masses of caldera-moat basalt. The hole encountered basement much shallower and temperatures much lower than a Unocal well 900 m to the southeast.

Scientific Implications

Results from drilling in the northern portion of the chain confirmed the hypothesized close relationship between shallow dike emplacement and the Inyo lava dome eruptions. Evidence from volatile distribution for the close approach of magma to chemical equilibrium at locally controlled lithostatic pressure indicated that ascending magma is a chemically open system. A model for porous-flow degassing of magma was developed to explain this behavior and was based upon physical and geometrical constraints obtained from the drilling observations. An implication of the model is that eruptive behavior is strongly influenced by permeability of the shallow intrusive environment. Analysis of crystalline and glassy rocks at multiple depths permitted reconstruction of the degassing history and led to the conclusion that degassing is a two-stage process, with loss of water-rich vapor during isothermal decompression, and loss of chlorine-rich aqueous vapor during isobaric second boiling. Distribution of crystalline and glassy rocks within the system indicates that water loss plays as great a role as heat loss in "quenching" magma to glass. Chemical zonation of the system reflects a mafic to silicic sequence of magma emplacement during dome extrusion that apparently repeated a similar sequence during the tephra eruption. This may have resulted from an inversion of reservoir zonation during withdrawal, or a temporary, unstable zonation of the magma reservoir related to a mixing event. Much of the

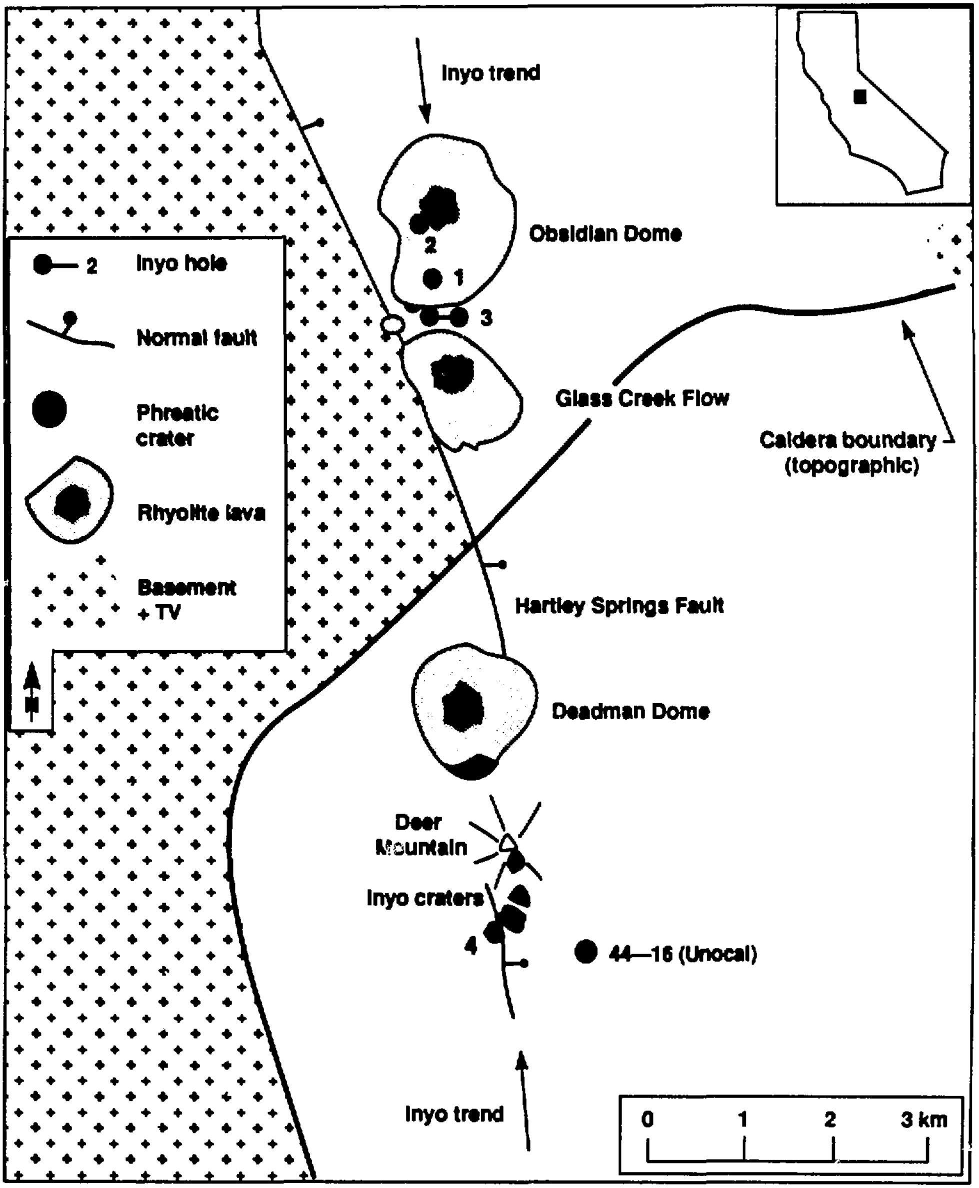

Figure 34. Inyo project drilling sequence and locations of holes.

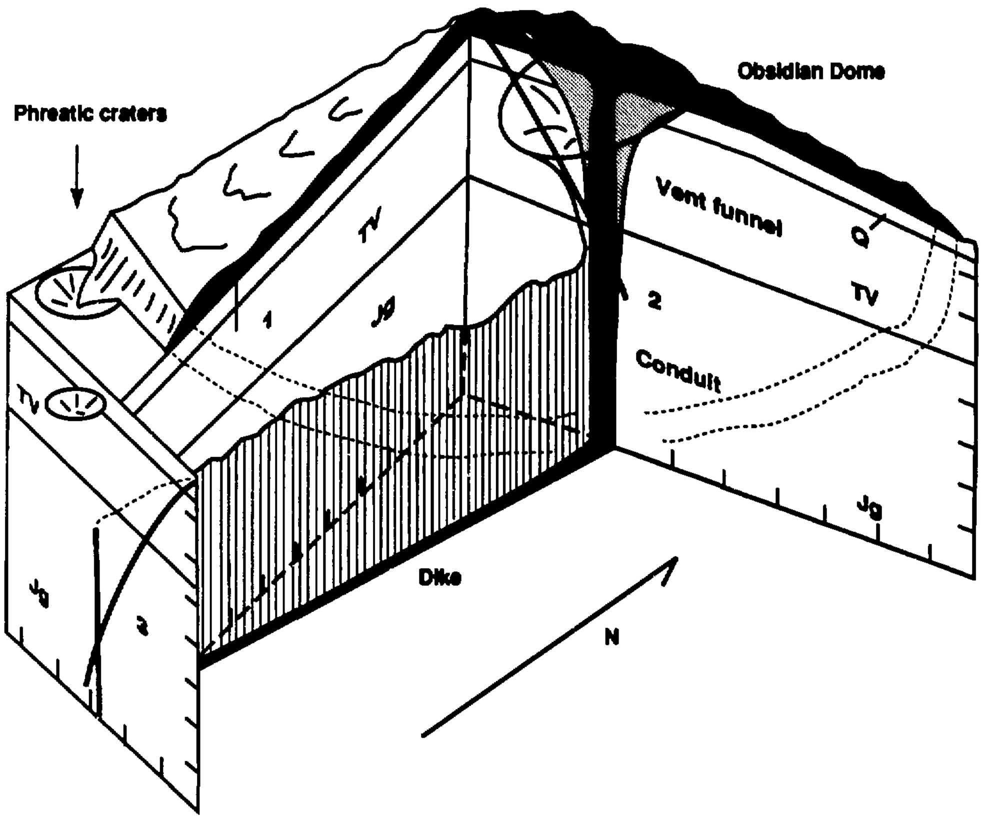

Figure 35. Cutaway section showing Inyo holes 1, 2, and 3, penetrating the flow, vent, and dike, respectively.

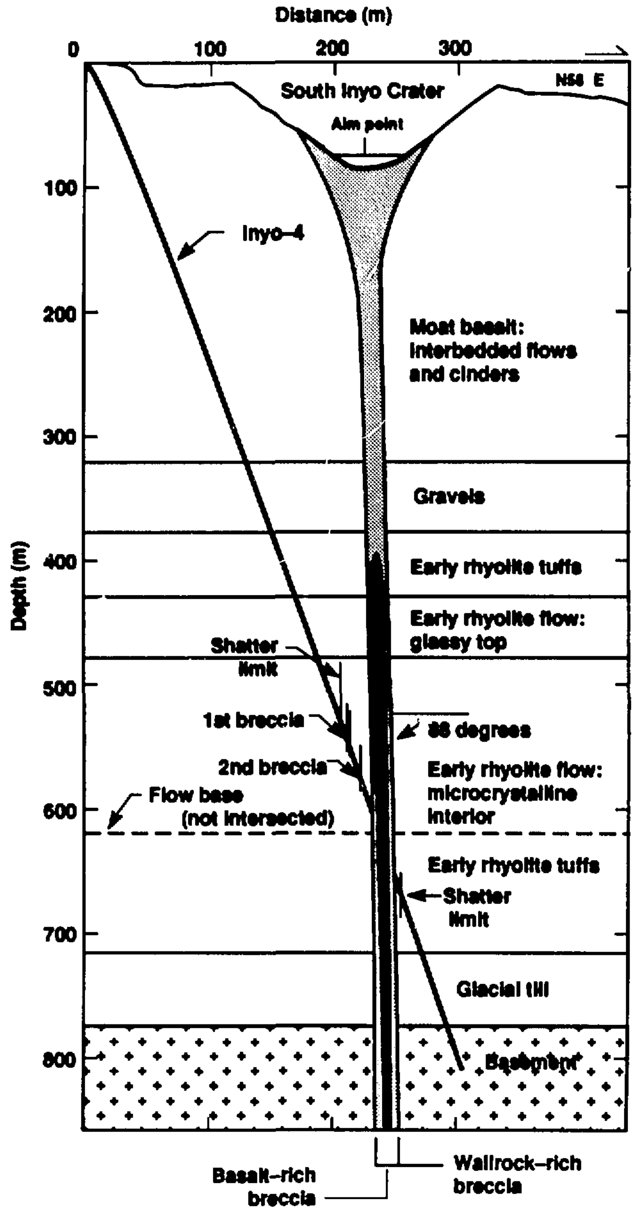

Figure 36. Vertical cross section through Inyo-4.

chemical variation can be explained by mixing with basaltic magma. This compositional problem remains unsolved.

Because drilling at South Inyo Crater did not intersect a dike comparable in composition to that beneath Obsidian Dome, it was not possible to carry out the comparison of magmatic behavior in the contrasting caldera and basement environments. However, the core provides the first view of intrusive structures beneath a young phreatic volcano and is now under study by a variety of techniques in order to understand the mechanisms of magma-water-wall-rock interaction that give rise to phreatic events. Drilling also constrained the position of a major portion of the structural boundary of the caldera, suggesting that much of the western moat is a cold, shallow shelf. The problem posed by surface extension well in excess of intrusion width is unsolved. The Inyo drilling was a joint project between Sandia National Laboratories, LLNL, USGS, and several universities.

IGPP – Seismic Investigation of the Continental Crust

Studies of the Crust and Upper Mantle—Northern California

G. Zandt is collaborating with K. P. Furlong (Penn State University) on the study of the seismic velocity structure, tectonically driven thermal processes, and geologic evolution of northern California. The Mendocino Triple Junction (MTJ) currently located off Cape Mendocino in northern California, represents a profound tectonic and thermal boundary. North of the MTJ, the western U.S. is underlain by a "cold" subducting oceanic lithosphere; whereas south of the MTJ, the base of the thin northern and central California lithosphere is exposed to "hot" mantle (in the "slabless window"). During the past 25 million years, western North America lithosphere has been progressively exposed to this tectonic and thermal perturbation as the MTJ migrated northward along the California coastline. The development and growth of the "slabless window" has produced an evolving system of mantle upwelling, crustal melting, volcanism, and crustal accretion in central and northern California. The eruption of the Clear Lake volcanics and the origins of the Geysers Geothermal Area are directly related to this process.

We believe the evolution of the San Andreas Fault System is also controlled by the thermal-mechanical processes associated with the development of a "slabless window." Lithospheric structure at the MTJ and the thermal evolution of the lithosphere associated with the San Andreas Fault System result in a plate boundary where the location for the deeper extent (10–100 km depth) of the plate boundary is offset 30–50 km (or more) to the east of the surface location of the plate boundary (i.e., the surface trace of the San Andreas Fault). The two vertical segments of the plate boundary must be connected along a horizontal or subhorizontal detachment surface in the mid- to lower-crust. Seismological and geodetic evidence in support of this hypothesis was presented by Furlong and Zandt (1986). Thermally controlled lithospheric strength calculations based on our tectonic model imply that the development of the offset fault is a natural consequence of the formation of the "slabless window," and may also explain the apparent inland migration of the Pacific-North American plate boundary over the past 25 million years.

Inversion of Teleseismic Receiver Functions for Lithospheric Structure

G. Zandt, G. R. Randall, and S. R. Taylor in collaboration with T. J. Owens (University of Missouri) are continuing work on the new broadband receiver function technique for the determination of lithospheric velocity structure. Long-period teleseismic body waveforms have often been used to infer crustal structure beneath isolated seismic stations. Recently we have developed an inversion technique to take advantage of new digital data from broadband seismograph stations in order to examine the detailed crustal and upper mantle structure beneath these stations. We completed the study of the Regional Seismic Test Network (RSTN) operated by the Department of Energy and found that, at sites where other seismic constraints exist, the structures inferred from teleseismic waveform modeling are generally in good agreement with the other studies.

With the exception of RSSD (in the Black Hills, South Dakota), the RSTN sites are characterized by relatively simple structure. This result is not unexpected due to their location in Precambrian shield regions. Station RSCP (Cumberland Plateau, Tennessee) exhibits the most complex waveforms which are due to the presence of late Paleozoic sedimentary sequences at the site and the southern termination of a Precambrian rift system just to the northeast. A gradational crust-mantle boundary is observed at RSCP as well as at the RSNY station in the Adirondacks, New York. At RSNY a high-velocity region in the mid-crust correlates well with a set of high-amplitude reflectors observed in nearby multichannel seismic reflection lines (COCORP). The crust beneath stations RSON (Ontario, Canada) and RSNT (Northwest Territory, Canada) are relatively simple, as indicated by uncomplicated receiver functions. In both cases, the crust-mantle boundary is abrupt, and RSNT is characterized by a remarkably simple crustal structure.

Converted Seismic Phases in Volcanic Regions -- Long Valley Deployments

Teleseismic *P*-waves are often utilized to determine the velocity structure beneath the recording station (see above), nowever, in regions with complex, laterally heterogeneous structure, deterministic methods such as waveform modeling are not currently practical. Volcanic regions are often characterized by complex heterogeneous structure but also by large impedance contrast interfaces (e.g., magma/solid contact) which should generate large *P-S* converted phases. Identification of such phases would be an important first step in the application of teleseismic waveform recording in volcanic regions.

In 1985 G. Zandt and S. R. Taylor deployed three three-component portable seismographs near Medicine Lake volcano, a Holocene shield volcano situated about 50 km east of Mount Shasta in the southern Cascade Range in northern California. Despite the voluminous volcanism exhibited at Medicine Lake volcano, no velocity feature indicative of a crustal magma chamber has been found near Medicine Lake. The teleseismic waveforms we recorded appear normal, and the vertical components area highly correlated over distances of at least 20 km.

In contrast to Medicine Lake, at Long Valley there is abundant geophysical evidence of one or more crustal magma chambers beneath the caldera. S. Mangino and G. Zandt in collaboration with L. Steck and W. Prothero (U.C. Santa Barbara) deployed portable seismographs within the Long Valley Caldera in eastern California during the summer and early fall of 1986. Steck and Prothero deployed three 3-component digital, broadband seismic stations on the Long Valley resurgent dome for two months. Mangino and Zandt deployed similar instrumentation at three different sites for about one month following the UCSB deployment. Steck and Prothero observed anomalously large energy on the horizontal components which they interpreted as strong *S-P* conversions, possibly from small magma bodies in the crust beneath Long Valley. Mangino and Zandt observed similar features in the seismograms recorded at sites off the resurgent dome but still within the caldera. We felt that the data was inconclusive as to whether it represented upward-traveling, converted shear phases or laterally traveling surface waves produced by *P*-to-surface wave conversions at the edges of the caldera. In both cases the vertical components were poorly correlated over distances as little as 5 km. All the investigators agreed that a small array deployment was necessary to address these questions and identify the nature of the large energy on the horizontal components.

In August 1987, a 3-km diameter array was deployed in the northwest corner of Long Valley Caldera as a joint project involving J. Zucca (LLNL), G. Zandt (LLNL), L. Steck (UCSB), and W. Prothero (UCSB). The array consisted of 10 stations telemetered to a continuously recording central site and 6 additional individually triggered portable recorders. The deployment lasted about two months, during which at least a dozen teleseisms, several large regional events, and numerous local events were recorded. Preliminary analysis of the teleseismic data indicates that at least the initial portion of the anomalous energy on the horizontal components is due to a *P-S* conversions beneath the array.

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