DOE/ER-0349

Summaries of Physical Research in the Geosciences

Published: September 1987

U.S. Department of Energy
Office of Energy Research
Division of Engineering & Geosciences

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DOE/ER-0349
Dist. Category: UC-11 & 70

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Washington, D.C. 20545

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FOREWORD

The Department of Energy supports research in the geosciences in order to provide a sound foundation of fundamental knowledge in those areas that are germane to the Department of Energy's many missions. The Division of Engineering, Mathematical and Geosciences–part of the Office of Basic Energy Sciences, which is under the Director of Energy Research–supports the Geosciences Research Program. The participants in this program include Department of Energy laboratories, industry, universities, and other governmental agencies. Their support, formalized by a contract or grant between the Department of Energy and the organization performing the work, provides funds for salaries, equipment and other materials, and an overhead allowance.

The summaries in this document, prepared by the investigators, describe the scope of the individual programs. The Geoscience Research Program includes research in geology, petrology, geophysics, geochemistry, solar-terrestrial relationships, aeronomy, seismology, and natural resource analysis, including their various subdivisions and interdisciplinary areas. All such research is related either directly or indirectly to the Department of Energy's technological needs.

INTRODUCTION TO THE GEOSCIENCES RESEARCH PROGRAM OF THE OFFICE OF BASIC ENERGY SCIENCES

The Geosciences Research Program is directed by the Department of Energy's Office of Energy Research, within the Office of Basic Energy Sciences, Division of Engineering and Geosciences. Research supported by this program may be directed toward one or more energy technologies, national security, conservation of the environment, or the safety objectives of the Department of Energy. The purpose of this program is to develop geoscience or geosciences-related information relevant to one or more of these Department of Energy objectives or to develop the broad, basic understanding of geoscientific materials and processes necessary for attaining long-term Department of Energy goals. In general, individual research efforts supported by this program may involve elements of all four objectives.

The Geoscience Research Program is divided into four broad categories:

- Geology, geophysics, and earth dynamics
- Geochemistry
- Energy resource recognition, evaluation, and development
- Solar-terrestrial-atmospheric interactions.

The following content outline of these categories is intended to be illustrative rather than exhaustive, and will evolve with time. Individual research efforts at the Department of Energy, university, college, corporate, not-for-profit, and other Federal agency laboratories supported by this program frequently have components in more than one of the categories or subcategories listed.

1. Geology, Geophysics, and Earth Dynamics

A. Large-Scale Earth Movements. Research related to the physical aspects of large-scale plate motion, mountain building, and regional scale uplift or subsidence.

B. Evolution of Geologic Structures. Research bearing on the history and development of geologic structures (e.g., folds, faults, landslides, and volcanoes) on a local or subregional scale.

C. Properties of Earth Materials. Research on physical properties of rocks and minerals determined in the laboratory or in the field *(in situ)* by direct or indirect techniques.

D. Rock Flow, Fracture, or Failure. Research related to response of minerals, rocks, and rock units to natural or artificially induced stress, including the strain rates that range from those appropriate to drilling to viscoelastic response.

2. Geochemistry

A. Thermochemical Properties of Geologic Materials. Research related to thermodynamic and transport properties of natural geologic materials and their synthetic analogues. Emphasis is on generic rather than site-specific studies.

B. Static Rock-Water Interactions. Research on chemical, mineralogical, and textural consequences of interaction of natural aqueous fluids, or their synthetic analogues, with rocks and minerals.

C. Organic Geochemistry. Research on naturally occurring carbonaceous and biologically derived substances of geologic importance, including the origin and development of coal, petroleum, and gas.

D. Geochemical Migration. Research on chemical migration in materials of the Earth's crust, emphasizing a generic rather than specific understanding, which may lead to predictive capability. These experimental and theoretical studies focus on chemical transport induced by pressure, temperature, and composition gradients within, between, and by a phase or phases. This component is part of a multiagency (Department of Energy, National Science Foundation, U.S. Geological Survey) joint program.

3. Energy Resource Recognition, Evaluation, and Utilization

A. Resource Definition and Utilization. The principal goal of this research is to develop new and advanced techniques that are physically, chemically, and mathematically based, for energy and energy-related resource exploration, definition, and use.

B. Reservoir Dynamics and Modeling. Research related to dynamic modeling of geothermal and hydrocarbon reservoirs in their natural and perturbed (by production, injection, or reinjection) states.

C. Magma Energy Resources. Field, laboratory, experimental, and theoretical research bearing on the origin, migration, emplacement, and crystallization of natural silicate liquids or their synthetic analogues. These studies emphasize the extraction of energy from such liquids.

D. Information Compilation, Evaluation, and Dissemination. These research activities are principally oriented toward evaluating existing geoscientific data to identify significant gaps, including the necessary compilation and dissemination activities.

E. Continental Scientific Drilling Program (CSDP). Research on advanced technology and services as well as scientifically motivated projects concerned with utilizing shallow (0.3 km), intermediate (0.3 to 1 km), and deep (> 1 km) drill holes in the United States continental crust to obtain samples for detailed physical, chemical, mineralogical, petrologic, and hydrologic characterization and interpretation; correlate geophysical data with laboratory-determined properties; and use the drill hole as an experimental facility for studying crustal materials and processes. The Department of Energy focuses on drilling through an active hydrothermal system (or systems) into a magma chamber or into high-temperature igneous rocks. Research includes aspects of drilling technology development for such hostile environments and is part of a multiagency (USGS, National Science Foundation, and DOE) coordinated program under the aegis of an Interagency Accord on Continental Scientific Drilling.

4. Solar-Terrestrial-Atmospheric Interactions

A. Magnetospheric Physics. Research directed toward developing a fundamental understanding of the interactions of the solar wind with the terrestrial magnetic field. Research related to the Earth's magnetosphere as a model magnetohydrodynamic generator and associated plasma physics research.

B. Upper Atmosphere Chemistry and Physics. Research on thermal, compositional, and electrical phenomena in the upper atmosphere, and the effects induced by solar radiation.

C. Solar Radiation. Research on the solar constant, spectral distribution, and characteristics of solar radiation of the earth, including the long-term effects of solar radiation on the climate.

D. Meteorology and Climatology. Interrelationships of weather and climate with energy systems.

PART I

ON-SITE

Contractor:	ARGONNE NATIONAL LABORATORY Argonne, Illinois 60439
Contract:	109 ENG 38
Category:	Geochemistry
Person in Charge:	F. A. Cafasso

The geochemistry of hydrothermal processes and the geochemical distribution of actinides are the two principal topics of our program. Chemical, isotopic, and mineralogic analyses of naturally occurring solid, liquid, and gaseous materials that compose active hydrothermal systems are pursued in the first program element to date the system, understand fluid/rock interactions within them, and contribute to the objectives of the Continental Scientific Drilling Program. The actinide program element is currently concerned with distinguishing between possible nuclear and nonnuclear hypotheses for the occurrence of actinide isotope enrichments in volcanic rock.

A. Hydrothermal System Evolution *(N. C. Sturchio, C. M. Binz, J. K. Bohlke, and C. E. Johnson)*

The objective of this program is to achieve a deeper understanding of the geochemical processes involved in fluid/rock interactions that occur in active hydrothermal systems in the Earth's crust. Specific problems being addressed include: the source of hydrothermal fluids and their dissolved components, the mechanisms by which dissolved components are enriched or depleted in these fluids, the effects of these fluids on the enveloping rocks, the rates of hydrothermal processes, the longevity of hydrothermal systems, and the relation of hydrothermal systems to large scale tectonomagmatic processes.

Recent efforts of this program were devoted to studies of materials from active magma-hydrothermal systems. Our approach has employed chemical and isotopic analyses of drill cores, surface deposits, thermal water, and gases from a number of hydrothermal systems, with emphasis on the application of uranium-series disequilibrium and the stable isotope ratios of hydrogen, oxygen, sulfur, and carbon.

Our uranium-series disequilibrium studies of samples from Valles caldera (New Mexico) to determine the age determination of calcite veins in VC-1 drill core have shown that many of the veins were formed prior to the present hydrothermal regime and that relatively thick, coarse-grained, and vug-rich calcite forms under present conditions. The analysis of U concentrations and ($^{234}U/^{238}U$) activity ratios in thermal water samples has shown the U concentrations increase when thermal water leaves the high-temperature intracaldera reservoir and that U behaves conservatively in the hydrothermal outflow plume. Other uranium-series disequilibrium studies in progress include: 1) age determination of sinters and travertines from the Yellowstone and Long Valley calderas and 2) a study of ($^{226}Ra/^{230}Th$) disequilibrium in Yellowstone drill cores Y-7 and Y-8. Preliminary data for Y-7 show unsupported ^{226}Ra in clinoptilolite-rich samples that correlates well with added Ba and clinoptilolite content. The *in situ* distribution coefficient for Ba agrees with laboratory measurements. These results suggest dynamic redistribution of Ba and Ra by clinoptilolite-water ion exchange.

Numerous hydrothermal silica and calcite minerals from Yellowstone drill cores were analyzed for oxygen and carbon isotope ratios. The $^{18}O/^{16}O$ ratio in these minerals generally decreases with increasing depth, reflecting the temperature gradient. Oxygen in calcite is apparently near isotopic equilibrium with thermal water under present conditions. The silica minerals have oxygen isotope ratios that are mostly higher than the equilibrium ratios. Layered silica veins display a consistent decrease in oxygen isotope ratio toward the vein interior, which corresponds to a change in mineralogy from chalcedony to quartz. Carbon isotope ratios in calcite are relatively high, suggesting a sedimentary marine carbonate source for dissolved carbon.

A comprehensive set of chemical and isotopic data was acquired for samples of thermal and surface water and steam from the Nevado del Ruiz volcano, Columbia. This study was initiated shortly after the catastrophic eruption of November 13, 1985, to determine the effects of the volcanic activity upon the associated hydrothermal system. The data indicate that there are two separate hydrothermal circulation systems within the volcano: 1) an alkali-chloride system that discharges from boiling springs near 2500 m elevation on the western slope of the volcano and 2) an acid-sulfate system that discharges widely at higher elevations around the northern and eastern slopes. Significant increases in sulfate and chloride have occurred steadily in acid-sulfate springs following the eruption, suggesting increased magmatic volatile input to the system at depth.

B. Actinide Geochemistry *(G. W. Reed, Jr., S. Jovanovic, and E. Olsen [University of Chicago])*

This program is concerned with understanding the details and mechanisms that influence the geochemical and isotopic distribution of actinide elements. Consequently, factors, such as isotopic abundances and mechanisms responsible for migration and immobilization, are objects of study. Current emphasis is on the determination of radionuclide abundances in natural materials, such as lava and volcanic ash, and on testing hypotheses devised to account for actinide isotope anomalies that have been reported for such materials. Confirmation of $^{239}Pu/U$ ratios in excess of the values observed in U minerals and of isotopically anomalous U in volcanic rocks, possible outcomes of current work, would have important geoscience implications. One implication would be the presence of long-lived superheavy elements in the earth. Another would be the original accretion of isotopically anomalous solar nebular matter and the failure to completely homogenize it with respect to uranium during the entire history of the earth. A third would be the collection of additional information on the background levels of Pu that can be expected in geological material.

Contractor: LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

Contract: DE-AC03-76SF00098

Category: Geology, Geophysics, and Earth Dynamics

Person in Charge: T. V. McEvilly

A. Deep Electromagnetic Sounding of the Crust *(H. F. Morrison and N. E. Goldstein)*

The electrical conductivity of the shallow crust is related mainly to the degree of connected pores and open fractures, the degree of liquid saturation and salinity of the pore fluids, as well as past and present-day thermal-tectonic processes that increase rock conductivities due to increased fracturing, hydrothermal alteration, and elevated temperatures. It is now well established that conductivity anomalies extend to mid-crustal depths in certain areas of the continental crust. Although it was initially believed that a few of the conductors were extensive regions of magma, recent information suggests that hot, brine-filled and/or graphite-lined fractures are likely causes for some of the deep anomalies.

The objectives of our investigations are to develop and apply advanced techniques for carrying out deep electromagnetic soundings, to develop better numerical methods for data processing and interpretation, and to develop better conceptual models for the conductivity of the crust. After a theoretical review and numerical tests of the EMAP technique were made, we attempted to apply the method in an experiment across the Long Valley caldera. EMAP is a variation of magnetotellurics in which the orthogonal electric field dipoles at separated sounding points are replaced by a long, continuous line of E-field measurements. A selective frequency-dependent numerical filter is applied to the data, which helps suppress the effects of local surface inhomogeneities that complicate normal MT data.

A major accomplishment has been the theoretical development and numerical testing of a new method for processing and interpreting electromagnetic sounding data. Central to the method is the fact that when the EM wave equation is transformed into a pure wave equation, solutions for the fields at the surface over buried conductors look like reflections of seismic wavelets from the surfaces of the conductor.

B. Center for Computational Seismology *(T. V. McEvilly and E. Majer)*

The Center for Computational Seismology (CCS) has now been in existence for four years. It has expanded from a several user facility occupying 10 to 25% of a VAX/780 to a 20 to 30 user community utilizing an equivalent of one to one and half VAX/780's. The purpose of CCS has been to provide a facility with a wide range of computational tools to serve DOE programs in the basic energy sciences and other areas of energy research. Research over the entire spectrum of seismology is carried out at CCS, from basic studies in earthquake source mechanisms to the applied work of reflection seismology. The software base comprises four years of CCS efforts in coding internal analysis routines in addition to the processing tools of DISCO, INGRES, and the AIMS package. The principal areas of activity are with DOE programs involving seismic projects relating to basic and applied research. During the past year this has included work on the Salton Sea drilling project and the Long Valley data synthesis. Another area of work has been for geothermal programs, encompassing Vertical Seismic Profiling for fracture detection and microearthquake studies for reservoir management. CCS also conducts work for the DOE nuclear waste program, relating the seismic response of fractured media to the hydrologic response. This program will soon involve field work, but the main thrust of the present study is to develop 2- and 3-D models for ray-tracing P-, SV-, and SH-waves through fractured rock. The goal is to use seismic tomography for mapping fracture density, spacing, and orientation. Hopefully, sufficient resolution can be achieved to aid the hydrologist/reservoir engineer in predicting fluid flow. Work related to mapping fluid flow in natural and induced (hydrofracture) fractures remains underway.

C. Microcrack Growth in Crystalline Rock *(L. R. Myer, N. G. W. Cook, and J. M. Kemeny)*

We are presently investigating the growth, interaction, and coalescence of microcracks in brittle rocks when subjected to compressive stresses up to and past the strength of the rock. Previous laboratory studies have revealed that under compressive stresses large enough to cause microcracks to grow, the microcracks initially grow in the direction of the maximum principal stress (axial direction in most laboratory tests). Under uniaxial or very low values of confining stresses, the axially growing cracks grow to form macroscopic splitting cracks, whereas under higher values of confining stresses, the axially growing cracks stabilize as shear localization processes occur, resulting in the formation of one or two distinct shear bands. These modes of deformation based on microcrack growth also characterize the macroscopic stress-strain behavior of the laboratory test. In general, the initial axial growth of microcracks is associated with strain hardening and the formation of macroscopic splitting cracks or shear bands is associated with strain softening. Using theoretical models based on linear elastic fracture mechanics, we are investigating the above phenomena. We have developed a model for the splitting phenomenon based on a doubly periodic array of "sliding cracks" and a model for the formation of shear bands based on a co-linear row of shear cracks. These models predict the transition from splitting to shear band formation as the confining stress is increased, and also the predicted stress-strain curves from the models exhibit the appropriate strain hardening and strain softening regimes.

These models have also been used to determine fracture parameters associated with different scales of fracturing. The primary fracture parameter that we have studied is the fracture energy. We find that for Westerly granite, the G_C associated with microcracking is three orders of magnitude less than the G_C associated with the propagation of the sample-size fractures. This is due to the fact that the propagation of large scale fractures under compressive stresses is associated with the creation of a large amount of subsidiary crack surface area, which absorbs strain energy and causes an apparent G_C that is much larger than the actual G_C at the tip of the crack. This gives an explanation for the large variation in G_C (10^2 to $10^8\,J/m^2$) for earthquake faulting that is reported in the literature.

D. Development of a Numerical Approach to the Study of Coupled Thermohydromechanical Processes in Geological Systems *(C. F. Tsang and J. Noorishad)*

Various aspects of petroleum reservoir engineering such as isothermal and non-isothermal hydraulic fracturing and permeability variations near injection or production wellbores involve coupled thermohydromechanical processes. The code ROCMAS was developed to address these coupled phenomena. Work is under way to improve the numerical solution approach used in the code. This involves the implementation of new matrix solution schemes and linearization schemes. Also, ground work is being prepared for implementing a generalized macroscopic failure criterion for brittle and ductile behavior of rocks. This is an essential feature required for hydraulic fracturing investigations.

E. Process Definition in Fractured Hydrocarbon Reservoirs, Element I: Hydromechanical, Seismic, and Electrical Properties of Natural Fractures *(L. R. Myer and N. G. W. Cook)*

A new research program with the objective of developing relationships between the hydromechanical properties of naturally fractured hydrocarbon reservoirs and their seismic and electrical properties was initiated. Theoretical models will be developed to describe the electrical conductivity of single, fluid-filled fractures and their effect on the transmission of seismic waves. Complementary laboratory measurements will be made of the hydrologic and electrical properties of single natural fractures and seismic properties of both single and multiple natural fractures.

Our effort has concentrated on two studies concerning the electrical and seismic properties of single fractures. In the electrical properties study, the effect on electrical conductivity of the geometric distribution of contact areas in a fracture was studied by representing a saturated fracture by a piece of conductive paper. Holes were punched in the paper to represent areas of contact in a fracture while the paper itself represented a conductive fluid in fracture voids. A DC voltage was applied and the potential field mapped to evaluate the effect of the holes (fracture contact areas). Different geometrical distributions of holes were used to evaluate the effect of the geometric distribution of contact areas on the potential field.

The second study was a theoretical investigation of the existence of an interface wave for the case of two media of equivalent elastic properties separated by a nonwelded interface in partial contact. (This describes a single, infinite fracture in an elastic rock mass.) This work is an extension of previous wave propagation studies in which a fracture is mathematically represented by a displacement discontinuity; the differential displacement between the fracture surface is defined to be inversely proportional to the specific stiffness of the fracture. In general, two distinct dispersive interface waves were found. At high frequency or low stiffness, both waves approach an asymptote defined by the Rayleigh wave velocity. At low frequencies or high stiffness, the slow wave approaches the shear wave velocity with essentially a zero slope while the fast wave approaches with a finite slope and ceases to exist below a threshold frequency. An important application of this work is the evaluation of seismic waves generated during propagation of hydrofractures.

F. Test of MHD Source for Crustal Electromagnetic Sounding *(H. F. Morrison and N. E. Goldstein)*

An engineering test was made of a controlled-source electromagnetic sounding system powered by a magnetohydrodynamic (MHD) generator. The MHD generator is an experimental device that uses a high electrical conductivity plasma to generate pulses of very high currents in low resistance loads. In this case the plasma is the combustion product from a small hybrid rocket combustor, and the load is a horizontal 200 × 250 m loop with a resistance of 0.07 ohm and an inductance of 800 μH. The generator delivered two current pulses of 6500 and 7250 A to the transmitter, and we recorded the resulting magnetic fields by means of 3-component SQUID magnetometers located 1.2 and 21 km from the center of the loop. Large levels of uncorrelated 60 Hz noise could not be removed from the data. It was impossible, therefore, to ascertain the secondary magnetic fields following interruption of loop current.

The maximum magnetic moment generated in this experiment was 3.6×10^8 A·m^2, which is comparable to moments we have been able to generate in the past only by employing very large loops, several km on a side, driven by conventional power sources. The use of the MHD generator dictates the deployment of small but very heavy transmitter loops that are awkward to deploy in most field environments. Also, an MHD source requires a detection system with a very large dynamic range capability when working at short offset distances from the loop. An MHD source provides very high current (and dipole moment) at the expense of an easily repeatable signal. Therefore, the usual stacking (or signal averaging) technique to improve signal-to-noise cannot be used.

G. Advance Geoscience Research Concepts *(T. V. McEvilly)*

Several novel projects received support under this program for encouraging development of advanced ideas in the geosciences. The two most substantial concepts developed were the initiatives on the Center for Isotopic Studies in the geosciences and interdisciplinary approach to process definition in fractured petroleum reservoirs. Both efforts involved seminar and discussion groups with Berkeley scientists and university and industry colleagues with expertise and interest in advancing research activity in this area. Another new development, also related to the need for high-resolution mapping of subsurface properties, is the borehole vibrating seismic source needed for seismic tomography studies. A particular aspect of this newly developing project needing special attention is the electromechanical feedback system for shear-wave polarization control. Some preliminary modeling has been supported.

Contractor: LAWRENCE BERKELEY LABORATORY
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Contract: DE-AC03-76SF00098

Category: Geochemistry

Person in charge: T. V. McEvilly

A. Thermodynamics of High Temperature Brines *(K. S. Pitzer)*

This project covers theoretical and experimental studies concerning the thermodynamic properties of aqueous electrolytes at high temperatures. The components important in natural waters and brines are emphasized. The resulting data are important in understanding certain geothermal and other natural resources and in fission-product waste disposal. Moreover, this information has a wide range of applicability, since similar solutions arise in many industrial processes and in high-pressure steam power plants.

The experimental program involves measuring the heat capacity and the density of solutions in the range 0 to 300°C and 0 to kbar. Recently, heat capacity measurements on KCl(aq) were completed and earlier work on Na_2SO_4(aq) is being extended from 200 to 300°C and 0 to kbar. A theory has been developed for the Gibbs energy of hydration of ions that is valid over a wide range of conditions to 1000°C and 5 kbar. This is an extension of the successive hydration model proposed recently for NaCl(aq) for more limited conditions. It makes use of the mass-spectrometric measurements of ion hydration to characterize the inner shell around an ion together with a Born-equation model for outer-shell effects. This model should give good results for aqueous system of widely varying density including the critical region. Parameters are available for the singly charged ions of geochemical interest. Other theoretical work has yielded equations predicting the properties of mixtures based on the knowledge of the pure component solutions in water. These equations have been applied to solubility calculations for a series of minerals and to calculation of water vapor pressure over mixed brines at temperature up to 300°C.

B. Thermodynamic Properties of Silicate Materials *(I. S. E. Carmichael, R. A. Lange, and D. A. Snyder)*

The focus of our project is to experimentally determine the thermodynamic and physical properties of silicate liquids relevant to natural lavas. Recently, there has been a rapid growth in the number of thermodynamic and fluid dynamic models of magmas. This growth has produced a renewed need for accurate measurements on melts. We have been fulfilling this need by performing measurements of densities, compressibilities, and enthalpies of silicate liquids.

To resolve the controversial issue of whether multicomponent silicate liquids mix ideally with respect to volume, the volumes of 23 liquids in the system K_2O-Na_2O-CaO-MgO-TiO_2-Al_2O_3-SiO_2 have been determined using the double-bob Archimedean technique. These volumes have been fit with a linear mixing equation except for an interaction term between CaO and TiO_2. To further investigate this interaction and to delineate the TiO_2 interaction among alkali and alkaline earth oxides, more detailed studies are under way.

A fundamental application of our one bar measurements of volumes is for the reduction of ultrasonic velocity data to calculate isothermal compressibilities. Our new volume data were used to rederive the pressure derivative of the partial molar volumes of the oxides. For minerals such as diopside, whose fusion curves and thermodynamic data are well determined, our volume and compressibility values for the melt can be used to derive values of the second derivative of volume with respect to pressure that compare well with results obtained from shock wave experiments at much higher pressure.

C. Generation of Petroleum and its Precursor Compounds *(O. Weres)*

The objective of this project is to simulate the generation and evolution of petroleum hydrocarbons and their precursor compounds in the laboratory. The ultimate purpose is to improve the understanding of the chemical reactions that produce petroleum in nature. This knowledge may lead to improved methods of finding and recovering oil and gas. This work has contributed to a better understanding of the hydrothermal chemistry of organic compounds, a topic with applications broader than petroleum geochemistry. A variety of organic compounds and polymers have been reacted with clay and brine in an autoclave at 315°C. Experiments run for several days, providing adequate reaction time at this temperature. The reaction products are extracted and identified using gas chromatography, coupled gas chromatography-mass spectrometry, and mass spectrometry. This project is near completion, and effort during the current fiscal year has emphasized writing up the results for publication.

D. Studies of the Interactions Between Mineral Surfaces and Ions in Solution *(D. L. Perry)*

This task is a fundamental study to determine the basic surface chemistry of common minerals (both synthetic and natural) and the chemical reactions of metal ions with the mineral surfaces. Pertinent to the occurrence of hydrocarbons, reactions of mineral surfaces with organic molecules act as models for petroleum precursors interacting with geologic materials. The research encompasses: 1) basic spectroscopy of natural minerals and their synthetic counterparts, 2) spectroscopic studies of metal ions that have been adsorbed onto the mineral surfaces, 3) syntheses and spectroscopy of model compounds that form in metal ion-petroleum precursor organic compound reactions, and 4) spectroscopy of organic compound-petroleum precursors that have been chemisorbed onto minerals with metal ions associated with petroleum deposits (i.e., uranium with humic and fulvic acids, a chemical system that exists in many coal deposits).

This research elucidates the metal ion-organic intermediates in petroleum and coal deposits, their interaction with mineral/rock media, and the new compounds that are formed. Surface/solution interface reactions, such as metal ions reacting with a petroleum-related thin film, serve as direct experimental models for studying the chemical bonding involved in such a complex. The results provide a better experimental understanding of the chemistry involved in the interactions among heavy metal ions, organic compounds that are petroleum precursors, and geologic substrates. The information also provides a larger database for theoretical models used to predict these interactions.

E. **Abiogenic Methane Production from Igneous and Metamorphic Rocks** *(J. A. Apps)*

The purpose of this project is to determine the origin and conditions of formation of methane associated with igneous rocks. The possibility exists that methane derived from abiogenic sources may have contributed substantially to the world's oil and gas accumulations. The problem is approached from three directions: 1) through examination of the thermodynamics of methane stability in the upper mantle and lower crust, 2) by theoretical simulation of the hydrolysis from mafic and ultramafic rocks between 25 and 500°C, and 3) through autoclave experiments of mafic rock hydrolysis between 150 and 400°C.

F. ***In Situ* Sampling of the SSSDP Well** *(A. White)*

The LBL fluid sampler was used last year in obtaining water samples from two producing zones in the Salton Sea well. The last samples obtained at the depth of 10,700 ft and a temperature in excess of 350°C represented one of the hottest fluid samples ever retrieved from a geothermal well. During the current year, chemical and isotopic analyses were preformed. Results indicated extensive contamination with drilling fluids. Interestingly, considerable variations were also observed between *in situ* samples obtained at comparable depths using the LBL flow-through sampler and the evacuated sampler used by LANL. This discrepancy may be due, in part, to design differences or rapid convective cycling in the wellbore. Due to a lack of accessibility, no new sampling occurred at the Salton Sea yet this year although plans are made if the defective liner can be replaced. Two sampling trips were made to the DOSECC Cajon Pass hole near the San Andreas Fault. Five successful runs were conducted at depths of 7,000 ft and a downhole temperature of 80°C.

G. **Nonisothermal Reservoir Dynamics** *(C. F. Tsang)*

This project encompasses a wide range of fundamental studies of fluid, heat, and solute transport in rocks. These studies are relevant to geological disposal of nuclear waste, chemical transport in ground water systems, underground energy storage, geothermal energy, and other energy-related problems. The goal is to better understand various physical and chemical transport processes in porous or fractured porous media and their effects, through theoretical considerations, mathematical modeling, and laboratory investigations. New measurement techniques to provide key data needed for these investigations are explored. A new wellbore fluid conductivity logging method was developed to measure fracture inflow parameters by means of a time sequence of electrical conductivity logging of the borehole fluid. The procedure is applied to an existing set of data, which shows initiation and growth of nine conductivity peaks in a 900-meter section of a 1690-meter borehole, corresponding to nine fractures intersecting the borehole. In co-operation with the Weizmann Institute of Science and Ben Gurion University in Israel, we are studying the thermohydraulics of unsaturated-soil heat-storage systems. A one-half scale field test is currently being constructed and carried out in Israel. We will perform mathematical modeling to study thermohydraulics of the system and to understand the basic physical processes involved.

H. **Chemical Transport in Natural Systems** *(C. L. Carnahan and J. S. Jacobsen)*

The objective of this program is to gain increased understanding of processes affecting the movement of chemically reactive solutes in ground water flow systems. This objective is being approached through development of theoretical models that can be rendered into numerical simulators. These studies are relevant to the understanding and quantitative description of geothermal energy reservoirs, hydrothermal ore deposits, subsurface migration of toxic and radioactive wastes, and other energy-related phenomena. We have used the thermodynamics of irreversible processes to construct a numerical simulator of direct and coupled transport processes that are driven by gradients of temperature, hydraulic potential, and chemical potential. The direct transport processes are those described by the phenomenological laws of Fourier, Darcy, and Fick. The coupled processes include chemical osmosis, thermal osmosis, thermal diffusion, ultrafiltration (reverse osmosis), and coupled chemical diffusion. We have applied our theoretical approach and numerical methods to technical problems of interest to the energy community. In the case of application to the near-field region of a geologic repository for nuclear waste, we have found that the coupled osmotic processes contribute significantly to transport of dissolved materials with a semi-permeable packing material. However, because of a restriction against fluid flow at the canister-packing interface, the coupled processes interact with the direct processes in such a way that the resulting flow of solute mass is not very different from the flow that would be predicted without consideration of coupling. On the other hand, simulations of coupled transport processes in less constrained, natural settings indicate a need to account for coupling in the interpretation of natural analogs of waste repositories.

I. Impacts and Mass Extinctions *(L. Alvarez, F. Asaro, H. V. Michel, and W. Alvarez)*

The overall objective of this project is to determine the relationship between asteroidal or other large-body impacts on the Earth and repeated massive extinctions of life that have occurred in the last 570 m.y. The primary mechanism for the research consists of intensive chemical and selective mineralogical studies (on sediments near both major and minor extinction boundaries) that are run in parallel with floral and faunal fossil studies by collaborating geologists and paleontologists. A secondary but major objective is to ascertain if a series of time markers of very high precision and accuracy (in the form of iridium and other geochemical anomalies) can be developed for relative dating and correlation of sediments in many different parts of the world. A minor objective is to evaluate the major chemical and mineralogical alterations that have occurred in the sedimentation of the 67 m.y. old Cretaceous-Tertiary (K-T) boundary, and one most closely linked to a large body impact, in order to predict the behavior expected in older boundaries.

We have studied highly calcareous samples from a deep sea core, taken from between New Zealand and Australia. The samples studied so far cover 53 meters of section and $\sim$ 3 million years of deposition. A scan of these samples with the iridium coincidence spectrometer showed only a single IR peak centered in 11.7 m.y. old sediment. This is approximately coincident with the middle Miocene extinction reported by others. Our data indicate that the Ir anomaly is not due to a temporary decrease in the $CaCo_3$ sedimentation rate and is probably not due to volcanic aerosols such as those erupted from the volcano Kilauea. The explanation for the Ir anomaly most consistent with the data is the impact of an extraterrestrial body on the Earth. If 11.7 m.y. old Ir-enriched rocks are found world-wide, then the evidence for the impact of a large asteroid or comet would be very convincing. There would then be 3 such horizons at 66.7, $\sim$ 39.4, and 11.7 million years with an average spacing of $\sim$ 27.5 million years. These data would strongly suggest a periodicity in Ir anomalies very close to those found for extinctions and crater ages and hence lend support to the periodic extinction proposal of Raup and Sepkoski and the astrophysical hypotheses that entail periodic impacts on the Earth.

Contractor:	LAWRENCE BERKELEY LABORATORY University of California Berkeley, California 94720
Contract:	DE-AC03-76SF00098
Category:	Energy Resource Recognition, Evaluation, and Utilization
Person in Charge:	T. V. McEvilly

A. Hydrothermal Chemistry *(A. F. White and H. A. Wollenberg)*

Activities were focused primarily on the Long valley caldera. Isotopic and chemical compositions of fluids and rocks in the Long Valley hydrothermal system were investigated. Deuterium and oxygen-18 distributions in precipitation across the valley indicate that significant recharge to the hydrothermal system occurs in the western moat area and on the southwest rim. The presence of hot shallow fluids intersected in a recently drilled hole (described below) confirmed this interpretation. The detailed distribution of hydrothermally indicative elements, including chloride, lithium, and boron, is being determined in the hydrothermal fluids and in altered and unaltered reservoir rocks. Hydrothermal bomb experiments have been completed between 100 and 200°C to assess leach rates. Linear rate kinetics will permit estimates of reservoir extent based on observed fluid flux from the hydrothermal system. Excess boron release in the altered tuffs implies open system transport, possibly from underlying meta-sedimentary rock of the Sierran basement.

To better understand the Long Valley hydrothermal circulation system, a hole was continuously cored to a depth of 715 m in the caldera's southwest moat. The hole encountered sharply increasing temperatures with depth to 335 m in rock of younger caldera fill. Below that depth and to the bottom of the hole, near-isothermal conditions at 200 to 205°C occurred in fractured, predominantly welded Early rhyolite and Bishop tuff. Following completion of coring, equilibrium temperature profiles were measured and the casing was perforated for fluid sampling. Resulting chemical analysis and associated chemical geothermometer temperatures indicated that the fluid encountered is the supply for the Casa Diablo geothermal field, $\sim$ 6 km to the east. This supports the concept of a predominantly eastward-flowing hydrothermal system, recharged from the Sierra Nevada, with an upwelling source of hot water in the caldera's west moat.

B. Continental Scientific Drilling Review Group *(T. V. McEvilly and H. Wollenberg)*

The twelve-person group reviews on-going, planned, and proposed Continental Scientific Drilling (CSD) projects, primarily in the thermal regimes sector, that are supported by the Department of Energy. Meetings are also held periodically with the Science Advisory Committee of DOSECC to cover topics of interest to both the thermal and non-thermal regimes sectors of the national CSD program. The Review Group is made up of scientists from Federal agencies, universities, industry, and DOE laboratories.

C. Fundamental Studies of Fluid Flow in Fractured Rock Masses under Stress *(P. A. Witherspoon, Y. W. Tsang, and L. Myer)*

Experimental observations in single fractures ranging from the laboratory scale (centimeters) to the field scale (meters) show evidence that fluid flow in a single fracture can be very uneven, taking place in only a few preferred channels. The theoretical phase of this program therefore focuses on the channel description of flow and transport in the single fracture. A conceptual model to interpret tracer tests in fractured media in terms of flow in a system of one-dimensional channels with variable apertures was developed earlier. More recently, calculations for flow and transport in two-dimensions in a single fracture with variable aperture were carried out. Our calculations show that the flow and transport takes place in channels rather than throughout the entire plane of a fracture and that the channeling phenomenon becomes more pronounced with increasing normal stress on the fracture. Excellent agreement was found between the predictions of the one-dimensional conceptual model and the two-dimensional calculations, suggesting the potential utility of the one-dimensional channel model to interpret the flow and transport in two-dimensions (single-fracture) as well as in three-dimensions (fractured media). In the laboratory phase of this program, a comprehensive study of the mechanical displacement, hydraulic conductivity, and void geometry of single natural fractures in a quartz monzonite was completed. Fluid flow tests were conducted on fractures oriented roughly orthogonal to the long axis of cylindrical samples under normal stresses ranging from about 1.5 to 75 MPa. Careful measurement of the mechanical deformation of the fracture permitted evaluation of the change in mean fracture aperture with effective stress. Results of the deformation and fluid flow tests were combined to analyze the relationship between hydromechanical properties and the geometry of the voids and asperities within the fracture.

D. Geomechanics Laboratory Studies of SSSDP Samples *(L. R. Myer)*

The objective of this study is to obtain physical properties of core recovered from the Salton Sea borehole. Emphasis has been on a study of the anisotropy in acoustic wave velocity and attenuation in shales present at the site. These data are important to evaluation of VSP surveys that already have been completed.

Five samples of core two inches in diameter with bedding parallel to the long axis of the samples were prepared for testing. The test apparatus permitted propagation of compressional and shear waves at any angle to the bedding direction. The apparatus allowed adjustment of the shear wave polarization direction so that measurements could be made with particle motion at arbitrary angles with respect to the bedding direction. In preliminary tests of the apparatus, anisotropy of a calibration specimen of Bandera sandstone was studied. In this material anisotropy is caused by diffuse bands of clay associated with the bedding planes. Minima and maxima velocities and amplitudes at 90° intervals were observed for compressional and shear waves. Maximum compressional wave velocity and amplitude were found when the wave propagated in a direction perpendicular to the axis of symmetry of the material (parallel to bedding). Upon saturation with water the trends in anisotropic behavior persisted while velocities and amplitudes changed. The compressional wave velocity increased by 15% and shear wave velocity increased slightly. However, shear wave amplitude decreased by more than an order of magnitude and compressional wave amplitudes decreased by a factor of two.

E. Aqueous Solutions Database *(S. L. Phillips)*

The result of this project is a computerized geochemical database with values for the following four thermodynamic properties: Gibbs energy of formation, enthalpy of formation, entropy, and heat capacity. The thermodynamic data are consistent with auxiliary Key Values that serve as the reference data. These Key Values were obtained mostly from CODATA and the National Bureau of Standards, as well as from our critical evaluation. The data are consistent with the fundamental relationship $\Delta_r G^\circ = \Delta_r H^\circ$ - 298.15 $\Delta_r S^\circ$ to $\pm$ 1000 J/mol, for any geochemical reaction. If this criterion is exceeded, then the thermodynamic properties are recalculated.

Besides this generic database, a similar database is being developed together with SNLA with major emphasis on Am, Pu, Np and U. This joint effort will result in a database that will be used to assess the performance of a nuclear waste repository. The basic question is, what is the solubility and speciation of selected waste nuclides in natural groundwaters? To fill a number of gaps in data, we are developing correlation equations, such as the heat capacity and entropy of individual species. We have found that the Gibbs energy of formation and the enthalpy of formation of complex ions are linearly related to the number of ligands. This may be a useful approach for predicting the formation constants of complex ions, when experimental data are not available.

F. Reflection Profiling at the Salton Sea Deep Hole Site *(T. V. McEvilly and E. Majer)*

The vertical seismic profile executed in the SSSDP borehole has been interpreted and modeled; the study forms the MS thesis of T. Daley and will be submitted in September 1987. A reflector at 6800–7000 ft is seen in both P- and S-waves, apparently fracture-related, and strong scattering is seen from a presumed heterogeneity near 3000 ft. Shear-wave anisotropy is evident in S-wave splitting, with up to 1% variation in the split-wave velocities. Particle motion studies yield encouragement for the potential of detecting and mapping split-wave orientation as an indicator in defining fracture orientation.

G. Geophysical Measurements Facility *(T. V. McEvilly and H. F. Morrison)*

Research programs at LBL Earth Sciences Division have always had a large component of field studies. Along with this effort runs a substantial instrumentation development program (e.g., downhole fluid sampler, automated seismic processor, electromagnetic geophysical sounding, etc.) and a large fleet of more than 20 special-purpose field vehicles (logging trucks, seismic network van, vibroseis trucks, reservoir engineering vehicles, etc.) and conventional equipment (seismic and electrical field systems, logging tools, recording systems, telemetry networks, etc.). The Geophysical Measurements Facility was created to manage this extensively used resource, maintaining, repairing, and upgrading the systems as needed. During this past year the VSP equipment was used in the CSDP program, as was the downhole sampler. The telemetered seismic network was deployed and maintained, and the MHD source was tested. Modest upgrades were effected on several items of equipment.

H. Synthesis of Long Valley Geophysical Data *(N. E. Goldstein, T. V. McEvilly, H. F. Morrison, and H. A. Wollenberg)*

The Long Valley caldera, located at the eastern edge of the Sierra Nevada, California, is one of the best studied Pleistocene silicic, ash-flow volcanoes in the world and a prime candidate for both CSD Thermal Regimes drilling and for exploratory drilling to penetrate into the "near-magmatic" environment. To help determine sites for future drilling, LBL has coordinated and expedited the processing and interpretation of critical data sets. The work resulted in a two-day symposium held at LBL on March 17-18, 1987. Thirty-one technical talks were presented by members of the three scientific study groups: geology-geohydrology-geochemistry, seismology, and potential fields and electromagnetics. One of the key findings presented at the symposium is: There is little evidence that a large, well-connected body of magma exists today at depths less than 10-12 km. Magma bodies at drillable depths may occur as small, discontinuous regions of partial melt, less than 2 km in horizontal dimension.

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Title:	Geology, Geophysics, and Earth Dynamics
Person in Charge:	L. W. Younker

A. Rock Mechanics *(H. C. Heard, B. Bonner, W. B. Durham and F. J. Ryerson)*

The rock mechanics program involves high pressure/high temperature research in two broad areas: 1) effects of porosity on the mechanical and transport properties of rocks and 2) intrinsic physical properties of rocks and minerals. Under 1) we are pursuing two subtasks: rock joint profiling in the laboratory and a study of thermal cracking in rocks as a function of pressure and temperature. Under 2) we are pursuing one subtask, the measurement of the effect of cation impurities in the deformation of rock salt. The rock joint profiling is peformed using a high-precision, computer-controlled surface profiling device recently constructed specifically for this task. Profiling the opposing faces of a rock joint gives us the "composite topography" of the joint. Theory suggests that joint stiffness and fluid flow depend not so much on joint roughness as on the composite topography. One of the most important characteristics of a joint is how "well" its two faces are correlated. Joints that are highly correlated tend to be less permeable and stiffer than joints that are less correlated. The second subtask is an investigation of microcrack generation in granite during heating while under confining pressure. The total number of acoustic emission (AE) events show very little activity up to 100°C. Then the critical temperature for onset of significant AE varies linearly with the confining pressure. The difference in compressional velocity between the heating and cooling portions of the thermal cycle seems to be a very sensitive indicator of the crack porosity in the rock. This difference could be exploited to monitor the physical state of a waste repository by seismic techniques. The third subtask concerns potentially important effects in the deformation of rock salt formations. Published laboratory data indicate that most natural salt formations have closely similar mechanical properties. However, at least two natural halites are stronger than the average by approximately 50%. The anomalously strong materials contained Ca, K and Mg impurities in the 0.1–0.5 wt% range. The work to date has shown that the effects of cation impurities on steady-state creep behavior are easily measureable in halite. Hence, the halite impurity-cation system is an excellent system in which to systematically investigate the effects and mechanisms of solid solution hardening in ionic crystals.

B. Diffusion in Silicate Materials *(F. J. Ryerson and W. B. Durham)*

The primary focus of this project is the experimental determination of diffusion coefficients in rock-forming minerals and melts and the application of these data to geochemical and geophysical problems. We have also broadened the focus of this study to include other experimentally tractable problems such as those involving mineral-melt equilibria and trace element partitioning. Oxygen diffusion has been measured in San Carlos olivine. The primary goal of this work is to constrain the mechanisms of plastic deformation in olivine and to further constrain its point-defect chemistry. The most striking feature of the data is the positive dependence of oxygen diffusion on oxygen fugacity. The increase in oxygen diffusivities with oxygen fugacity argues against the diffusion of oxygen by a vacancy mechanism. Also, a major host for LREE and the heat producing elements U and Th in peraluminous granites is monazite, and the stability of monazite will affect the redistribution on the elements within the crust during anatexis. The compositional stability of monazite in "granitic" melts ranging from peraluminous to metaluminous compositions has been investigated under water saturated conditions between 850–1000°C, at 8 kb. Monazite solubility, measured as the concentration of LREE's in monazite saturated melts is inversely correlated with the Si concentration of the melt and positively correlated with the concentration of alkali and alkaline earth cations in excess of that needed to charge balance tetrahedrally coordinated aluminum. Application of the monazite solubility model to crustal anatexis of typical shales indicates that for fusion temperatures at or below 800°C, anatexis of aluminous source rocks may lead to an enrichment of monazite in the restitic lower crust. At temperatures approaching 850°C, enrichment of monazite in the lower crust due to anatexis is unlikely due to the high saturation concentrations. The TiO_2 contents of rutile-saturated melts ranging from basalt to rhyodacite have been investigated at P = 8-30 kb and T = 1000-1300°C under hydrous, CO_2-saturated, and volatile-absent conditions. For ranges of probable solidus conditions, rutile saturation in basaltic, andesitic, and dacitic liquids requires 7–9, 5–7, and 1–3 wt% TiO_2, respectively. These concentrations are well in excess of those found in the respective rock types, so depletion in Nb, Ta, and Ti and reduced Nb/Th ratios in volcanics from collisional margins cannot be attributed to residual rutile in their source regions. Thus, Nb, Ta, and Ti depletion must be an inherent property of the source region.

C. Electrical Conductivity, Temperature, and Radiative Transport in the Earth
(A. G. Duba, joint research with T. J. Shankland, LANL)

Results of both the electrical and optical research efforts help determine temperature distributions in the crust and upper mantle. The thermoelectric effect S and electrical conductivity σ in the mantle minerals olivine and pyroxene are being measured as a function of temperature, orientation, oxygen fugacity, and iron content. The results apply to inference of upper mantle temperatures from electrical data. Although there are seismic models to explain the low velocity zone (LVZ) as a solid-state phenomenon not requiring partial melting, the most well-constrained laboratory electrical measurements are more consistent with the partial melting hypothesis for the high conductivity layer (HCL) apparently associated with the LVZ. If the LVZ/HCL is not a partial melt layer, then mantle geotherms would be considerably lower than previously inferred. We are evaluating the constraints on temperature imposed by electrical studies.

In addition to measuring S and σ in the three principal directions in olivine from San Carlos, Arizona, at 1200 to 1500°C under controlled oxygen fugacity, we have obtained most of this information for the related, iron-free mineral forsterite under oxidizing and reducing conditions. From the sign change of S at about 1390°C we infer the olivine to be a mixed semiconductor. Forsterite is more complex: at low oxygen pressures it appears to be a good ionic semiconductor via extrinsic magnesium vacancies along the crystallographic c-axis, whereas it is an electronic semiconductor along the other two axes. We have used these results to obtain a best-fitting conductivity-temperature curve for determining upper bounds on mantle temperatures and to argue for a high-temperature mantle geotherm on the basis that the abrupt rise in mantle conductivity at the HCL is due to partial melt. From radiative heat transport calculations for silicic magmas, we infer that these materials are among the most highly thermally conductive materials in the Earth, a matter of some consequence for those studying evolution of silicic magma chambers. We have accomplished a similar suite of measurements for (Mg,Fe)O, the most likely Fe-bearing phase in the lower mantle. The results will apply to heat transport and convection in the largest uniform part of the Earth's interior.

D. Attenuation and Dispersion in Partially Saturated Rocks *(J. G. Berryman, B. P. Bonner, Y. Chin, G. W. Hedstrom, and L. Thigpen)*

Our objective is to combine theory and experiment to analyze attenuation and dispersion of waves in partially or fully saturated rocks over a broad range of frequencies. The techniques developed in this work will be applicable to many basic problems in energy recovery, particularly hydrocarbon and geothermal exploration and resource assessment. The results will also impact code calculations for the Nuclear Test Containment Program and waveform analysis for the Seismic Verification Program. Our recent experimental efforts have concentrated on verifying theoretical predictions for wave propagation in fluid-saturated porous media. Measurements of the electrical conductivity of saturated rock and the saturating pore fluid can be used to estimate the tortuosity of the pore space. Acoustic microscopy shows promise as a new tool to evaluate the morphology of porous rock. We have produced high contrast images of fractures in Climax Stock granodiorite and find indications of reabsorption of the fracture by the matrix. Acoustic images may prove useful for determining the chronology of fracture emplacement, giving insight into the geologic history of a rock mass. Recent theoretical efforts have led to a comprehensive theory of wave propagation in partially saturated porous media. A new explanation of the observed magnitude of the attenuation of waves in partially saturated porous media has been proposed based on a local-flow generalization of Biot's theory. This idea provides very plausible explanations of the discrepancies previously observed between theory and experiment. It also shows that acoustical methods may not be used directly to measure global permeability of rocks, although bounds on permeability may be obtained from attenuation measurements. The image processing method for analyzing rock topological structure being developed here has also been shown to be a promising method for determining the values of the local permeability and formation factor required in a predictive theory.

E. Surface Wave Method for Determining Earthquake Mechanisms with Applications to Regional Stress Field Studies *(H. J. Patton and S. R. Taylor)*

This project utilizes seismic surface waves to map lateral shear-velocity variations in the Basin and Range of western United States. In addition, surface-wave observations and moment-tensor inversion methods are applied to determine source mechanisms and depths of earthquakes in selected areas of the Basin and Range and surrounding geologic regions. Interpretation of the velocity structures, including effects of anisotropy, will give insights into the processes controlling lithospheric extension of the Basin and Range and into possible flow of magma in the crust and upper mantle. Source mechanisms and depths along with better structural information will improve knowledge of the regional tectonic stress field and provide useful constraints for geophysical models of convective hydrothermal systems. We have pursued our investigations into lateral variations of shear-velocity structure using standard tomographic methods applied to Love- and Rayleigh-wave dispersion curves. As a check on the tomographic results, several field experiments, consisting of 350 km long linear arrays of seismometers, were carried out to supply independent velocity measurements and to study the structure in greater detail in northwestern Nevada. Array data have been collected for three nuclear explosions at the Nevada Test Site, and frequencywavenumber analysis has yielded information on surface-wave velocities, improving our tomographic results. In addition to these structural investigations, we have carried out a joint study with the University of Texas, El Paso, into the source mechanism of a Borah Peak aftershock in central Idaho. The purpose of this study was to test our methodology for determining earthquake source mechanisms and for extracting directions of principal tectonic stress and source depth. The test results gave a source depth in agreement with studies of the aftershock distribution and gave principal stress directions in agreement with three independent seismic determinations of the source mechanism.

F. Advanced Concepts *(R. N. Schock and L. W. Younker)*

The Advanced Concepts project allows us to develop capabilities that are or will be needed by LLNL or DOE programs and to test hypotheses and prove feasibility before seeking major program funding. New topics are selected each year, based on scientific merit and relationship to the mission and interests of the Earth Sciences Department. We are currently funding a project aimed at direct observations of silicate melt properties at elevated pressures and temperatures using infrared spectroscopy. The goal is to construct and operate an apparatus necessary to obtain infrared and optical spectra at high temperatures (to 1000°C) and high pressures (to 500 MPa) and to use this capability to study the specification and properties of water in silicate melts. The first observation to be made will be of water in a granitic melt at temperatures of 700–1000°C and an argon pressure of 200 MPa. We will examine the ratio of water to hydroxyl groups in the melt as a function of temperature. Although this is a simple goal, it is fundamental to the study of water in melts. We will demonstrate hydrogen speciation by direct, equilibrated measurements for the first time.

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Contract: W-7405-ENG-48

Title: Geochemistry

Person in Charge: L. W. Younker

A. Thermodynamics, Kinetics, and Transport in Aqueous Electrolyte Solutions *(J. A. Rard and D. G. Miller)*

Transport of dissolved chemical species is important in a wide variety of aqueous geochemical phenomena. Geochemical applications include radioactive and chemical waste isolation, diagenesis, ore formation, and mineral crystal growth and dissolution kinetics under some conditions. Mutual diffusion coefficients are required to understand and model these processes, but relatively little diffusion data have been published. Diffusion data at 25°C are available for most of the major and minor brine salts and for several salts of diagenetic interest, and a small but growing amount of data is now available for mixtures. Activity/osmotic coefficients are available for many single salts but only some mixtures in water.

Mutual diffusion coefficients have now been measured for eleven of the twelve desired compositions of aqueous $SrCl_2$-NaCl (total molarities of 0.5, 1.0, 2.0, and 3.0 $mol{\cdot}dm^{-3}$ and molarity fractions of 1/3, 1/2, and 2/3). Additional experiments were performed for several of the compositions reported previously in order to improve the quality of the data. All diffusion data for NaCl-$SrCl_2$ mixtures were recalculated using tighter convergence criteria for the nonlinear least-squares calculations.

We have been measuring data for aqueous NaCl-$MgCl_2$, which is of interest for sea water and its evaporites. This work is part of a collaboration among USA, Australian, Canadian, German, Italian, and Argentinian laboratories to characterize the transport properties of an electrolyte mixture containing one higher valence salt. Our part of this effort is: 1) extensive isopiestic measurements were performed for NaCl-$MgCl_2$, and activity coefficients were calculated using Pitzer's and Stachard's neutral electrolyte methods, 2) diffusion and density data are being measured for NaCl-$MgCl_2$, in collaboration with visitors from Texas Christian University and the University of Naples (Italy), and 3) preliminary calculations for Onsager l_{ij} ionic transport coefficients were started but cannot be completed until data are available from the other laboratories.

B. Compositional Kinetic Model of Petroleum Formation *(A. K. Burnham, J. J. Sweeney, and R. L. Braun)*

The objective of this project is to derive and verify quantitative chemical kinetic models for petroleum formation. We showed a few years ago that our detailed pyrolysis model of Green River oil shale, developed mostly from experiments related to oil shale processing, predicted the occurrence and composition of petroleum in Utah's Uinta basin. However, the Green River formation is a lacustrine deposit having a significantly different type of kerogen than the marine deposits from which most petroleum is generated. Over the past year, we have redirected our project to determine kinetics for the marine kerogens to account for their lower hydrogen and higher oxygen content, which caused less oil and more carbonaceous residue to be formed during pyrolysis, and their larger spread in the generation temperatures of different kinds of organic compounds.

We systematically investigated the influence of a distribution of activation energies on the apparent activation energy derived if no distribution were assumed. We found, for example, that an energy distribution of only ±2% about a typical average value of 50 kcal/mol is sufficient to distort the apparent energy so that predicted oil formation temperatures for geological time scales are off by about 40°C. This study also led to a simple approximate method and an easy to use computer program for determining activation energy distributions.

We next used our computer program to derive hydrocarbon generation kinetics for a variety of petroleum source rocks using reaction rate data. Activation energy distributions were determined for nine source rocks. In contrast to some earlier studies, all energies are in the 40 to 60 kcal/mol range, which makes sense chemically. The reactivity of Green River shale and an African lacustrine kerogen could be described almost completely by single activation energies, but the marine kerogens usually required a distribution over several kcal/mol. In contrast to most previous assumptions, we found a wide variation in the principal energy and distribution width of the marine kerogens.

We have used these kinetic parameters to calculate two important characteristics of petroleum source rocks: the dependence of Rock Eval T_{max} on maturity and the oil generation profile at a geologic heating rate. T_{max} is the temperature of maximum hydrocarbon generation rate during standard Rock Eval pyrolysis and reflects the average reactivity of the remaining organic matter. If a distribution of activation energies is present initially, T_{max} will increase with maturity. Our kinetic parameters predict the T_{max} trends observed in typical well logs. Predicted oil generation profiles were calculated at a heating rate of 10°C/m.y. The temperature of maximum oil generation rate varies from about 110 to 160°C. Green River shale, at the high end of the scale, is within the range predicted for oil generation from marine kerogens and is comparable to Woodford shale. New Albany shale from Kentucky showed the lowest oil generation temperature, followed by Phosphoria and Kimmeridge shales. Preliminary modeling of the North Sea and Rocky Mountain basins indicates that the predicted oil generation temperatures for Kimmeridge and Phosphoria shales are consistent with observed occurrence of oil, but more detailed modeling is required for definitive verification.

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A. Continental Drilling Program Information and Data Management Unit *(G. Pawloski)*

The focus of this project has shifted from the general goal of collecting and disseminating information about wells available for scientific studies to a more specific activity: collecting, archiving, and analyzing well log data collected from the Salton Sea Scientific Drilling Program well. A data base system, with data from about 15 wells from the Salton Sea geothermal field, was taken to the SSSDP site before drilling began. It was maintained on site to provide researchers access to previously collected data and to construct an on-site data base of the data from the SSSDP well. The well logging data are currently being studied to develop log analysis methods that will allow the degree of metamorphism to be estimated without examining samples and to understand the physical changes caused by metamorphism. The data management program has ensured that the logging data from the SSSDP well were available to scientists during the drilling, were archived in an accessible manner, and are being studied to understand the hydrothermal system at the Salton Sea.

B. Viscosity and Electrical Conductivity of Rock Melts: Continental Scientific Drilling Program *(F. J. Ryerson and H. C. Weed)*

The viscosity of magmatic systems strongly influences their ability to transport matter and energy. Since subliquidus systems are of considerable practical importance in petrologic processes, we have measured viscosities in both the superliquidus and subliquidus regions and correlated the rheological behavior with the melting behavior of the sample to determine the influence of temperature, fluid composition, and solid phase volume fraction. We measured the viscosity of a Medicine Lake high-Al basalt for which the crystallization sequence had previously been determined. The basalt shows negligible yield stress from 1315 to 1240°C and rapidly rising yield stress from 1229 to 1170°C. The rapid increase correlates well with the increase in crystal concentration. The curvature of the flow curve displays Newtonian behavior above 1240°C and pseudoplastic behavior below 1240°C. The range of the steady-state viscosity at unit shear rate (μ) was from 10 to 1600 Pa·s. An arrhenius plot of log μ vs 1/(T,K) shows two branches intersecting at 1244°C. The high-temperature branch corresponds to viscous flow in single phase fluid with an apparent activation energy of 46 $\pm$ 50 kcal/mol. The low-temperature branch corresponds to viscous flow in a multiphase suspension with an apparent activation energy of 280 $\pm$ 50 kcal/mol. Although an increase in fluid viscosity in the low-temperature region would be expected because of the changing composition of the melt, this change (as calculated from the Bottinga-Weill scheme) is small compared with the observed increase in suspension viscosity. Hence, we attribute the observed rapid increase to hydrodynamic interaction between fluid and crystallites.

C. Seismic Studies of Possible Magma Injection and Magma Chambers in the Long Valley Region *(J. J. Zucca and P. W. Kasameyer)*

We have performed a passive seismic experiment in the Long Valley caldera region of California. A small network of 14 three-component digital seismographs in the Mono craters area recorded small earthquakes located to the south of Long Valley. One earthquake recorded shows a clear, high amplitude phase arriving between the normal P and S arrivals. A similar phase has been recorded by other researchers corroborating our observation. Through amplitude and travel time modeling we suggest that the phase is a P to P reflection from the base of a low-velocity layer with a high-velocity floor that extends to near the base of the crust. A second passive seismic experiment has been planned for late summer 1987. Recent observations of teleseismic P waves recorded in Long Valley show large anomalous arrivals on the horizontal components. These phases may be due to converted energy from interfaces five to eight kilometers below the surface of the caldera and could provide a new method for mapping the magma chamber in the region. To confirm the exact nature of these arrivals, ten three-component stations, using high-quality 1 Hz seismometers, will be deployed in the resurgent dome area to measure both the phase velocities and particle motions of these arrivals.

D. Shallow Hole Investigations of Long Valley, Valles, and Salton Sea Thermal Regimes *(L. W. Younker, P. W. Kasameyer, R. L. Newmark,* and *N. R. Burkhard)* (Cooperative program with SNL, LANL, and LBL)

During November and December 1985, Lawrence Livermore and Sandia National Laboratories cooperated in drilling a series of shallow (80 m or 250 ft) holes in the southern Salton Sea as part of the Thermal Regimes shallow drilling initiative. The intent was to complete the surficial coverage of the thermal anomaly offshore in the region north of the line of volcanoes. Temperature profiles were logged periodically in these holes to establish equilibrium temperatures. These data allow us to close the contours around the thermal anomaly, revealing its shape and extent. The contour map of the thermal gradients shows the thermal anomaly to be of arcuate shape, about 4 km wide and about 12 km long. This is in contrast to earlier predictions of a circular shape. These observations will be used to constrain models of the evolution of the hydrothermal system and of continental rifting.

The purpose of drilling at Inyo dome volcanic chain of eastern California is to understand the behavior of silicic magma as it intrudes the upper crust. This behavior,which involves the response of magma to decompression and cooling, is closely related to both eruptive phenomena and the establishment of hydrothermal circulation. In early June 1987 a steeply dipping 1000-m hole will be cored across the trend of the chain from a site near Inyo craters, passing beneath the largest of the phreatic craters. This is the fourth in a series of research holes that have explored both the extrusive and intrusive Inyo systems. Outside Long Valley caldera, holes have penetrated the largest of the Inyo lava domes and probed the parent intrusion within Sierran basement. The results have demonstrated the close relationship between eruption and shallow dike emplacement for silicic magma, delineated chemically tagged flow paths in the extensive/intrusive system, documented the excavation of a vent funnel prior to extrusion, and demonstrated the contrasting crystallization behavior of extruded and shallowly intruded magma. One of the conclusions reached is that silicic magma ascends as permeable foam and that the extent of degassing and hence eruptive behavior depends strongly on the permeability of the intruded environment. Observations in the planned hole will test these ideas by describing the behavior of the same magma in a more permeable environment, where both more rapid degassing and cooling are expected to have occurred.

E. SSSDP: Constraints from Borehole Gravity on Geothermal System Models and Resource Definition for the Salton Sea Geothermal Field *(J. R. Hearst, P. W. Kasameyer,* and *L. W. Younker)*

We use observations with a borehole gravimeter to learn about the density structure in the vicinity of the SSSDP well and use that knowledge to understand more about the evolution of the hydrothermal system at the Salton Sea. Since density indicates the degree of metamorphism and the hole was near the edge of the geothermal field, it was thought that extending the range of investigation about the borehole might detect the lateral border of the metamorphosed zone, if it lies within several hundred meters of the borehole. Measurements were collected between 3400 to 5700 feet depth, and the vertical gradient of gravity was measured. We found that the gravimetric density is within 0.02 g/cm^3 of the log density over the depth interval studied, and the above-ground vertical gradient at the site is anomalously high. Two hypotheses can explain these observations. Either the SSSDP well is surrounded by high density material between 3000 and 6000 feet, or there is low density material near it at a range of 0 to 2000 feet. Because of the high densities observed in the SSSDP hole, the second hypothesis is preferred.

F. SSSDP: Physical and Chemical Laboratory Studies of Cores from the Salton Sea Scientific Drilling Project *(W. D. Daily* and *W. Lin)*

We planned to measure the ultrasonic wave velocities, electrical resistivity, and brine permeability on SSSDP samples under *in situ* pressure and temperature conditions. The experiment will provide insight into the interpretation of well log and surface geophysical data, understanding of brine transport mechanism, interpretation of flow tests, and the extrapolation of properties measured in the borehole to greater depths. So far a SSSDP siltstone core from 1158-m depth has been studied in the laboratory to determine electrical resistivity, ultrasonic velocities, and brine permeability at pressures and temperatures close to the estimated borehole conditions. The maximum pressure and temperature during the experiment were 50 MPa and 245°C. At the mid-plane of the sample, impedance imaging was used to map the spatial variation of resistivity as a function of time. Also, in the same plane ultrasonic tomography was used to map the spatial variation of P-wave velocity. In addition to these tomographs, resistivity was measured with 6 pairs of electrodes along the sample axis. P-wave and S-wave velocities were also measured along the sample axis. Sonic P-wave velocities at 245°C, 30 MPa confining pressure, and 12 MPa pore pressure were slightly higher than measured by the well logs, and resistivities were much higher.

G. Underground Imaging *(W. D. Daily and J. G. Berryman)*

The thrust of the underground imaging effort is development of data collection methods, data processing procedures, integrated data interpretation techniques, and enhanced means of data presentation in order to characterize the subsurface environment. Our work involves developing improved laboratory and field instrumentation, acquiring fundamental data on the properties of materials under varied conditions in the laboratory, and improving the overall data interpretation process. The results of this project will benefit many DOE programs including nuclear waste emplacement and monitoring, test ban verification through on-site inspection and cavity detection, enhanced oil recovery, and basic research through imaging the detailed flow patterns of fluids in fractured rocks. A program is in progress to continue development of electrical impedance tomography (EIT) for geophysical applications. We have continued developing algorithms to solve the inverse problem of EIT. We have compared our algorithms against the iterative Newton-Raphson method and concluded that our least-squares method has the most potential for accurate reconstruction. We have improved the model for the impedance distribution in the least-squares solution. Our ability to construct realistic models of rocks has therefore been significantly enhanced. Besides EIT, we are also continuing development of high frequency electromagnetic and seismic tomography methods, especially for application to borehole-to-borehole geometry. A new algorithm for travel time inversion tomography in regions with large wave-speed contrasts has been formulated and is currently being tested on synthetic data.

Contractor:	LOS ALAMOS NATIONAL LABORATORY University of California Earth and Space Sciences Division
Contract:	W-7405-ENG-36
Category:	Geology, Geophysics, and Earth Dynamics
Person in Charge:	T. J. Shankland

A. Electrical Conductivity, Temperature, and Radiative Transport in the Earth *(T. J. Shankland, joint research with A. G. Duba, LLNL)*

The thermoelectric effect S and electrical conductivity σ in the mantle minerals olivine and pyroxene are being measured as a function of temperature, orientation, oxygen fugacity, and iron content. Results of this research help determine temperature distributions in the crust and upper mantle. Because temperature differences drive tectonic motions on the Earth's surface and interior, improved knowledge of thermal patterns is a requirement for evaluating seismic and volcanic hazards to waste isolation and power plant sites. Further, locating high temperatures is an essential for regional geothermal prospecting. The results should clarify our understanding of the regional geophysics needed for Continental Scientific Drilling site selection and for nuclear event detection and discrimination.

In measuring S and σ in iron-free mineral forsterite under oxidizing and reducing conditions, we infer this material to be a mixed electronic and ionic semiconductor. At low oxygen pressures it appears to be a good ionic semiconductor via extrinsic magnesium vacancies along the crystallographic c-axis; whereas, it is an electronic semiconductor along the other two axes. We have used these results in two ways. One has been to use spatial averages to obtain a best-fitting conductivity-temperature curve for determining upper bounds on mantle temperatures from field electrical work. The other was to argue for a high-temperature mantle geotherm on the basis that the abrupt rise of the mantle high conductivity layer is due to partial melt.

From radiative heat transport calculations for silicic magmas, we infer that these materials are among the most highly thermally conductive materials in the earth. We have accomplished a similar suite of measurements for (Mg, Fe)O, the most likely Fe-bearing phase in the lower mantle. The results will apply to heat transport and convection in the largest uniform part of the Earth's interior.

B. Nonlinear Generation of Acoustic Beams *(T. J. Shankland and J. N. Albright)*

We are using the nonlinear elastic properties of rocks to generate low-frequency, long-wavelength acoustic beams in analogy with the case in laser optics. Two narrow beams of high-frequency sound can interact in a nonlinear medium to produce a narrow beam at their much lower difference frequency. The lower frequency beam has the narrow width of the generating beams, but it can travel much farther because of lower attenuation. Such a narrow beam would permit examination of acoustic interfaces from mine interiors and wellbores without the ambiguities of conventional seismology that use undirected sources, for example, transducers or explosives that broadcast energy in an almost spherical pattern. Should beam formation prove possible, there would be numerous applications to problems such as mapping fractures, the boundaries of ore and coal bodies, burn fronts in underground retorts, and fluid locations in oil, gas, and geothermal reservoirs. Of more interest to basic research in rock physics is the investigation of nonlinear properties of rocks and frequency dependence of elastic properties.

Preliminary results showed difference frequency generation from vibroseis transducers operating in the field and from piezoelectric transducers on laboratory specimens at high frequencies. In the laboratory, we have shown that the intensity of the difference beam is proportional to the product of intensities of the driving beams as predicted by theory. The definitive work has come from observations of the general case of two driving beams intersecting at arbitrary angles to produce a difference beam at a still different angle. In this case we have been able to verify the selection rules that govern these angles when sample velocities and frequency ratios are specified.

C. Time-Dependent Deformation of Rock *(R. L. Kranz and J. D. Blacic)*

Assurance of long-term isolation of nuclear wastes in mined cavities in hard rock requires knowledge of the time-dependent strength and transport properties of these rocks. Normal, short-time engineering tests do not encompass the full effects of phenomena such as stress-aided corrosion, hydrolytic weakening, and stress generation resulting from hydration of dehydration of susceptible minerals. It is known, for example, that water-related geochemical effects are coupled with stress-induced mechanical effects, but the magnitude and time-dependency of this coupling is poorly understood.

The objectives of this research are: 1) to understand and evaluate the effects of water on time-dependent brittle rock deformation, including rock swelling and contraction, and 2) to evaluate changes in transport properties, such as permeability, that accompany this deformation. To accomplish these objectives, we perform creep experiments on candidate repository host rock such as basalt, granite, and tuff under simulated *in situ* repository conditions.

Experiments have demonstrated a number of interesting and important phenomena. Increases in water content, internal pore pressure, or temperature accelerate the static fatigue of rock, lowering strength and time to failure under constant load. We have demonstrated the competing effects of microcrack generation and solution and deposition processes on rock fluid-transport properties. The former results in increased permeability, whereas the latter results in decreased permeability as rock continues to deform in time. We have also demonstrated that the time-dependent absorption of water by zeolite minerals in confined tuff can create large compressional internal stresses. We are now studying the reverse situation where dehydration causes extensional stresses, possibly resulting in microcrack generation, which would again reflect on the transport properties. It is important to understand the complicated interaction between thermomechanical effects and geochemical effects during the lifetime of the repository.

D. Advanced Geoscience Concepts Research *(N. Marusak)*

A major aspect of subsurface geologic interpretation is the comparison and correlation of geophysical logs by geoscientists. This research project proposed to create an expert system by applying pattern matching techniques developed in speech recognition technology to geophysical log analysis or comparison.

The approach used was to divide the project into four modules. The first was a forward chaining inference or a database with interpolation. The geologic and geophysical parameters for a specific location are predicted from data in nearby drill holes. The second module was a backward chaining inference. A site must be selected that meets many different criteria and includes appropriate heuristics. The third module was the dynamic pattern matching used to correlate geophysical logs. The last module was that the expert system should incorporate a natural language query, i.e., interactions should be in English.

The prototype for the project used an existing large database of geological and geophysical data from the Nevada Test Site as its basis. Dynamic pattern matching and natural language query were activated. Dynamic pattern matching of geophysical logs could be done using certain algorithms related to speech recognition. Now, allowable variability and lateral variation are being considered for the module. The natural language query module was operational last year. A format was setup that included discrete information for over 300 holes. The first two modules, which were the most difficult, were partially completed. As part of both modules, a polynomial fit routine was developed to be used on each stratigraphic layer to help determine structure and tectonic activity.

This year, simple problems such as future site selection and anticipated geological structure were set up to prove feasibility studies of both the forward chaining and backwards chaining modules. Toward the end of this year, the feasibility of this prototype was realized. All the modules can be implemented to some extent on the IBM PC AT. The current goal is to have this expert system interface with the existing database. This database includes all geophysical and geological information from the Nevada Test Site. The database resides on a VAX 8650 under the VMS operating system. After extensive investigation of currently available equipment and software, it has been decided that KEE will be the system used for this interface to the existing database on the VAX.

Contractor:	LOS ALAMOS NATIONAL LABORATORY University of California Los Alamos, New Mexico 87545
Contract:	W-7405-ENG-36
Category:	Geochemistry
Person in Charge:	R. W. Charles

A. Coal Maturation: Occurrence, Form, and Distribution of Inorganic Phases within the Peat-to-Lignite Transition *(R. Raymond, Jr., A. D. Cohen, and D. L. Bish)*

Peat, the precursor of coal, is composed predominantly of plant components and secondarily of mineral matter derived from various sources. The elemental, mineralogic, and petrographic compositions of a peat are controlled by a combination of botanical and depositional environments. The coal resulting from this peat is controlled by digenetic alterations during peatification and later coalification. To evaluate the occurrence of inorganic phases in a coal deposit, we must understand the mechanisms for their introduction into the original peat deposit and the physical and chemical conditions affecting the peat during its transformation into coal.

The objectives of this research are: 1) to identify and correlate authigenic and detrital inorganic phases found in different peat types and compare these with those found in lignites, 2) to identify the processes that enhance and/or inhibit distribution and preservation of inorganic material in the initial coal-forming environment, and 3) to construct geochemical models for formation, preservation, alteration, and distribution of inorganics in peats and lignites based on the first two objectives. To achieve the above objectives, we will investigate the occurrence of inorganics within peat and lignite deposits and the physical and chemical conditions affecting these deposits. Deposits will be chosen such that the most reasonable correlations can be made between the depositional environments of the peats and those of the lignites. Our approach is to use state-of-the-art analytical instruments to characterize the modes of occurrence and content of biogenically and nonbiogenically derived inorganic phases in the peats and lignites. We will then establish geochemical models for the alteration of those phases during the peat-to-lignite transition. These models will allow us to predict the occurrence and distribution of inorganics within various lignite and higher rank coal seams.

Results to date suggest that factors controlling the amount and type of inorganic material in peats are: 1) underlying bedrock or sediments, 2) detrital source areas, and 3) the ecology of the peat-forming botanical communities. Thus, inorganic phase contents and major and trace element contents of peats relate directly to depositional and ecological settings rather than geographic provinces.

B. Rock-Water Interactions and Element Migration *(R. W. Charles, D. R. Janecky, T. M. Benjamin, and P. S. Z. Rogers)*

The emphasis of this project is experimental and computational modeling of rock-fluid reactions in hydrothermal systems applicable to environments of general interest for the discovery and recovery of energy whether geothermal or fossil.

The major thrust at this time in the Continental Scientific Drilling context consists of sample collection and experimental hydrothermal reactions investigating various natural hydrothermal systems. The discrimination of major, minor, and trace elements (via nuclear microprobe) chemistry and associated phase equilibria during mobilization, transport, and deposition is the thrust of this investigation. Experimental systems are used to develop models for element migration in strong brines using single minerals as well as rocks. The results will aid in developing a model relating portions of the various hydrothermal systems using the mineral assemblages defining the state of local equilibrium. Solubility (mass transport) models, reaction path calculations, and coupled flow and rock-water interaction calculations are upgraded as the experimental data are analyzed.

The modeling of natural systems has yielded important new results from CSDP wells. From the naturally observed phase assemblages, we are able to define the state of equilibrium in VC-2a (Sulphur Springs, Jemez Mountains, NM) and constrain the thermodynamic properties of the molybdenite deposits encountered there. Alteration assemblages are used to constrain the hydrologic environment of RDO-2b, Long Valley, California, and perturbations due to volcanic events. In effect the rock-water reactions show the rhyolite dike dams and diverts the ground water flow. At Salton Sea we can demonstrate total dissolved sulfur had to be much higher in the past or temperatures significantly lower than those currently observed to stabilize the bulk rock mineral assemblages. Evaluation of coupled volcanic-hydrologic processes and their chemical-thermal-hydrologic consequences is important for making long-term predictions of hydrogeochemical processes in areas with significant probabilities of volcanic activity. The experimental program, closely coupled to the above, used Au-Ti reaction cells to examine reaction pathways, mineral reaction rates, alteration mineralogy, solution composition, and effects of salinity, temperature, and pressure. Work is coordinated with the calorimetry and Raman projects described below. Current experiments at high salinity react magnetite-hematite-kspar-epidote and hematite-pyrite-kspar-epidote defining several chemical parameters of the system that are compared with computed values.

C. Thermodynamic Properties of Aqueous Solutions at High Temperatures and Pressures *(P. S. Z. Rogers)*

Knowledge of the thermodynamic properties of aqueous solutions is basic to an understanding of many geochemical systems. Hydrothermal alteration, element migration, and geothermal activity are a few examples of processes largely dependent on the properties of the associated aqueous fluid. Studies of these processes require information on the heat content and ion activities of mixed electrolyte solutions over a wide range of composition and temperature. A high temperature/high pressure flow calorimeter has been constructed to measure the heat capacities of aqueous electrolyte solutions. Operation and calibration of the calorimeter have been sufficiently refined so that heat capacities can be determined with an accuracy of better than 0.05%. Heat capacity data have been obtained for mixtures of $NaCl$-Na_2SO_4-H_2O, an important system in many cases of hydrothermal transport and deposition. Work presently underway is extending these measurements to 200 bar and nearly 350°C. The ultimate goal is to provide data to 400°C at 400 bar, in order to study the behavior of electrolyte solutions in the region very near the critical point of water.

D. Geochemistry of Technetium: Geochemical Controls of the Transport and Retention of Multivalent Elements in the Geosphere *(D. B. Curtis, R. E. Perrin, and D. J. Rokop)*

Technetium is an extremely rare element in nature. A single isotope, ^{99}Tc, exists in the geosphere as a product of the fission of isotopes of uranium. This nuclide is radioactive, with a half life of 2.13×10^5 y. Consequently, it is a transient element in nature, constantly being produced by a nuclear reaction and destroyed by radioactive decay. If uranium and technetium are unfractionated for time periods of the last million years, they will establish a state of nuclear equilibrium, where the rate of production of technetium is equal to rate of radioactive decay. The result is an invariant ratio in the relative abundances of the two elements. The object of the research is to establish a means of predicting the relative abundances of the two elements at nuclear equilibrium. Such a predicted ratio will serve as a comparison for measured abundances of the two elements to evaluate aspects of the physiochemical state of the system over the last 10^6 y. For example, correspondence between the measured ratio and the ratio at nuclear equilibrium might signify a closed system with respect to these two elements for the last million years. We have used this technique to analyze samples from the Koongarra uranium deposit in the Australian Northern Territory and to make the first known measurement of the concentration of technetium in water. The ultimate goal is to use these methods to study chemical and temporal aspects of processes in the geosphere.

E. Trace Element Geochemistry of Volcanic Gases and Particles from Basaltic Volcanoes and Geothermal Fluids *(B. Crowe and D. Finnegan)*

Field and laboratory studies are being undertaken to investigate the trace element compositions of volcanic gases and particles of active volcanoes. We have sampled volcanic gases during four separate eruptions and at the cooling vents preceding and following eruptions of Kilauea and Mauna Loa Volcanoes, Hawaii. The collection system used consists of a series of filters contained in a polyethylene canister. After exposure to volcanic aerosols, the filters are analyzed using INAA for about 35 to 40 elements. The major goals of the project are: 1) determine the characteristic trace element contents of volcanic fume associated with the eruption of Hawaiian magmas, 2) evaluate the variations in the trace element composition of aerosols through eruption cycles, and 3) evaluate the speciation of highly enriched metals directly upon release from the magma. This information will be used to examine the geochemical mechanisms of trace element enrichment in volcanic fume for the prediction of future volcanic eruptions. The most promising use of trace metal monitoring for eruption prediction would be at silicic volcanoes that commonly show a phase of increased gas emissions and preatic outbursts prior to major eruptions (for example the 1975–1976 activity of Soufriere de Guadeloupe and the 1980 eruption of Mt. St. Helens).

F. Raman Spectroscopy of Aqueous Solution Species *(N. Marley, T. Benjamin, and P. Rogers)*

Knowledge of the speciation behavior of metal-ligand complexes is important to modeling mineral solubilities, metal ion transport, and ore deposition. However, data for the quantitative determination of metal-ligand complexes in aqueous solution at geologically significant pressures and temperatures are quite limited. Few complexes have been studied above 100°C whereas there is a need for data to at least 600°C. Speciation of geologically important complexes will be determined by high temperature, high pressure Raman spectroscopy. Laser Raman spectroscopy provides one of the most direct methods for the quantitative determination of complex species in aqueous solution. Unlike the complementary technique of IR spectroscopy, it is relatively free of interferences from the water solvent. Although absolute quantitation of Raman spectra is nontrivial, it is our goal to obtain sufficient accuracy to generate equilibrium constants as a function of temperature and pressure. These experiments will be coordinated with calorimetry measurements and hydrothermal studies to narrow the possible interpretations.

G. A Search for Evidence of Large Comet or Asteroid Impacts at Extinction Boundaries *(C. J. Orth)*

There is considerable evidence that a large extraterrestrial body collided with Earth at the end of the Cretaceous Period, about 65 million years (m.y.) ago, and that the impact probably led to the mass extinction that characterizes the Cretaceous-Tertiary (K-T) boundary. Although no distinctive crater has been identified, the occurrence of microspherules, shocked-mineral grains, and a strong Pt-group (Ir) anomaly at the boundary is consistent with the impact scenario. The objectives of this work are to search for evidence of large-body impacts at the extinction boundaries in the fossil record, to study the consequences of the local release of ultra-high amounts of energy, and to study the effects of "impact winter," nature's equivalent of "nuclear winter." In this new study we have found several Ir anomalies, which have generally proven to be derived from terrestrial processes. Currently, we are concentrating our effort on the 92-m.y. Cenomanian-Turonian stage boundary. This globally recognized extinction occurred 26 m.y. (one "cycle") before the massive K-T extinction, and the results of our study should provide an important test of the periodic comet-swarm hypotheses.

H. Development of a Borehole Hydrothermal Solution Sampler for High Temperatures, Brine Salinities, and Gas-Tight Operation *(R. Charles, C. Navarro, and D. Janecky)*

Investigation of the composition of hydrothermal fluids has important applications to resource evaluation, both in energy and materials development. Studying fluid compositions can lead to understanding of the source and pathway of fluids and indicate geothermal energy potential, hydrocarbon resources, and metal deposit formation. However, many, if not most, hydrothermal solutions do not appear at the Earth's surface for sampling and those that are accessible may be significantly modified by the venting process. Thus, sampling solutions from boreholes is a necessary part of hydrothermal research efforts. Due to the inherent limitations of previous sampler designs, simultaneous collection of uncontaminated and unfractionated fluid and gas from discrete horizons under commonly encountered hydrothermal conditions cannot be assured or even expected. Our objective is to develop a wireline-based tool for simultaneous collection of uncontaminated and unfractionated gases and fluid in the difficult environment encountered in boreholes drilled as part of the CSDP project. We have modified a commercially available slim-line, flow-through sampler that will be used to collect fluids from these extreme conditions. Different sealing mechanisms and sampler metals are incorporated in the new design. A prototype is under construction at this time.

Contractor:	LOS ALAMOS NATIONAL LABORATORY Los Alamos, New Mexico 87545
Contract:	W7405-ENG-36
Category:	Energy Resource Recognition, Evaluation, and Utilization
Person in Charge:	C. W. Myers

A. Search for Magma Chambers and Structures Beneath the Northern Jemez Volcanic Field: An Integrated Geological, Geophysical, and Petrochemical Study *(K. H. Olsen and W. S. Baldridge)*

The Jemez volcanic field of northern New Mexico, which includes one of the world's largest and youngest calderas, is a complex volcanic field with a history of eruptions from more than 14 m.y. ago to 130,000 years ago. Volcanism is broadly coincident with reactivation of the Rio Grande rift, with Basin and Range extensional deformation, and with regional basaltic activity. Recent seismic tomography experiments by us have delineated a large (greater than 15 km diameter by 15 km deep) pluton at shallow crustal depths beneath the Valles and Toledo calderas, which were the sites of two cataclysmic Bandelier ash flow eruptions 1.45 and 1.12 m.y. ago. The Bandelier pluton includes the magma chambers that were the sources for the ignimbrite eruptions; these are large enough and young enough that they may still contain pockets of residual magma. The objective of this study is to closely integrate geophysical and geological/petrological techniques in an area immediately northeast of the Valles caldera where a long record of volcanic history (> 10 m.y. to < 2 m.y. ago) of the Jemez is preserved.

Our work is directed toward a better understanding of the evolution of a complex intermediate-to-silicic volcanic field, of processes leading to formation of major calderas, and of the present structure of the volcanic field. By focusing on this region we will: 1) search for upper crustal magma chambers and/or plutons associated with a young (> 3.0 m.y.-old) andesite/dacite dome and flow field (Tschicoma formation) and with a group of young (2.0 m.y.-old) rhyolite domes (El Rechuelos formation), 2) quantify the thermal and composition-volume-structural development of the (composite) pluton underlying the Jemez volcanic field, and 3) correlate geophysical data (including density and seismic velocities) with petrographic studies to facilitate interpretation of subsurface geophysical data and to develop a detailed model of the structure and evoluton of the magma chambers underlying this major silicic volcanic field.

This interdisciplinary project, which will also incorporate and synthesize a large amount of existing geophysical, geological, and geochemical data, will augment the research goals of the CSD project in the Jemez volcanic field directed toward a better understanding of physical and chemical processes surrounding a major, shallow silicic magma system. The results will have general application to other large intermediate-to-silicic magmatic systems in the continental crust, including Long Valley and Yellowstone.

B. Valles Caldera: Fluid Sampling and Core Studies of Sulphur Springs *(F. E. Goff and J. N. Gardner)*

Valles caldera has been a high-priority site since the earliest days of Continental Scientific Drilling. Because of the size, youth, and excellent preservation of this caldera complex, its high-temperature hydrothermal system, and the available data base, Valles caldera has appealed to both the thermal regimes and mineral deposits communities as an ideal laboratory for the study of magmatic processes and active hydrothermal systems.

The first CSDP core hole in Valles caldera was VC-1. This core hole investigated: 1) a hydrothermal outflow plume near its source, 2) structural and stratigraphic changes at the intersection of the caldera ring-fracture zone and the pre-caldera Jemez fault zone, and 3) the Banco Bonito obsidian flow, the youngest eruption in Valles caldera. VC-2A was the next core hole of the long-range plan for continued scientific drilling in the Valles caldera and was to investigate a small vapor-dominated geothermal system. Vapor-dominated systems are important to the geothermal industry because they may yield dry steam, which is the most economically desirable geothermal resource. Characteristic of vapor-dominated systems is a high-temperature boiling interface at depth between vapor- and liquid-dominated zones. Also, these boiling interfaces have important implications for ore genesis. Studies of fluid and gas samples and the altered cores from VC-2A helped characterize the Sulphur Springs system. These data will be integrated with geologic and geophysical studies to be conducted in the well. Preliminary results from VC-2A show a rather complete sequence of intracaldera tuffs, rotation of tuff units that may document structural resurgence, an orderly configuration of hydrothermal zones, and a sub-ore grade molybdenum deposit.

VC-2B will be a continuation of CSDP efforts at Sulphur Springs, Valles caldera, that began with the coring of VC-2A. The objectives of scientific drilling in the Sulphur Springs area are: 1) direct measurement of physical conditions and sampling of fluids of zones within the Sulphur Springs hydrothermal system, 2) sampling of products of active hydrothermal mineralization in the system, 3) development and evolution of vapor-dominated geothermal systems, 4) obtaining important structural and stratigraphic information on the western flank of the resurgent dome of Valles caldera for caldera process models, and 5) studying the heat transfer from the deep cooling magma chamber through the conductive thermal regime that underlies the Sulphur Springs hydrothermal system.

C. Downhole Fluid Sampling of Salton Sea Scientific Drilling Program Well *(F. E. Goff, C. O. Grigsby, and P. E. Trujillo, Jr.)*

The Salton Sea geothermal field is one of the largest, hottest, and most saline geothermal systems in North America. The Salton Sea Scientific Drilling Program (SSSDP) will explore the roots of this system and could yield more data to the public domain than any commercial geothermal well drilled to date. The geochemistry of *in situ* fluids will be an important set of these data.

Our objective was to acquire uncontaminated samples of formation fluids to provide the chemical analyses required to identify the sources and flow paths of ground water and quantify metasomatic and metamorphic processes in Salton trough sediments due to burial and heating by magmatic intrusion. Because fluid inclusions do not provide a large enough sample for comprehensive, precise chemical analyses, we proposed to collect large-volume, *in situ* samples from several different aquifer horizons using new high-temperature (350°C) downhole sampling devices.

The goal of the sampling was a comprehensive chemical and isotopic analysis of the samples. Samples were obtained from 3110 m at 350°C and 1860 m at 300°C. These samples are believed to be the most saline *in situ* samples ever collected at depth. Los Alamos and Lawrence Berkeley Laboratories analyzed splits of samples for major trace element chemistry, stable isotopes, tritium, bulk gas composition, ^{13}C isotopes of CO_2, ^{36}Cl isotopes of water, and ^{10}Be isotopes of water. Splits of samples were provided to other researchers. This suite of carefully collected and analyzed fluid samples from many horizons in the extremely hot and saline environment will form a major part of the research aims of the SSSD Project.

D. Development and Initiation of Sample Management Policy Procedure for CSDP *(S. J. Goff)*

The Curation Office, managed from Los Alamos, operates a core curation facility at Grand Junction, Colorado. This facility is designed to provide the scientific community with access to geologic samples from CSDP core holes. The core repository occupies about 7,200 square feet of space in Building 7 at the DOE Grand Junction facility. In addition to the core-storage area, the repository contains office space for the curator, a receptionist, and visiting scientists, as well as rooms housing specialized sample preparation equipment. Core can be viewed in a large enclosed and heated area, which is equipped with sample tables designed for laying out many boxes of core at once. Equipment includes a 24-slab saw, a trim saw, a drill press, and a core splitter. Also available for scientists are binocular and petrographic microscopes. Presently archived at the repository are ~ 8000 feet of drill core from various CSDP drilling projects.

The Curation Office has also published Curatorial Policy Guidelines and Procedures for the Continental Scientific Drilling Program, which includes the Field Curation Manual for the Inyo domes, Salton Sea, Shady Rest, and Valles caldera drilling projects.

E. Scientific Assembly of the International Association of Volcanism and Chemistry of the Earth's Interior *(S. Baldridge, G. Heiken, and K. Wohletz)*

The 1989 Scientific Assembly of the International Association of Volcanism and Chemistry of the Earth's Interior (IAVCEI) will be partially supported by the DOE Office of Basic Energy Sciences. The meeting will be held in Santa Fe, New Mexico and emphasize volcanology and geochemistry-petrology. Numerous scientific sessions and symposia are planned as well as a field excursion into the nearby Jemez volcanic field, Valles caldera, and Taos plateau volcanic field. Los Alamos geoscientists (S. Baldridge, G. Heiken, and K. Wohletz) are members of the organizing committee. Those interested in receiving future circulars regarding the meeting should contact IAVCEI/1989 c/o Protocol Office, Los Alamos National Laboratory, Mail Stop P366, Los Alamos, NM 87545, USA.

F. Evaluation of Data Base Systems for OBES CSDP *(N. Marusak)*

During this past year, a joint effort was made to address the database needs, implementation, and protocol for the Department of Energy/Office of Basic Energy Science

(DOE/OBES) and the Deep Observation Sampling of the Earth's Crust (DOSECC) community. The major activity was a workshop held in Lakewood, Colorado to evaluate the various database needs. Due to lack of representation by DOE personnel, much of the discussion was weighted toward the needs of DOSECC. In spite of the sparse attendance, significant progress was made. Many of the database needs, potential pitfalls, and current as well as upcoming hardware and software availability were discussed. Some specific concerns to be addressed initially were establishing data format standards and guarding against mishandling and/or loss of data. It was decided the organization of a sub-committee to evaluate database requirements of both communities and to provide recommendations would be mutually beneficial.

Contractor: LOS ALAMOS NATIONAL LABORATORY
University of California
Los Alamos, New Mexico 87545

Contract: W-7405-ENG-36

Category: Solar-Terrestrial-Atmospheric Interactions

Person in Charge: S. P. Gary

The objective of this program is to carry out theoretical and experimental research on the plasma physics of the solar wind and the Earth's magnetosphere and ionosphere. There are four goals of this research: to understand the flow of plasma energy in the near-earth space environment from a small-scale point of view, to understand the plasma physics of the solar wind-magnetosphere interaction, to understand the details of the acceleration processes affecting energetic particles in the magnetosphere, and to understand certain astrophysical plasma physics problems that have implications for solar-terrestrial plasmas. Since the solar wind and magnetospheric plasma are the media through which solar-generated disturbances propagate and in which solar wind convection energy is stored and subsequently released to the auroral ionosphere, these studies help us understand the coupling of solar variations to the near-earth environment.

A. Energy Transport in Space Plasma *(S. P. Gary)*

The long-term goal of this research is to understand the flow of plasma energy in the near-earth space environment from a small scale point of view. Specifically, we use electron and ion distribution functions observed by Los Alamos plasma instruments to carry out fundamental studies of plasma instabilities and associated transport in and near the Earth's bow shock, magnetosphere, and ionosphere. Our most important accomplishment of 1986 has been our explanation of the ion-acoustic-like electrostatic noise upstream of the Earth's bow shock. We first carried out a broad theoretical examination of the ion/ion acoustic instability, then coupled the results of this study to a study of data from Los Alamos instrumentation on the ISEE-1 and -2 satellites. We showed that steep sides of observed ion beam velocity distributions at oblique angles to the magnetic field can drive the ion/ion acoustic instability and are therefore the most likely source of the observed noise.

B. The Solar Wind-Magnetospheric Interaction *(E. W. Hones, Jr., and J. Birn)*

In its simplest terms the interaction of the solar wind with the magnetosphere is that of a fast flowing, highly conducting plasma with a stationary source of magnetic field, i.e., it is completely analogous to the action of a magnetohydrodynamic (MHD) electric generator (although much more complex) and is thus electrodynamical in nature. The purpose of this research is to extend the understanding of this complex magnetoelectrical plasma system by examining its global structure and dynamics through correlative studies of data from multiple sites within and near the magnetosphere (including the Earth itself and appropriate scientific satellites) and by the development and use of theoretical models of the structure and dynamics of the magnetosphere. Our most important experimental achievement in 1986 was the organization and execution of the PROMIS project. In the spring of that year there were three satellites making measurements of the magnetotail and one satellite making measurements in the solar wind, while two other satellites carrying unique, newly developed imaging devices were recording images of the northern and southern polar auroras. Foreseeing this situation a year ahead of time, we organized Project PROMIS, with the support and collaboration of NASA organizations, to maximize the acquisition of data from these and other magnetospheric data sources. Our most important theoretical achievement of 1986 was the use of our MHD computer models to demonstrate that reconnection in the magnetotail can give rise to significant plasma flow parallel to magnetic field lines in the plasma sheet boundary layer. This demonstration has supported the neutral line model of the magnetotail against a major criticism and has established this model more firmly as an appropriate description of magnetospheric dynamics.

C. Energetic Particle Acceleration *(D. N. Baker)*

By energetic particles we mean that population of ions and electrons that extends from just above the bulk thermal plasma population all the way to the highest velocity charged particles of the measurable plasma energy distribution function. Our studies examine energetic particle phenomena from a few keV to many MeV, and we have considered energetic particle processes in a variety of magnetospheric systems (Jupiter, Mercury, and Comet Giacobini-Zinner) as well as the terrestrial system. Although the primary effort of this research involves the analysis of energetic particle data from Los Alamos spacecraft, we also make extensive use of theoretical ideas drawn from various magnetospheric models. One of our most important results in 1986 has been the measurement of highly relativistic electrons in the Earth's outer magnetosphere for the first time from Los Alamos geostationary spacecraft. It is possible that relativistic electrons result from processes occurring entirely within the Earth's magnetosphere. If this is the case, then this implies the frequent and efficient generation of highly energetic particles of the sort required in many other astrophysical contexts, such as astrophysical jets. On the other hand, these electrons may arise directly from the Jovian magnetosphere; in this case the relativistic electron population marks a surprising example of heliospheric particle transport and coupling between two major magnetospheric systems.

D. Radiation from Space and Astrophysical Plasmas *(G. Gisler and S. P. Gary)*

The goals of this study are diverse: using both analytic and computational techniques, we seek to understand how relativistic charged particles originate in both astrophysical and Solar System plasmas and then how these energetic particles couple with background thermal plasma and electromagnetic radiation. Our most important achievement in 1986 has been the development of a computer simulation model for particle acceleration in astrophysical jets. We are using a widely accepted model of jets that involves a conducting accretion disk that rotates through a magnetic field thereby generating an intense electric field. Electrons and positrons are extracted from this "foilless diode" configuration and are accelerated to highly relativistic energies, accompanied by intense electromagnetic radiation. Our simulations typically show a single pulse of energy emitted from the diode, but under some conditions we find that the diode pulses between two modes, a particle-flux dominated mode and an electromagnetic-radiation dominated mode. This pulsing may be responsible for the discrete nature of structures often seen in jets.

Contractor: OAK RIDGE NATIONAL LABORATORY
Martin Marietta Energy Systems, Inc.
Oak Ridge, Tennessee 37831

Contract: DE-AC05-84OR21400

Category: Geochemistry

Person in Charge: R. E. Mesmer

A. Metal-Acetate Complexing in Hydrothermal Systems *(S. E. Drummond, D. A. Palmer, D. Wesolowski, and T. Giordano [New Mexico State University])*

A series of experimental studies has been undertaken to assess the role of organic complexes in the transportation of metals in hydrothermal fluids with access to organic material. Recently developed EMF techniques have been employed to investigate the coordination of Fe^{2+} and Zn^{2+} with acetate between 50 and 300°C. Preliminary results from gibbsite ($Al(OH)_3$) solubility experiments indicate that the formation constant for the first acetate complex of aluminum is approximately 50,000 at 50°C. These results demonstrate that acetate is very effective in complexing metals in hydrothermal solutions. In fact, it appears that the acetate complexes will dominate the metal speciation in most natural hydrothermal solutions when the acetate concentration exceeds 0.01 mol. Consequently, acetate plays a significant role in the dissolution and reprecipitation of the diagenetic mineral phases that control the permeability of hydrocarbon reservoirs. Attempts to model the mobility of actinide and other elements in sedimentary radioactive waste disposal environments must consider the effects of organic complexing.

B. Effects of Common Minerals on Acetate Decarboxylation Kinetics *(S. E. Drummond, D. A. Palmer, and J. Schleusener [Pennsylvania State University])*

Previous work has shown that acetate plays an important role in the primary migration of natural gas and in the transportation of metals in hydrothermal systems. To further define the importance of acetate in these processes, we are continuing the experiments on acetate decarboxylation kinetics that have established a mechanistic framework for the decarboxylation reaction at solid surfaces. New experiments have been designed to identify the mineral classes that are active natural catalysts and to test and refine the overall reaction mechanism. Recent results have defined the decarboxylation rates of acetic acid in the presence of quartz, montmorillonite, and pyrite and of sodium acetate in the presence of calcite—all at 340°C. Quartz and calcite have catalytic effects that are indiscernible in titanium reaction vessels that introduce background decarboxylation with a first-order rate constant of about $1.0 \times 10^{-8} s^{-1}$ at 340°C. In the presence of montmorillonite and pyrite, the reaction rates are approximately ten times the background rate and are apparently independent of surface area.

C. Ionization of Water in Noncomplexing Media at Elevated Temperatures *(S. E. Drummond and D. A. Palmer)*

In an effort to identify a noncomplexing electrolyte that could be used in speciation studies at elevated temperatures, the ionization of water was measured in sodium trifluoromethanesulfonate (triflate) at ionic strengths up to 6.5 and up to 250°C. These EMF experiments showed that water is generally less ionized in sodium triflate than in sodium chloride—a result indicating that proton association is greater with chloride than with triflate and that triflate is an excellent noncomplexing anion that is stable with H_2 at high temperatures. This result is particularly significant because it is now possible to perform EMF and solubility studies wherein the data can be interpreted without the ambiguity imposed by complexing effects of the media.

D. High Temperature-High Pressure Properties of C-O-H Fluids *(S. E. Drummond and B. Nesbitt [University of Alberta at Edmonton])*

A vibrating tube densimeter has been developed that is capable of precise measurements of the density of fluids at pressures to 4000 bars and 600°C. This pressure and temperature capability substantially extends the operating range of vibrating tube densimetry from the $\sim$ 100°C, 100 bar limit of the available instruments that similarly operate on the principle that the resonant period of oscillation of a vibrating tube is related to the density of the fluid in the tube. Experiments at 100 and 200°C and pressures up to 1000 bars, using published data for H_2O and CH_4 to calibrate the instrument, have produced density measurements for CO_2 ($\pm$0.2%), which are well within the errors of the accepted values.

E. Sulfur Mobility in Silicate Melts *(D. R. Cole, M. T. Naney, and E. Ripley [University of Indiana])*

An understanding of how magmas evolve from depth to the site of emplacement (or eruption) requires a knowledge of the original volatile content of the melt, the speciation of the volatiles, and their mobilities. Since magmatic rocks may contain only a fraction of their original C, H, and S as a result of degassing, original compositions (both chemical and isotropic) of the exsolved or separated volatiles must be reconstructed either by tracing their effects on the rocks or by calculating compositions from experimental or theoretical data. We have focused our initial effort on the determination of sulfur diffusivities in silicate melts at 950 to 1300°C at 100 kPa and with two oxygen fugacities (QFM and NNO). Sulfur diffusion in a mafic silicate liquid was investigated by heating $\sim$ 125 mg samples of Duluth complex troctolite to 1200, 1250, or 1300°C at 100 kPa for periods ranging from 2 to 6510 minutes. The systematic decreases observed in S concentration with increasing experiment duration are the result of a two-stage process. In general, 80–90% of the total sulfur is lost within the first 60 minutes of heating during the evolution of a vapor phase and bubble migration. Subsequent sulfur loss is modeled assuming the concentration-time profiles result from diffusion of one or more sulfur species in a spherical liquid drop.

F. An Improved Shaw Hydrogen Osmotic Membrane *(M. T. Naney)*

Shaw hydrogen osmotic diffusion membranes of various designs have been used to control and monitor hydrogen fugacity in studies of oxidation-reduction processes important to the geosciences. In most cases, membranes have been designed for use in cold seal pressure vessel apparatus that are operated at temperatures below 800°C. Some design improvements were made to accommodate the extended operating temperature capabilities of an internally heated pressure vessel apparatus and to enhance the service life of a membrane. The configuration of internal support components minimizes deformation of the membrane, which consists of thin-walled noble metal tubing. This is accomplished by using a single-bore soft-fired crushable alumina thermocouple insulator to provide structural support as well as a porous gas pathway from the metal membrane to the axial capillary conduit connected to a pressure gauge and hydrogen reservoir. A hydrogen osmotic membrane of this design has been successfully used in continuous operation for greater than 1440 hours at temperatures ranging from 600 to 1000°C, with a constant external pressure (250 MPa) and internal pressure varying from 0 to 250 MPa.

G. Salinity Effects on Oxygen and Hydrogen Isotope Partitioning Between Geothermal Brines and Other Phases at Elevated Temperatures *(D. Wesolowski and D. R. Cole)*

The stable oxygen, hydrogen, carbon, and sulfur isotope compositions of fluids and minerals have become standard geochemical tools for determining the sources of fluids, flow paths, water/rock ratios, and temperatures of fluid/rock interactions in geothermal systems, as well as in the study of other geologic processes where fluids play a dominant role in heat and mass transfer. One of the most fundamental, yet least understood, aspects of this research is the effect of electrolytes on the partitioning of ^{18}O, ^{13}C, ^{34}S and D between the aqueous solutions and other phases. The addition of various salts to liquid water at room temperature strongly alters the $^{18}O/^{16}O$ and D/H ratios of H_2O and the $^{18}O/^{16}O$ of CO_2 in the vapor phase coexisting with this liquid. These effects have been ascribed to partitioning of the isotopes of liquid-water between "free" water and "bound" water in hydration spheres around ions. Experimental studies of this phenomenon at elevated temperatures are extremely limited, imprecise, and conflicting. To date, a theoretical framework has not been presented that would explain these effects, reconcile the discrepancies in reported studies, or enable prediction of the isotopic activity coefficients of mixed-electrolyte brines. We have initiated a series of experiments to directly measure the hydrogen and oxygen isotope partitioning between water vapor and aqueous solutions of NaCl, KCl, $CaCl_2$, $MgCl_2$, and Na_2SO_4 and mixtures of these salts.

H. Stable Isotope Exchange Between Geothermal Minerals and Fluids *(D. R. Cole)*

Equilibrium fractionation factors and isotope exchange rate data for a variety of mineral-fluid systems are required to quantitatively model the thermal and temporal evolution of geothermal systems, respectively. Partial isotope exchange experiments have been conducted on the following systems: Fe-rich chlorite-H_2O, biotite-H_2O, hematite-H_2O, and scheelite-H_2O. Oxygen isotope exchange in the chlorite-water system at 350°C is very sluggish. Only about 5% exchange was measured for 8 weeks of reaction, and most of that occurred during the first week. The data suggest that minor recrystallization of very fine-grained (< 1 to 10 μ) material occurred early in the experiment, with subsequent exchange controlled by a diffusional process. Oxygen isotope data on hematite and biotite suggest that some recrystallization of fine-grained material probably occurred during reaction, about 5% exchange for hematite and 12% for biotite after 5 months. The magnitude of oxygen isotope exchange measured in the scheelite-water system is somewhat higher, approximately 10% after 4 weeks and 24% after 8 weeks. These data indicate scheelite probably continued to recrystallize during the course of reaction.

I. Kinetics of Isotopic Exchange at Elevated Temperatures and Pressures *(D. R. Cole)*

Isotopic disequilibrium provides an opportunity to investigate temporal relationships in geologic systems. However, a knowledge of the rates and mechanisms of stable isotope exchange is needed for the interpretation of isotope disequilibrium processes in nature. In this study, we conducted the experimental and computational techniques used in determining rates and mechanisms of isotope exchange for a wide variety of geological systems, including gas-gas reactions, interaction of solutes in aqueous solution, and the reaction of solids (or melts) with either gases or fluids. In addition to the theoretical aspects, we also have calculated isotopic rate constants or diffusion coefficients for a wide variety of mineral-fluid and mineral-gas systems not previously treated from a kinetic basis. This work demonstrates how isotopic rate laws vary according to the type of system studied and that slow rates of isotope exchange are not restricted to heterogenous mineral-volatile systems. They may also occur in homogeneous systems, i.e., in solutions or gases.

J. Oxygen and Hydrogen Isotopic Investigation of the Experimental Basalt-Seawater System *(D. R. Cole, H. Ohmoto [Pennsylvania State University], and M. Mottl [Hawaii Institute of Geophysics])*

Oxygen and hydrogen isotopic exchange reactions between basalt and seawater at 300 to 500°C were investigated using oceanic tholeiitic basalt, natural seawater, and artificial seawater as starting materials. The starting basalts varied in crystallinity from holocrystalline to glass. In general, depletion of ^{18}O and enrichment of D in basalts occur at all temperatures. The degree of isotopic exchange (F value) increased with increasing temperature and duration of experiment and also with decreasing crystallinity of the starting materials. The calculated rate constants and the activation energy for the oxygen isotope exchange reactions are similar to those for various minerals-fluid systems in which isotopic exchange accompanied the formation of new minerals. The equilibrium oxygen isotopic fractionation factors between the altered basalt and seawater fall within ±0.5% of the values computed from the equilibrium fractionation factors between various alteration minerals and water, weighted according to the abundance of alteration minerals. These data suggest that the dominant mechanism of oxygen isotope exchange between basalt and seawater in our experimental systems involved surface chemical reactions and the formation of alteration minerals, rather than the simple diffusion of isotopes through solid phases. An application of our experimental data to natural systems suggests that the oxygen isotope equilibrium between basalt and seawater in the mid-oceanic ridge may take place within approximately 1000 years at 350°C. The observed hydrogen isotopic fractionation factors between the altered basalts and seawater are probably attributable to the equilibrium fractionation between Fe-rich secondary phases and seawater.

K. Rates of Stable Isotopic Equilibration in Icelandic Geothermal Systems *(D. R. Cole)*

The effect of variations in temperature, mineralogy, and fluid chemistry on the degree of isotopic equilibration has been studied in five high temperature ($T > 200$°C) areas and one low temperature ($T < 200$°C) geothermal area in Iceland. The high temperature systems exhibit striking similarities in their lithologies and structural setting but differ markedly in their fluid chemistry and intensity of rock alteration. Specifically, two are dominated by seawater-like fluids and intense hydrothermal alteration, whereas the other systems are dominated by dilute, meteoric fluids with weak-to-moderate alteration signatures.

In all areas, rocks have undergone extensive oxygen isotopic exchange with the thermal fluids. Vertical profiles of $\delta^{18}O$ in whole rocks generally exhibit increased ^{18}O depletion with increasing depth and temperature. A comparison between the measured bulk rock-fluid fractionation factors and equilibrium fractionation curves estimated from theoretical mass transfer calculations indicates that the high chloride systems have attained fractions of isotopic equilibrium (F) ranging from 0.85 to nearly 1.0, whereas the dilute meteoric-dominated systems are far from equilibrium with F values ranging from 0.4 to 0.75. Using the rate data and our models for basalt-water isotope exchange, we estimate that the high-temperature chlorite-epidote zones in the high chloride systems can attain F values of 0.9 in 10 to 100 years, depending on grain size. Equilibration times of an order to magnitude more are required for the dilute meteoric systems under similar temperature-grain size conditions. Although isotopic exchange rates are fast, the observed isotopic disequilibrium in systems known to be several tens of thousands of years old implies that local self-sealing of the fracture system occurred prior to isotopic equilibration. This suggests that once a local domain seals, it may be closed for the duration of hydrothermal activity, or at the least until the hydrothermal regime declines in temperature to a level where reaction rates are too slow to allow for equilibration.

L. Generation and Migration of Methane-Bearing Fluids in a High-Grade Metamorphic Setting *(D. Wesolowski and M. S. Drummond [University of Alabama at Birmingham])*

The synmetamorphic Rockford granite intrudes lower Paleozoic, graphite-bearing amphibolite grade (500–700°C, 4–5 kb) metasediments in northeastern Alabama. We have performed 67 whole-rock oxygen and 45 reduced carbon isotope analyses of the granites and their host rocks. These data are consistent with our petrologic, major, and trace element studies, which indicate that the Rockford granite originated by partial melting of metagraywacke and was later altered by exchange with Na-, ^{18}O-, and ^{13}C-enriched metamorphic fluids generated in the volumetrically dominant metapelites. Thermochemical calculations indicate that these fluids would have consisted predominantly of CH_4 (5–10 mole %), CO_2 (5–10%), and H_2O (80–90 %). The isotope data clearly demonstrate the ability of graphite-bearing metamorphic assemblages to generate a CH_4-bearing fluid phase, which is then able to migrate over many kilometers at high integrated fluid/rock ratios, even at extreme depths in the crust ($\sim$ 20 km). This suggests the possibility for accumulation of economic concentrations of metamorphically derived methane in regions of the Earth previously considered unsuitable for hydrocarbon exploration.

M. Crystalline Overthrust Structures in the Platform Localizing Unconventional Methane (COSPLUM) *(D. Wesolowski and D. R. Cole)*

In our reconnaissance investigations of rocks in the ADCOH site region in northeast Georgia, we discovered several areas in the Blue Ridge thrust sheet that contained abundant CH_4-rich fluid inclusions. Geophysical results from the ADCOH site indicate that these geochemical anomalies are associated with domal structures in the unmetamorphosed platform sediments beneath the Blue Ridge thrust sheet. We hypothesize that this methane was generated in the platform rocks during overthrusting and migrated upward into the overlying crystalline rocks. We further propose that significant accumulations of methane may still be trapped in the sediments beneath the thrust sheet in such domal features.

Contractor: PACIFIC NORTHWEST LABORATORY
Battelle Memorial Institute
Richland, Washington 99352

Contract: DE-AC06-76RLO 1830

Category: Geochemistry

Person in Charge: J. C. Laul

A. Chemical Migration in Continental Crustal Rocks *(J. C. Laul and J. J. Papike [South Dakota School of Mines and Technology])*

The major objectives of this research program are to gain a quantitative understanding of chemical migration over a range of temperatures in diverse geological media. The study includes the understanding of dispensing solutions into country rocks, partitioning of mobile elements between mineral phases and solutions derived from granite and pegmatite, and composition and evolution of the solutions. While the study focuses on some forty major, minor, and trace elements, specific emphases are on the rare earth elements and Ba, Sr, K, Rb, Cs, As, Sb, Pb, Cl, Zr, Hf, Ni, Th, and U. The trace elements study may enable us to understand and predict the long-term ($10^3 - 10^7$ year) behavior of their analog: fission products, activation products, and transuranic elements in the high-level radwaste to be stored in a geological repository. It is a far-field study using a natural analog approach.

The site for this study has been pegmatite/country rock interactions in the Black Hills, South Dakota. Five pegmatites have been under investigations. The study is now extended to Harney Peak granite in Black Hills and carbonatite intrusions (rich in REE, U and Th) in Bear Lodge Mountain, Wyoming. The later site is to evaluate the migration of REE, U, Th, Zr, and Hf in country rock. Chemical studies of the pegmatites showed that there is virtually no migration of REE, Al, V, Sc, Cr, Hf, Th, U, Co, Sr, and Ta elements. On the other hand, elements K, Li, Rb, Cs, As, Sb, Zn, and Pb have migrated 4 to 90 meters. The degree of migration varies depending on the element. Minerals biotite and muscovite are effective trace element traps for Li, Rb, and Cs. Chemical data of the Harney Peak granite suggest that: 1) within individual units, volatile transfer mechanisms may have resulted in selective mineral and chemical segregation, 2) a high degree of fractional crystallization (75-80%) of a primitive biotite-muscovite granite may be the dominant mechanism in producing the more evolved tourmaline bearing granites, and 3) extreme fractional crystallization aided by high volatile activity may be the dominant mechanism in producing the associated rare-element pegmatite.

Earlier chemical studies in pegmatites were limited to chemical migration on a smaller scale. Now the study of granite-pegmatite/wall rock interactions is extended to investigate chemical migration to a much larger scale ($\sim$ km scale). The overall aim is to understand the chemical fractionation and migration processes in the pegmatite-granite/wall rock interactions.

Contractor: PACIFIC NORTHWEST LABORATORY
Battelle Memorial Institute
Richland, Washington 99352

Contract: DE-AC06-76RLO 1830

Category: Energy Resource Recognition, Evaluation, and Utilization

Person in Charge: R. A. Stokes

A. Remote Sensing: Geoscience Data Analysis and Integration *(H. P. Foote, G. E. Wukelic, and J. R. Eliason)*

Since 1976, we have been conducting research in areas of remote sensing, image processing, and computer graphics. The goal of this task is to develop advanced, interactive computer techniques for processing, analyzing, and displaying combinations of remote sensing and geosciences data so scientists can interpret complex data combinations, involving resource discovery, energy development, environmental conservation, and national security. Beginning in 1985, task emphasis was placed on procuring, installing, and developing a second-generation interactive, image-processing, and data-integration system for geoscientific analysis (referred to as geodata). The new system incorporates selected knowledge representation techniques (developed under artificial intelligence research) with conventional image-processing/data-integration functions previously performed on the initial geodata system.

In addition to hardware and software advancements, this task has emphasized assessment of the energy-related applications of satellite multispectral data, primarily geoscientific uses. Most of this research has involved analyses of NASA's Landsat Thematic Mapper (TM data). To date, this task has made extensive qualitative use of TM acquisitions to prepare multisource, computer composites (combining Landsat, topography, and geologic data) mostly for the Continental Scientific Drilling and wind energy sites. Major progress included the ability to vary the viewing angle to simulate an apparent view point on or near the Earth's surface. Also, programs have been developed and successfully tested for reducing topography-induced variations in the Landsat reflectance data, which significantly increases the geologic mapping potential of such data.

Currently, software for correlation of stereo pairs is being developed. Stereo imagery with a ground resolution of 10 m is now available from the French SPOT satellite. These stereo pairs can be combined to produce digital elevation maps, or DEMs, of at least the quality of 15 minute topographic maps. The program, now in a testing phase, will accept stereo data sets from satellite or conventional sources. Corresponding picture elements in the images are correlated and the stereo displacement computed. The resulting map of stereo displacements can be processed to produce an array of elevations, or a DEM. The digital elevation files are a basic input for many geodata analysis programs. Results of exploratory studies to develop digital, quantitative spatial analysis techniques for determining the relationships among geological, geophysical, and geochemical structures were promising for aiding both geoscientific and geoexploration studies.

Contractor:	PACIFIC NORTHWEST LABORATORY Battelle Memorial Institute Richland, Washington 99352
Contract:	DE-AC06-76RLO 1830
Category:	Solar-Terrestrial-Atmospheric Interactions
Person in Charge:	R. A. Stokes and E. W. Kleckner

The isolation/aeronomy program encompasses the area of aeronomy in the upper atmosphere and the area of insolation and radiative transfer in the lower atmosphere. Specifically, the aeronomy program is concerned with the plasmasphere/magnetosphere regions and the ionosphere/upper atmosphere regions. Significant advances have been achieved over the past two decades in expanding our basic knowledge of the Earth's atmosphere and magnetosphere and the Sun as an interacting system. The physics of this coupling region must be well understood to obtain definitive solar-terrestrial cause-effect relationships.

The insolation program relies on a database of direct and diffuse solar radiation measurements made in visible and near-infrared spectral passbands. The research has two goals. One is to quantify the spectral characteristics of scattered and direct sunlight. This is germane to energy generating solar technologies, including photovoltaics and day-lighting. However, the primary emphasis of the insolation task is to characterize the influence of trace species in the troposphere and lower stratosphere on solar radiation. These man-made or naturally produced trace species include aerosols, molecules, and clouds.

A. DOE Insolation/Aeronomy Studies *(E. W. Kleckner, D. W. Slater, J. J. Michalsky, B. A. LeBaron, N. R. Larson, and E. W. Pearson)*

The entire Rattlesnake Mountain Observatory data set of direct solar measurements (1977–1986) has now been analyzed. Our attention has focused on extracting the effect of volcanic aerosols on the stratospheric aerosol burden. In particular, we have made a detailed examination of the effect of the El Chichon eruption. Our analysis required us to remove the effect of tropospheric aerosols. Lidar measurements made by NASA Langley implied that the stratosphere was almost devoid of aerosol during 1977–1979; thus our measurements for this period represented a true tropospheric background determination. With this information, and with the application of a number of new statistical estimators, we were able to determine the time history of stratopsheric aerosols at the observatory site for the entire period 1977–1986. The outstanding features of the stratospheric data are the El Chichon peak, the decay of the peak from a maximum that includes an annual cycle that is out of phase with the tropospheric variation, and previously unreported, a summer maximum in 1981 that requires further explanation. We are in the process of making a wavelength-dependent inversion of this turbidity data to recover the aerosol size distributions as a function of time.

Further analysis of the data for extracting total column ozone, in particular for the period from the end of 1985 when a different set of wavelengths was programmed in the MASP unit, is encouraging. We have found general agreement with the standard method of determining ozone via Dobson instruments, but we also found that the effect of stratospheric aerosols, due to El Chichon, strongly contaminated the results.

We use mid- and high-altitude auroral and ionospheric phenomena to reveal solar-terrestrial relations involving wide-ranging and complex interactions. A major goal of the aeronomy program is to investigate the coupling of the ionosphere, plasmasphere, and magnetosphere, primarily through the use of optical remote sensing. To accomplish this, a network of automatic photometers was engineered and deployed to acquire synoptic observations of the aurora and airglow above major portions of the North American continent. Catalogs of all data available through the end of 1986 have been created and are available for interested users.

A number of studies were concluded this year. Among the variety of auroral emission patterns that occur, the most striking at mid-latitudes is the Stable Auroral Red arc (or SAR arc). In collaboration with others, we have identified a new source of energy for SAR arcs. This is a flux of very low-energy (< 10 eV) electrons precipitating into the SAR arc region. The phenomena are persistent, occurring in all twenty-three cases of SAR arcs found coincident with satellite passes that measured plasma parameters. The phenomena were modeled with varying ratios of precipitating flux to heat conduction, with the result that the precipitating flux carries considerable energy into the SAR arc but does not directly contribute a significant amount to the 630.0 nm emission rate. Previous contradictory results, obtained in other satellite experiments, were examined, and an explanation was suggested that reconciles the disparity. The location of the source of the electron flux is uncertain; whether it is from low altitudes, or from regions nearer the equatorial plan, is yet to be determined.

A new study with the University of Michigan has been initiated that will use our photometric data, together with satellite data sets, to try to identify regions of the ring current within the equatorial magnetosphere that are associated with SAR arcs. The satellite data, used to characterize the composition and energy spectra of the ring current population,are combined with the ground-based photometric observations. A model is being developed to compare predictions as to the energy influx and resulting emission intensities from selected events.

An ongoing study of a major magnetic storm (February 8–9, 1986) has yielded *in situ* measurement of magnetic field strengths above a series of SAR arcs. The data are being examined to determine if plasma wave activity is present and, if so, the type and strength of these waves. The primary objective of this study is to determine the importance of plasma wave activity to the conversion of magnetospheric energy to the heating of the ionosphere above the earth.

Contractor: SANDIA NATIONAL LABORATORIES
Albuquerque, New Mexico 87185

Contract: DE-AC04-76DP00789

Category: Geology, Geophysics, and Earth Dynamics

Person in Charge: W. C. Luth

A. Crustal Strain *(J. B. Rundle)*

The objective of the crustal strain program is to understand the physical mechanisms responsible for large-scale, long-term deformation and strain in the earth. To accomplish this objective, it is necessary to construct physical models for the interpretation and analysis of a variety of geodetic data, and to a lesser degree, other data obtained on a continuous basis in regions undergoing active tectonic deformation. With viable models and sufficient data, it is possible to understand the physical mechanisms responsible for long-term deformation in the Earth and to evaluate the susceptibility of a given region to tectonic instabilities such as earthquakes. Of particular interest are long-term, time-dependent strains obtained from an examination of historic triangulation and leveling, modern microgravity and trilateration surveys, and space-based measurements such as GPS (Global Position System), VLBI (Very Long Baseline Interferometry), and SLR (Satellite Laser Ranging). Moreover, modeling techniques based upon emerging concepts in statistical mechanics, nonlinear chaotic dynamics, and catastrophe theory show considerable promise. Results to date, which focus on the construction of kinematic models, have had considerable success in explaining crustal motions in the western United States, Japan, Alaska, and South America.

B. Acoustic Emissions and Damage in Geomaterials *(D. J. Holcomb)*

Under compressive stresses, brittle polycrystalline materials fail as the result of the accumulation of multiple microfailures. Constitutive laws for such materials must incorporate the effects of the microfailures, in particular the inelastic strain and reductions in elastic moduli. A method of incorporating accumulating failures into a continuum model is to replace the details of crack density, size, orientation, and development with a material property that is commonly called damage. Although a number of theories of damage have been proposed, there is no generally accepted technique for detecting the measuring damage. The purpose of this research is to develop such techniques, using acoustic emissions as the basic tool, and to apply the techniques to study the development of damage in geomaterials. Developing and demonstrating the techniques to be used is the first goal. A method was developed for detecting various projections of the six-dimensional damage surface and the existence of the damage surface was demonstrated. The second goal, to study localization by measuring the spatial distribution of damage, requires location of the individual microcracks responsible. A system for acquiring the acoustic emission wave forms from which locational can be determined is operational. Knowledge of the spatial distribution of damage (microcracking) is important for two reasons: validation of computer codes based on damage models and study of the failure process.

C. Advanced Concepts *(W. C. Luth)*

Research conducted in this program involves exploratory research in several geoscience areas. Typically, such research efforts are of a short-term nature and may be oriented toward assessing feasibility of a particular research task.

Paleomagnetic and Rock Magnetic Studies of the Inyo Dike *(J. W. Geissman [University of New Mexico] and J. C. Eichelberger)*

Measurement of rock magnetic properties offers the potential of interpreting both the flow regime and thermal history of igneous bodies. Because of its youth, relative simplicity, and continuously sampled sections, the Inyo domes system has been selected for an early test of the utility of this approach. We have completed detailed work on several samples from the "finger" dike. Additional rock magnetic work on the material from the other Inyo dike holes is nearly completed. Bulk and anisotropy of magnetic susceptibility measurements are available on nearly all core segments from the conduit and dike. Work has begun on suevite units of the Ries meteor crater in southern Germany.

Anelastic Strain Recovery Method of In Situ Stress Determination *(L. W. Teufel)*

Knowledge of the principal *in situ* stresses at depth is critical in the design of many underground processes and workings, including hydraulic fracture stimulations for enhanced oil and gas recovery, problems of wellbore stability, and subsidence. A new stress measurement technique based upon anelastic strain recovery (ASR) measurements of oriented core has been developed. Limited field tests have shown the technique to be successful in determining principal horizontal stress directions and, in some cases, magnitudes in undeformed and horizontal lying clastic rocks. The results of these tests are encouraging, but additional field tests are required to complete the evaluation of the method, particularly on geologic structures where the rock has been highly deformed and bedding is not horizontal. During the past year cooperative field experiments with Phillips Petroleum were conducted in the Albuskjell and Ekofisk oil fields located in the Norwegian sector of the North Sea. Anelastic strain recovery measurements were made on shale and chalk cores from three wells. The results of our work were incorporated in a technology transfer workshop on the anelastic strain recovery method.

Mobile Geochemical Analysis Facility *(H. R. Westrich and W. F. Chambers)*

The JEOL scanning electron microscope, which will provide on-site chemical analyses for drill core glass and mineral phases, has been upgraded to include full-stage automation. The Tracor Northern EDS system has been upgraded to include advanced x-ray and video imaging capabilities, including multi-element mapping and size analysis. A remotely activated Faraday cup for automated measurement of beam current has been acquired and will be utilized during spectral acquisitions to ensure beam stability.

The Role of Crystal Defects in Mineral Dissolution Rates *(W. H. Casey and H. R. Westrich)*

Weathered minerals commonly contain an abundance of surface etch pits. It has been clearly shown that these pits nucleate and grow around the surface expression of edge dislocations of the crystal lattice. Such dislocations introduce strain into the mineral lattice that can accelerate the weathering rate. This research is intended to measure the effect of crystal defects on the dissolution rate and thus provide the first quantitative examination of the phenomena. Measurements are being made of the dissolution kinetics of TiO_2 (rutile) because samples with a well-characterized deformation microstructure are available at Sandia. Rutile is also a type of structure for a wide class of natural minerals. Samples are shocked at 27 GPa with high explosives and heat-treated to partly anneal the resulting deformation structure. In this manner we generated samples with several orders of magnitude variation in edge dislocation densities, point defect concentrations, and residual lattice strain as indicated by x-ray line broadening. The dissolution rate of these samples is then measured in 1.065 N hydrofluoric acid. Although previous workers have emphasized the importance of lattice strain in controlling the reaction rates, our results suggest that the effect is minor.

Contractor:	SANDIA NATIONAL LABORATORIES Albuquerque, New Mexico 87185
Contract:	DE-AC04-76DP00789
Category:	Geochemistry
Person in Charge:	W. C. Luth

The Geochemistry Program at Sandia National Laboratories is comprised of the following projects: A) Magmatic Volatiles, B) Clay-Water Interactions, C) Chemical Diffusion in Minerals, and D) Kinetics of Mica Dissolution. These projects include investigations of the role of volatiles in shallow magmas, the free energies and kinetics of clay minerals dissolution, the chemical diffusion processes in selected silicate minerals, and the kinetics of silicate dissolution. The research addresses fundamental problems and is relevant in a number of applied areas including geothermal energy, nuclear waste isolation, and the evolution of fluids in petroleum-bearing strata.

A. Magmatic Volatiles *(T. M. Gerlach, J. C. Eichelberger, H. R. Westrich, and H. W. Stockman)*

This project is intended to provide understanding of the role of volatiles in shallow magmas of volcanic environments. The research is focused on determining the *in situ* volatile contents of shallow magmas, the mechanisms and rates of their exsolution, and the chemical and isotopic trends that characterize escaping gases at various stages of the degassing process. The investigations include development of on-site fumarole data acquisition capabilities, laboratory techniques to measure the chemical and isotopic compositions of natural glasses and glass inclusions, experimental procedures to examine the kinetics of vapor exsolution and bubble growth in silicate melts at elevated pressures, and models for the mechanics of eruptive vesiculation and outgassing. Investigations are also being performed of trace metal transport by volcanic gases and of D/H fractionation between hydrous silicate melt and coexisting aqueous fluid. One of the long range goals of the work is to establish volatile budgets of volcanic systems. Such budgets are presently poorly defined and are needed as benchmarks for assessing the environmental impact of energy technologies relative to that of volcanism. These studies provide supporting research for DOE programs in Continental Scientific Drilling and advanced geothermal energy recovery. Our work over the past 18 months has shown the importance of plutonic degassing of CO_2 from the mid-oceanic ridges in the transfer of mantle volatiles to the crust-ocean-atmosphere system. Bubble nucleation and growth experiments have been completed in hydrous rhyolite glass at 0.1 MPa and at temperatures ranging from 450 to 1100°C. New, thick-walled gold tubing has been employed for D/H vapor-melt fractionation experiments at pressures of 20, 35, and 50 MPa and temperature of 950°C. The phase equilibria of hydrous rhyolites have been determined at low pressures (50 MPa).

B. Clay-H_2O Interactions *(J. L. Krumhansl)*

The dissolution behavior of smectite clays affects pore water chemistry in hydrothermal systems, sedimentary basins, and man-made nuclear waste disposal repositories. The work in progress is intended to study this problem for a variety of clays in neutral to acidic solutions. Clays studied to date include the Wyoming bentonite SWy-1 (Al rich), Ballarat saponite SACA-1 (Mg rich), and Hohen Hagen nontronite NG-1 (Fe^{+3} rich). Of these three, the saponite seems most resistant to change under hydrothermal conditions. The other clays react in a more complex fashion. These complexities are being examined and interpreted quantitatively with EDS spectra obtained from our JEOL T300 scanning electron microscope. A thermochemical data base applicable to the problems posed by iron, magnesium, and aluminum hydrolysis is also being assembled to support final interpretation of the solubility data.

C. Chemical Diffusion Processes in Silicate Minerals *(R. T. Cygan)*

The occurrence of disequilibrium behavior in geological materials is often attributed to the limited diffusion of chemical species through a silicate mineral. Knowledge of these transport processes is vital to the prediction and evaluation of a variety of geochemical, nuclear waste, energy, and materials problems. The goal of the present research is to examine solid state diffusion in silicate minerals utilizing both experimental and theoretical approaches; the latter complements the direct experimental measurement of diffusion coefficients by providing an atomistic description of the formation of a point defect and the eventual migration of an ion into the available lattice site. Recent experimental work has dealt with the construction of a high temperature furnace with a microprocessor-controlled gas mixing apparatus. Several additional garnet/MgO aneals were performed at temperatures up to 1100°C. The theoretical analysis has concentrated on the evaluation of lattice energies of selected garnet compositions using an ionic model to describe the chemical bonding. Recent simulations of the diffusion process have been directed towards evaluating the energy required for the formation of a defect.

D. Kinetics of Mica Dissolution *(W. H. Casey)*

Understanding the chemical composition and evolution of solutions in the Earth's crust is of critical concern for the disposal of radioactive and chemical waste, as well as for the development of geothermal energy, and for understanding the chemical evolution of sedimentary basins. The most important reactions commonly involve the formation, modification, or dissolution of phyllosilicate minerals such as micas. These reactions generally do not proceed to complete equilibrium but require time as a critical variable in their description. While a conceptual framework has been proposed to describe the kinetics of these disequilibrium reactions, the supporting experimental data are missing. The goal of this study is a series of experiments designed to obtain the dissolution kinetics of muscovite. The study is divided into three parts that examine 1) the dependence of the dissolution reaction rate on hydrogen ion activity in solution, 2) the dependence of reaction rates on temperature, and 3) the molecular controls on the dissolution rate. Essential to all of this work is the use of circulating cells to measure rates of mineral dissolution. We have constructed several Holdren cells for experiments at 25 to 80°C, and we are designing experiments to be performed in a flowing autoclave that can be used for rate measurements with a rotating disc up to 500°C and 500 bars.

Contractor:	SANDIA NATIONAL LABORATORIES Albuquerque, New Mexico 87185
Contract:	DE-AC04-76DP00789
Category:	Energy Resource Recognition, Evaluation, and Utilization
Person in Charge:	W. C. Luth

A. CSDP-High Temperature Geophysical Research Techniques *(H. C. Hardee, G. J. Elbring, and C. R. Carrigan)*

The objective of this task is the development of new or refined concepts and techniques in thermal, seismic, and electrical methods to locate and define subsurface anomalous thermal areas. Surface or near-surface thermal instrumentation includes development and field testing of thermopile heat flux, oriented convective heat flow sensors, and downhole fluid samplers. Seismic techniques involve use of surface geophones and a downhole controlled seismic source capable of swept-frequency operation at 250°C and eventually at 500°C. An oriented, 3-axis seismometer for use in drill holes has been developed. This instrument will be used in both hole-to-hole and surface-to-hole seismic studies. In addition to the instrumentation *per se*, each of these studies involves research on methods to interpret the data. Current research is concentrated in these areas: 1) a downhole, controlled, seismic shear-wave source under development provides control of energy content and frequency of the downhole seismic signal, 2) a new device has been developed that is capable of making triaxial heat flow measurement in a vertical borehole, 3) a downhole seismometer with extended temperature (250°C) capability has been designed and fabricated, 4) a fluid sampler has been developed for obtaining downhole samples of fluids and gases in hot thermal wells, and 5) a high temperature (800°C) thermal probe and associated cable and handling equipment have been developed for logging high temperature holes.

B. Magmatic Emplacement *(C. R. Carrigan)*

Heat and mass transfer across the magma-hydrothermal regime involves a wide range of processes that ultimately give rise to surface and borehole observables. Investigation of the modes of interaction between heat sources and hydrologic regimes provides a testable framework (through drilling) for the use of borehole and surface data as state-of-the-system indicators. Presently, quantitative models of magma-heat-source/host-regime interaction are being used to consider those physical, chemical, and thermal couplings that are responsible for the evolutionary behavior of magmatic systems. This includes investigating not only the long-term nature of volcanism but also the short-term, sometimes dramatic, processes associated with eruptive behavior. Significant recent results include the following: 1) boundary layer analyses indicate that the convective thermal regime in magma bodies is less accommodating to chemical separation by the Soret mechanism than is a purely conductive environment, 2) for two-phase hydrothermal zones, it was found that the heat-pipe mechanism, associated with capillarity, can increase heat transfer rates by an order of magnitude, and 3) models of magma-hydrothermal systems employing heat flow data from several calderas suggest that the host regime tends to dominate heat transfer owing to its much higher effective thermal resistance.

C. **Inyo Domes Research Drilling Project** *(J. C. Eichelberger, H. R. Westrich, and H. W. Stockman)*

The goal of drilling at the Inyo domes chain, California, is to understand the chemical mechanical, and thermal behavior of silicic magma as it intrudes the upper crust and the relationship of that behavior to properties of the intrusive environment. Such information is fundamental to determining the causes of eruptive phenomena and the origin and evaluation of igneous-related geothermal systems and is also applicable to the problem of man-made thermal perturbations of crustal regimes. The Inyo domes chain was chosen for study because it has a relatively simple and well-understood eruption history and is the youngest rhyolitic event in coterminus United States. Recognition that the 20-km-long linear array of Inyo vents erupted simultaneously 600 years ago led to the hypothesis that the eruption was fed by a dike at shallow depth. The Inyo trend runs northward through the west moat of Long Valley caldera and out into the Sierran block. Drilling into the Inyo system was proposed for sites both inside and outside the caldera in order to evaluate effects of the contrasting geologic environments upon magmatic behavior. Differences evident at the surface are the development of large lava domes outside the caldera and large phreatic craters and normal faults inside the caldera, along the Inyo trend. Drilling outside the caldera was completed in fiscal year 1985, and chemical analysis of the core was largely completed in fiscal year 1986. Site preparations are under way for drilling within the caldera. A 1000-m core hole (Inyo 4) will be slanted across the Inyo trend and pass directly beneath, at a planned vertical depth of 600 m, the largest of the phreatic craters.

Core from Inyo 4 will be compared with core obtained outside the caldera. Key observations will be the mineralogy, crystallization texture, character and distribution of glass and chemical boundary zones, and structure of the intrusion. An important question to be answered is why the intrusion stopped short of the surface within the caldera. This project is a cooperative effort with two other DOE laboratories, three universities, and the USGS.

D. **Geoscience Research Drilling Office** *(P. Lysne)*

The Drilling Office supports geoscientists by providing field logistics, generic hardware, drilling plan development, permits, contracts, and consultation for CSDP-thermal regimes research. In the past year, drilling activities took place at Long Valley (Shady Rest hole) and Valles caldera (Sulphur Springs hole). These efforts were in support of drilling research projects put forth by principal investigators from Lawrence Berkeley Laboratory, the USGS, Los Alamos National Laboratory, and the University of Utah Research Institute. Plans are being made for drilling at the Valles caldera, Long Valley, and Katmai. A limited instrumentation capability for borehole diagnostics is also being developed by the Drilling Office. This instrumentation was used to temperature log previously drilled holes in the Salton Sea for Lawrence Livermore National Laboratory. Personnel in the Drilling Office are also working on the calibration of neutron porosity logs for use in igneous formations.

E. **Katmai Workshop** *(J. C. Eichelberger)*

At the recommendation of the advisory groups, a workshop was convened to bring the project to the proposal stage. The workshop was announced in the *EOS* article and organized by J. C. Eichelberger, with help from W. Hildreth and members of 1543. Sixty-six scientists came to Durango, Colorado for the meeting, which lasted two and a half days.

Participants represented twenty universities (including three European universities), five DOE laboratories, and several private corporations and included some of the leading researchers in the field of magmatic processes. Three quarters of the participants were new to Katmai project planning, and only about half had participated in previous CSDP deliberations. Program managers from the NSF, DOE, and USGS were also present. The sessions consisted of a briefing on the concept of the Katmai project and on the Katmai eruption itself, presentations focusing on critical research issues, subgroup discussion on the adequacy of the science plan, and a plenary discussion of project priorities. Agency representatives met during the workshop and concluded that the initiative was ready for the formal proposal stage and that such a proposal should be considered for support by all three agencies. Accordingly, J. C. Eichelberger and W. Hildreth were directed to prepare a "streamlined" proposal for drilling and closely related scientific activities to be submitted by May 1, 1987.

F. Wellbore Sampling Workshop *(R. K. Traeger)*

Representatives from academia, industry, and research laboratories participated in an intensive two-day review to identify major technological limitations in obtaining solid and fluid samples from wellbores. Top priorities identified for further development include: coring of hard, unconsolidated materials; flow through fluid samplers with borehole measurements for T, P, and pH; and nonintrusive interrogation of pressure cores.

Grantee:	UNIVERSITY OF ALASKA Geophysical Institute Fairbanks, Alaska 99775-0800
Grant:	DE-AT06-7 ER70005
Title:	Magnetic Field Annihilation in the Magnetosphere and its Applications
Person in charge:	S.-I. Akasofu and L. C. Lee

Plasmas in the thermonuclear fusion research devices and in space around the Earth have much in common. The Earth's magnetosphere provides a unique opportunity to study some of the basic characteristics of plasmas. We have studied basic processes associated with the magnetic reconnection, ion heating across a collisionless shock, and the generation of electromagnetic waves through electron cyclotron maser mechanism that are taking place in the solar corona and the magnetosphere.

The latest progress in our study of magnetic reconnection is motivated by the attempt to explain the occurrence of FTEs, which is believed to be associated with the time-dependent reconnection process. In one of the attempts, we proposed a multiple X-line reconnection model for the dayside magnetopause to explain the occurrence and the observed properties of FTEs. In the model, magnetic field lines are assumed to reconnect at multiple sites of the magnetopause, and magnetic islands are formed as a consequence of the multiple X-line reconnection process. In a three-dimensional perspective view, magnetic islands become magnetic flux tubes with helical fields, which can then be identified as the open flux tubes observed in FTEs.

The multiple X-line reconnection is intrinsically a time-dependent process. As the magnetic islands formed between two neighboring X-lines grow to a large size, the reconnection of magnetic field lines will slow down and stop due to some nonlinear saturation process. Subsequently, reconnection will begin again when the saturated magnetic flux tubes are convected out of the reconnection region. Thus, the magnetic islands are expected to be formed intermittently and repeatedly, similar to the occurrence of the observed FTEs. Therefore, the time-dependent multiple X-line reconnection process is different from the classical single X-line reconnection models mentioned earlier. In order to understand the physical processes associated with multiple X-line reconnection, a series of theoretical and simulation studies was carried out. In particular, a criterion for the transition from the single X-line reconnection to multiple X-line reconnection was obtained.

Our researchers are also interested in energy-related geophysical problems in the Arctic region. In particular, they are studying the electric current induced by auroral activity in power transmission lines and in oil/gas pipelines. We have successfully demonstrated that auroral activity causes surges in protective relay systems in power transmission lines. Intense surges will open these relays causing blackouts, which are fairly common in Canada where many power transmission lines are long. By studying the characteristics of the surges, we are designing a protective relay system that will not be affected by auroral activity. This project is important for the proposed Anchorage-Fairbanks tie line.

Grantee: ARIZONA STATE UNIVERSITY
Department of Geology
Tempe, Arizona 85287

Grant: DE-FG02-85ER13320

Title: Drilling Investigation of a Young Magmatic Intrusion Beneath the Inyo Domes, Long Valley, California: Structural and Emplacement Studies

Person in Charge: J. H. Fink

The purpose of this project is to characterize the geometry and mechanisms of emplacement of silicic dikes beneath the Inyo domes. The investigation involves surface structural and textural studies in the Inyo area, mapping projects in analogous areas that offer better controls on either the three-dimensional geometry or emplacement conditions of dikes, and analytical studies.

The Inyo drilling project has provided the best constraints available on the shallow geometry of a silicic dike and conduit system. We have used the drill-hole data along with regional tectonic information, laboratory data on the rheology of crustal rocks, and surface mapping to arrive at a quantitative model for emplacement of the Inyo dike. One of the key features of our model is its inclusion of the effect that Long Valley caldera's high heat flow has on the fracture behavior of the invaded host-rocks. The failure of the dike to erupt magma at the Inyo craters may be due to the inability of the weaker crustal rocks within a few hundred meters of the surface to transmit tensile tectonic stresses. Finally, the model suggests that rotation and segmentation of dikes may result from depth-dependent changes in fracture orientations caused by changes in rheologic behavior of shallow crustal rocks.

One of the implications of our earlier mapping was that the Inyo dike propagated laterally as much as 11 km from the south. Oblique northward propagation across lithologic and topographic boundaries associated with the caldera margin may have been responsible for the transition from lateral or vertical flow, in turn causing the magmatic eruptions that produced Obsidian and South Glass Creek domes and the associated pyroclastic deposits.

The products of the Inyo eruptive activity show variations in texture, chemistry, and mineralogy. This distribution has been attributed previously to the mixing of laterally distinct magma source. An alternative hypothesis is that the different products all came from a uniform vertically stratified source region, but that different vents were able to draw up varying amounts of the superposed layers. In order to investigate the application of this model to the Inyo deposits, we have performed a theoretical and experimental study of selective withdrawal of magma from a vertically stratified dike. We find that the ability of a vent to draw up the lower of two density-stratified layers depends on the eruption rate, the density contrast between layers, the viscosity of the upper fluid, and the geometry of the dike.

Grantee: UNIVERSITY OF ARIZONA
Tucson, Arizona 85721

Grant: DE-FG02-87ER13670

Title: Solar Variability Observed Through Changes in Solar Figure and Diameter

Person in Charge: H. A. Hill

The objective of this program is to employ long-term changes in the figure and diameter of the Sun as an indirect diagnostic of changes in the solar constant. This indirect diagnostic of changes in luminosity offers a viable alternative to the difficult task of obtaining reproducible radiometric data over the period of years to decades necessary for a significant study of solar luminosity changes. The primary observations made at SCLERA are diameter measurements of approximately 9 hr observing runs per day. These observations are capable of detecting fractional change in a solar diameter of one part in 10^5 to 10^6 over climatically significant time periods. The quantification of the relationship between changes in the figure and diameter of the Sun and the solar constant is in process.

The results do not support the suggestion based on the 1983 and 1984 Mt. Wilson observations that the intrinsic visual oblateness of the Sun varies with the solar cycle. In our program to quantify changes in solar diameter in terms of changes in luminosity, our findings indicate that solar diameter observations have a relatively high sensitivity to changes in luminosity, a necessary prerequisite for an observable to be of value as a diagnostic for solar variability.

The first significant new development to come out of the quantification project was the finding of evidence of gravity modes in the total irradiance observations. For frequencies near 100 μHz, the evidence indicates that $\approx 29\%$ of the variability in the total irradiance is due to gravity modes. Since gravity modes are known to have very long coherence times, this finding has very important implications for the anticipation of future changes in the luminosity. The second significant development in the quantification project was the discovery of a group of gravity mode multiplets that exhibit evidence of mode coupling in the solar interior. Mode coupling is of interest to understanding luminosity variations because it indicates that these modes may alter the neutrino and fusion energy production rates in the core of the Sun. The third development was the discovery of apparent changes in the equilibrium conditions of the convection zone over a period of five years. Detection of these changes may also be important to anticipating changes in luminosity. The changes in the convection zone were inferred from changes in the eigenfrequencies of low-order, low-degree acoustic modes.

Grantee: BROWN UNIVERSITY
Department of Geological Science
Providence, Rhode Island 02912

Grant: DE-FG02-87ER13665

Title: Thermal Regimes of Major Volcanic Centers: Magnetotelluric Constraints

Person in Charge: J. G. Hermance

Our focus is on applying natural electromagnetic methods along with other geophysical techniques to studying the dynamical processes and thermal regimes associated with centers of major volcanic activity. We are presently emphasizing studies of the Long Valley/Mono craters volcanic complex, the Cascades volcanic belt, and the Valles caldera. This work addresses questions regarding geothermal energy, chemical transport of minerals in the crust, emplacement of economic ore deposits, and optimal siting of drill holes for scientific purposes.

Recent studies have stressed the possibiliy of renewed volcanism in Long Valley caldera. In October 1981, we initiated a regional magnetotelluric survey in east-central California to study active volcanic centers along the eastern front of the Sierra Nevadas and their relationship to regional extension in the Great Basin. The MT data reflect low resistivities associated with the caldera fill and/or features in the basement. In particular, in the southwest moat both the telluric field and magnetic induction parameters reflect a structurally controlled east-west current system at relatively shallow depth in the crust. This elongated east-west zone is aligned along a belt of seismic activity, a zone of seismic shear wave attenuation, and a zone of known hydrothermal alteration. Our present thinking suggests that the southwest moat is underlain by an intensely brecciated shear zone lubricated by clays and hydrothermally altered materials associated with the same hydrothermal reservoir as the nearby Casa Diablo geothermal field.

One of the principal tectonic elements in the Long Valley volcanic complex is a deep basin-like caldera bounded by steeply dipping normal faults having characteristic offsets of at least several kilometers. To characterize the subsurface geometry of this structure we have reinterpreted regional gravity and MT data in terms of simple 3-D models. The similarity between our gravity and MT models clearly underscores the fact that both types of data are largely influenced by the same geologic features: the caldera fill, the topography on the underlying basement, and the major boundary faults.

The most recent research undertaken involves a magnetic variation study of the Cascades volcanic system. During the summer of 1985, a detailed east-west profile was conducted in central Oregon. The profile stretchs for 225 km from Newport on the Oregon coast to a point approximately 50 km east of Santiam Pass in the Basin and Range province. Employing a new generalized 2-D inverse algorithm, we are able to resolve an intracrustal low resistivity zone at a depth of approximately 15 km beneath the Basin and Range province at the east end of our profile. This conductor extends laterally to the west at a more or less constant depth beneath the High Cascades and terminates beneath the older Cascades Range. The lateral extent of this feature and its relation to other geophysical and tectonic evidence is currently being studied.

Grantee:	CALIFORNIA INSTITUTE OF TECHNOLOGY Seismological Laboratory, Division of Geological and Planetary Sciences Pasadena, California 91125
Grant:	DE-FG03-85ER13422
Title:	*In Situ* Stress in Deep Boreholes
Person in Charge:	T. J. Ahrens

We have developed a new technique that allows measurement of all six components of the stress tensor in deep boreholes in the earth. To make this measurement we carry out stress relief by drilling a sidehole in the borehole. The displacements, with magnitudes of μm, resulting from this stress relief are measured with holographic interferometry. During the last year we have occupied boreholes in an oil shale mine in Colorado and a marble mine in California, where we carried out multiple *in situ* stress and *in situ* modulus measurements in various orientations. The new complete analyses allow full inversion of holographic data to yield the components of the stress tensor.

We have systematically investigated, using finite element methods in two dimensions, the possible quantitative errors incurred in our analysis. In our analysis, we use the displacement model for boreholes in a stressed plate as approximation to the displacements associated with stress relief in different orientations. For most of the holograms, the hoop stress is greater than the normal stress along the axis of the borehole, and thus our analysis should employ a plane strain case instead of a plane stress approximation. We need to develop procedures that will allow quantitative application of these calculational results.

A very important qualitative result we obtained from this modeling work was the observation that increasing the depth of the stress-relieving sidehole generally is more effective than increasing the hole diameter in producing stress relief displacement on the free surface of the borehole. This result has immediate application in future work when we need to adjust the amount of stress relief to obtain an optimum fringe spacing in holograms.

In order to invert the observed displacement into an *in situ* stress tensor determination, a measurement of the *in situ*, static elastic, modulus of the rock is also required. We determine the Young's modulus of the rock by applying a known force on the borehole wall with an indentor and measure the resultant displacement field using holographic interferometry. In order to further validate our initial field studies of *in situ* moduli both in boreholes in marble and in the oil shale, we have begun to carry out a series of laboratory elastic moduli calibration tests. Our objective is to develop a rigorous data reduction methodology. As in the *in situ* stress measurement, we calculate theoretical interference holograms on the basis of elastic models and compare these to observations.

Grantee:	CALIFORNIA INSTITUTE OF TECHNOLOGY Division of Geological and Planetary Sciences Pasadena, California 91125
Grant:	DE-FG03-85ER13445
Title:	Infrared Spectroscopy and Hydrogen Isotope Geochemistry of Hydrous Silicate Glasses
Person in Charge:	S. Epstein and E. Stolper

Infrared spectroscopic studies have shown that "water" dissolves in silicate melts and glasses both as molecules of water and as hydroxyl groups. The fact that water dissolves in amorphous silicates as at least two distinct species raises interesting issues in isotopic geochemistry. For example, is there a hydrogen isotopic fractionation between the molecular water and hydroxyl groups in glasses and melts? If so, is it temperature or composition dependent? The answers to these and related questions would contribute to our understanding of the basic physical chemistry of hydrogen in silicate melts and glasses, could be applied to geothermometry of volcanic glasses, and would provide data essential to understanding the evolution of volcanic systems and their associated hydrothermal circulation systems. These results could also be valuable in applications of glass technology to development of nuclear waste disposal strategies.

The focus of this project is the combined application of infrared spectroscopy and stable isotope geochemistry to the study of the various hydrogen-bearing species dissolved in silicate melts and glasses. During the current grant period, we have studied water and carbon dioxide concentrations and hydrogen isotopic ratios in a series of obsidians from the ca. 1340 A.D. eruption of the Mono craters chain in central California. The maximum water contents of the obsidian clasts declined as the eruption proceeded. The proportions of water dissolved as hydroxyl groups and as molecules of water in these glasses vary smoothly with total water content. At most stratigraphic levels there is a range of water contents from clast to clast, though each clast is homogeneous. The D/H ratio varies monotonically with the total water content. Carbon dioxide contents are low but roughly proportional to total water content. The proportions of molecular water and hydroxyl groups in the obsidians from the pyroclastic phase of the latest eruption of the Mono craters indicate temperatures of about 500-600°C. This is much lower than magmatic temperatures. We have suggested that these glasses are samples of the cool glassy margins of the feeder system of the volcano caught up in the explosive eruption. Modeling of the hydrogen isotopic chemistry and CO_2/H_2O ratios of the glasses suggests that degassing of the magma initially approached that of a closed system but changed to an open system when explosive eruptions ceased and quiescent lava flows and domes were extruded.

We have begun to conduct laboratory experiments aimed at determining the fractionation of D and H between melt species (OH and H_2O) and hydrous vapor. Knowledge of these fractionations, their compositional dependence, and their temperature dependence should provide critical insights into the degassing behavior of magmas such as those erupted at the Mono craters, perhaps into the temperatures at which degassing occurred, and into the local structural environments of hydroxyl groups and water molecules in melts.

Grantee:	UNIVERSITY OF CALIFORNIA Department of Geology and Geophysics Berkeley, California 94720
Grant:	DE-FG03-85ER13419
Title:	Advective-Diffusive/Dispersive Transport of Chemically Reacting Species in Hydrothermal Systems
Person in Charge:	H. C. Helgeson

Chemical interaction of fluids with their mineralogic environment is an integral part of many geochemical processes. The focus of this project is development of a comprehensive and quantitative model of fluid-rock interaction coupled to mass transport by advection, diffusion, and dispersion in porous media. The model is suitable for application to a wide variety of processes, including radioactive waste disposal, weathering, diagenesis, hydrothermal ore deposition, and metamorphism.

The ability to integrate governing equations over time spans of geologic significance for chemical processes in the Earth is essential for implementation of any numerical model applied to transport of fluids with concurrent chemical interaction in natural systems. Usual finite difference schemes are limited to relatively short time spans as a result of the stringent requirements imposed by accuracy and stability considerations, which restrict the size of the allowable time step used by the numerical algorithm. Our research during the past year focused on methods to overcome this difficulty by developing reliable techniques for approximating the transport equations and devising alternative numerical algorithms for their integration. Our results indicate that this approach offers considerable promise.

Considerable effort has been devoted to theoretical development of new techniques based on the quasi-stationary state approximation to coupled mass transport and chemical reactions, application of these techniques to weathering and fluid flow in hydrothermal systems, and investigation of conditions necessary for surface- or diffusion-controlled heterogeneous reactions to dominate in metasomatic processes. Emphasis was placed on developing efficient numerical algorithms to integrate the quasi-stationary state equations in the case of pure advective mass transport over geologically significant time spans and to justify the approximations made in simplifying the general transport equations. Toward this end, the method of quasi-stationary states was applied to metasomatic processes involving irreversible heterogeneous reactions of minerals and fluid. The quasi-stationary state method is based on the assumption that the motion of reaction zone boundaries of mineral alteration zones is slow compared to the time required to form a stationary state. Fluid composition and mineral reaction rates are assumed to adjust quasi-statically to changes in mineral reaction zone boundaries, surface area, porosity, and permeability. The time dependence of the positions of reaction zone boundaries can be determined directly without any additional assumptions of the functional dependence of the positions of the zone boundaries on time. Changes in system porosity, permeability, fluid composition, mineral abundance, and mineral surface area can be computed as a function of distance and time for mass transport by advection, diffusion, and dispersion. Because the time step used to integrate the quasi-stationary state equations is not restricted to stability and accuracy considerations, as is the case in the usual finite difference algorithms, geologically significant time spans are attainable for complex systems with the aid of this approximation.

Grantee:	UNIVERSITY OF CALIFORNIA Department of Physics Berkeley, California 94720
Grant:	DE-FG03-87ER13667
Title:	Isotopic Studies of Rare Gases in Terrestrial Samples and in Natural Nucleosynthesis
Person in Charge:	J. H. Reynolds

This project is concerned with research in rare gas mass spectrometry. The broad objective is to read the natural record that isotopes of the rare gases comprise as trace constituents of natural gases, rocks, and meteorites. In past years, these interests have led to the study of such diverse problems as the dating of rocks, the early chronology and isotopic structure of the solar system as revealed by extinct radioactivities, and the elemental and isotopic composition of trapped primordial rare gases in meteorites. In recent years, the project has focused progressively more on terrestrial problems.

The mobile laboratory for elemental and isotopic analysis of the noble gases in terrestrial fluids was readied for deployment in Los Alamos County, New Mexico, throughout 1987. The first project at the New Mexico site was of interest to our Los Alamos hosts who have been engaged in a geothermal study in Honduras in a range and basin area where the crust has been sufficiently thinned by stretching to cause geothermal activity. We find elevated $^3He/^4He$ ratios indicative of a deep gas component of mantle origin. The helium ratios exhibit an east-west trend, cutting across the north-trending graben systems that make up the Honduras depression. The trend shows the highest ratios (up to 2.5 times the air value) in the center. Also, we have studied gas samples from Lake Nyos, scene of the 1986 gas disaster in Cameroon, West Africa. Using samples collected within two weeks of the event, we have measured two lake samples and one sample from a spring 40 km south of the lake to find an R/R_a value of 5 to 6.5 for the $^3He/^4He$ ratio, the single most definitive datum indicating that the gas that accumulated in the lake was from a mantle source. Further sampling will monitor the helium isotopic ratio and help answer the question of whether the gas accumulation in the lake is constant or episodic.

Our group has hosted a study on metamorphic rocks using an instrument that we developed for our research on planetary materials. The instrument enables high sensitivity mass spectrometry of the noble gases to be carried out on submicrogram samples of rocks outgassed by vaporization with a targeted laser shot. Ion counting contributes to the sensitivity of the method. By exposing the samples to neutron irradiation before analysis, ^{39}Ar–^{40}Ar dates can be determined for microscopic domains in compositionally zoned individual crystals. Reconnaisance studies have been made on metamorphic rocks from Sri Lanka and Scotland. The former were already well studied by conventional isotopic dating and known to exhibit three distinct ages. In our microprobe study the same three dates were obtained but now with unequivocal identification of the domains of individual minerals that correspond to particular ages. A surprising retentivity for radiogenic argon despite subsequent metamorphic events has been found for quartz, garnet, and sphene. Age determinations down to 250 m.y. have been successful by this technique for such minerals at very low ($\sim$50 ppm) potassium concentrations.

Grantee: UNIVERSITY OF CALIFORNIA, LOS ANGELES
Department of Earth and Space Sciences
Los Angeles, CA 90024

Grant: DE-FG03-87ER13803

Title: To Complete the Thermodynamic Functions of Five Minerals Up to 1500°K and Up to Compressions of $V/V_o = 0.7$

Person in Charge: O. L. Anderson

With this effort we will complete the calculations and publications of the thermodynamic properties of minerals already measured and analyzed. The minerals are periclase, corundum, forsterite, NaCl, and KCl. For these minerals we expect to tabulate and publish the complete data. We also expect to finish most of the computational work for fayalite. The aim is to proceed with the computational work, which will optimize the application of the experimental and analytical work previously accomplished.

The computational work for MgO is presently nearly finished. More effort is needed to bring the work to a publishable state. For example, we need an error analysis and several contour maps (lines of constant entropy, constant internal energy, etc.).

The computational work for one other solid, Mg_2SiO_4, is partially completed, but nothing has been started for the other solids listed above. Completing the computations required to produce the thermodynamic tables of the thermodynamic functions of these solids would occupy our major attention in the next year.

Grantee:	UNIVERSITY OF CALIFORNIA, LOS ANGELES Department of Earth and Space Sciences Los Angeles, CA 90024
Grant:	DE-FG03-87ER13806
Title:	Thermal and Petrotectonic Evolution of the Central Klamath Island Arcphanerozoic Komatitic Lavas in Northwesternmost California
Person in Charge:	W. G. Ernst

Ongoing investigations in the central Klamath Mountains have documented the presence of a metamorphosed suite of highly magnesian basaltic rocks. The Yellow Dog metavolcanics, regarded as displaying komatitic affinities, have important significance for the thermal and petrotectonic evolution of this early Mesozoic island arc. They are thought to reflect the Permo-Triassic overriding of an oceanic spreading center by the stable, nonsubducted arc-capped lithospheric plate. Partial fusion at 150-200 km depths within garnet-bearing, LREE-enriched mantle may have been responsible for generation of the magnesian lavas.

The research will concentrate on elucidating the areal extent and structural/stratigraphic relations of these mafic/ultramafic volcanic units, the degree of crustal contamination of the melts, the timing of the thermal events, and the physical conditions of metamorphism and of water-rock interaction accompanying island arc accretion. The thermal structure and its evolution in the central Klamath Mountains evidently reflect surfaceward advective transport of energy derived from the subducted heat source; clarification and the generalization of this phenomenon are the ultimate goals of the proposed research.

Grantee: UNIVERSITY OF CALIFORNIA, RIVERSIDE
Institute of Geophysics and Planetary Physics
Riverside, California 92521

Grant: DE-FG03-87ER13408

Title: Sulfide-Oxide-Silicate Phase Equilibria and Associated Fluid Inclusion Properties in the Salton Sea Geothermal System, California

Person in Charge: M. A. McKibben

Our research program is centered on elucidating the sources of metals and sulfur in saline, high temperature, sediment-hosted geothermal systems and on determining mechanisms of hydrothermal metal transport and deposition. To do so we are studying authigenic minerals formed in mineralized fractures within the reservoir rocks of the Salton Sea geothermal system. Systematic documentation of authigenic mineral compositions, phase relations, and fluid inclusion properties allows detailed evaluation of the spatial and temporal variations in brine temperature and geochemistry that have occurred in this active geothermal system. Knowledge of these variations provides constraints on conceptual and quantitative geochemical models of geothermal processes. Most of our samples consist of cores recovered from the State 2–14 well drilled as part of the Salton Sea Scientific Drilling Project.

Our results to date indicate that the earliest fluids in the geothermal system were hot, reduced brines that precipitated carbonate and base metal sulfides. These fluids were heated and expelled upwards along vertical fracture networks by the initial intrusive event that formed the geothermal system. This thermal front was not accompanied by any significant chemical front, as wall-rock alteration associated with early veins is minimal. Rapid sealing of the wall-rock by carbonate precipitation probably prevented significant alteration. The initial heating event generated temperature in the system's upper 2 km that were as much as 100°C higher than the present temperatures.

As the geothermal system has matured, an interface has developed between deep hypersaline metamorphic brine and shallow, less saline brines derived from evolved lake waters. Economic reservoir brine production currently occurs from open fracture zones below this interface. Fluid inclusion studies of metamorphosed evaporites in the reservoir rocks indicate that the hypersalinity of the deep brines is due in part to metamorphic leaching of evaporitic salt. Fluid inclusion studies of vein mineralization reveal that a fluid mixing process is responsible for modern ore deposition. During ongoing intrusive and seismic activity, vertical fracture networks are developed and the deep, heated hypersaline brine upwells above the static fluid interface level. Mixing then occurs between the deep brine and the shallow oxygenated fluids, resulting in a modern vein set that is characterized by silicate and iron oxide mineral assemblages.

Our results provide constraints on models for the thermal and chemical evolution of geothermal systems and have a direct bearing on the successful exploitation of a known geothermal energy resource. We are currently testing geochemical codes to model the brine mixing processes to compare calculated precipitation sequences with those observed in the veins. Such modeling has applications to the prediction and prevention of precipitation processes during brine production and reinjection.

Grantee:	UNIVERSITY OF CALIFORNIA Scripps Institution of Oceanography La Jolla, California 92093
Grant:	DE-FG03-86ER13267
Title:	Long Valley Caldera: Monitoring Studies of Gas Composition and He, Ar, and Carbon Isotopes
Person in Charge:	H. Craig and D. Hilton

Dramatic changes in the level of seismicity, hydrothermal activity, and ground deformation have typified the Long Valley/Mono Lakes region of the Sierra Nevada Range in recent years. Since the first major earthquake ($M > 5$) in October 1978 we have monitored a number of hot springs and fumaroles, both within Long Valley caldera and from adjacent areas, to investigate the relationship between variations in the thermal and seismic activity and changes in the gas chemistry of the hydrothermal fluids. In addition we have obtained drillhole fluids from the Ben Hope Geothermal Plant and from the newly completed research borehole at Shady Rest. The focus of our analytical effort has been on helium isotope variations ($^3He/^4he$), because of its unique ability to distinguish between mantle and crustal provenance; however, we have also analyzed for major gas chemistry (CO_2, N_2, O_2, Ar), other trace gases (e.g., Ch_4), and the isotropic composition of carbon (CO_2 and CH_4) and argon ($^{40}Ar/^{36}Ar$).

We have found that the $^3He/^4He$ ratio (R) is significantly greater than the atmospheric value (R_a) for all sites within the caldera. The range in R/R_a (3.8–6.5) indicates that the helium is predominantly primordial and of magmatic origin. This in turn shows that the heat source driving the Long Valley hydrothermal system is also of magmatic origin. Also, we observe significant and systematic variations in the R/R_a ratio (~12%) at individual sampling localities even though 1986 has been seismically quiet (only one event in the caldera reached magnitude 3). We are now able to discern a seasonal perturbation to the R/R_a ratio. The consistently higher winter R/R_a ratios are probably related to the decrease in recharge characteristic of that period, which allows a greater proportion of the magmatic component to reach the surface. In the late spring, after significant snowmelt, the situation is reversed and the proportion of crustally derived radiogenic helium in the hydrothermal system increases. It is crucial to distinguish the background variation in R/R_a from variations that may be related to seismic activity.

Monitoring of the chemistry of the other gases has allowed us to define the characteristics of the magmatic component further. Winter increases in the R/R_a ratio are accompanied at most sites by decreases in the He/CO_2 ratio. Also, the absolute values ($\sim 10^6$) of the methane/^{3}He ratio show no discernable temporal trends at Long Valley. The narrow "magmatic" ranges of He/CO_2 and $CH_4/^3He$ are important because they show that there is not a significant sedimentary input to the gas inventory. This implies that the Bishop tuff aquifer is the probable source of the crustal component. Ongoing work on the carbon isotope systematics of the CO_2 and CH_4 should allow a more refined resolution of these two gases into their component structures and yield more information on their ultimate origin and potential for exploitation.

Grantee:	UNIVERSITY OF CALIFORNIA, SAN DIEGO Institute of Geophysics & Planetary Physics Scripps Institution of Oceanography La Jolla, CA 92093
Grant:	DE-FG03-87ER13779
Title:	Two-Dimensional Modeling and Inversion of EM Data
Person in Charge:	A. Chave and S. Constable

The objective of the proposed research is the development of numerical codes for the modeling and inversion of EM data in two-dimensional media. This work combines the extensive experience at LANL with large-scale numerical procedures on supercomputers and the theoretical and field expertise in EM methods and inverse theory at Scripps. The project would not be feasible without extensive cooperation between scientists at the two institutions. As for the seismic exploration methods, EM instrumentation and the software used for field data acquisition have become quite advanced in recent years. However, the approaches used to interpret and model EM data have lagged relative to those for seismics, largely due to the coupled vector nature of EM fields. This has posed an obstacle to the extensive application of EM geophysics for energy and mineral exploration and scientific investigations of the earth. Our proposed research will reduce this obstacle by developing modern 2D/3D EM modeling codes for the supercomputer that are both efficient and capable of dealing with realistic models and combining these with regularization approaches to inversion that find the simplest model consistent with a given set of data. We plan to test and assess the results using extensive data sets from the southwest U.S. available at LANL and the EMSLAB project in the northwest U.S.

The inversion of electromagnetic sounding data does not yield a unique solution, but inevitably one desires a single preferred model to interpret the observations. We recommend that this model be as simple, or smooth, as possible in order to reduce the temptation to over-interpret the data and to eliminate the arbitrary discontinuities that occur in simple layered models.

To obtain smooth models, the nonlinear forward problem is linearized about a starting model in the usual way but then solved explicitly for the desired model rather than for a model correction. By parameterizing the model in terms of its first or second derivative with depth, the minimum norm solution to the problem yields the smoothest possible model.

Rather than fit the experimental data as well as possible, which maximizes the roughness of the model, the smoothest model that fits the data to within an expected tolerance is sought. We present a practical scheme that optimizes the stop size at each iteration and retains the computational efficiency of layered models, resulting in a stable and rapidly convergent algorithm. The method is demonstrated using both MT and Schlumberger sounding data as well as joint MT-resistivity inversion.

Grantee: UNIVERSITY OF COLORADO
Department of Geological Sciences
CIRES, Campus Box 449
Boulder, CO 80309-0449

Grant: DE-FG02-87ER13804

Title: Seismic Absorption in Fluid Filled Porous Rocks as a Function of Seismic Frequencies, Pressure, and Temperature

Person in Charge: H. Spetzler

Laboratory measurements will be undertaken to examine the dependence of the inelastic damping of seismic waves in sedimentary rocks on parameters that are known to be significant for different proposed attenuation mechanisms. The expected data are needed to gain a better understanding of the attenuation mechanisms of seismic waves as an additional parameter for the lithological interpretation of seismic data. Samples of sedimentary rock will be subjected to harmonic stress, both shear and longitudinal. The inelasticity and the moduli will be measured by determining the resulting complex strain by means of optical interferometry. The strain amplitude will be in the range of 10^{-6} and smaller in order to meet linearity conditions. These measurements will be performed in the frequency range 0.01 to 300 Hz under confining pressure up to 100 MPa (1 kbar). The temperature range will be between 20 and 100°C. Variations of the mechanical and thermal properties of the pore fluids and different degrees of saturation will be explored to establish relationships between these parameters and the attenuation. This information should be very helpful for identifying the attenuation mechanisms in the seismic frequency range.

Grantee:	COLUMBIA UNIVERSITY Lamont-Doherty Geological Observatory Palisades, New York 10964
Grant:	DE-FG02-86ER13287
Title:	Energetics of Silicate Melts from Thermal Diffusion Studies
Person in Charge:	D. Walker and C. E. Lesher

A detailed characterization of silicate liquids is required for a predictive understanding of the evolution of natural magmas within the Earth's crust. A magma's crystallization behavior and interaction with its surroundings determine, among other things, the potential for geothermal energy extraction and the formation of ore deposits. The thermodynamic evolution of magmatic systems depends not only upon the thermochemical details of the solidification products but also on the thermochemical properties of the initial magmatic liquids. These properties are more poorly known for the liquids than for the solids. It is the purpose of this project to aid in the characterization of the thermodynamic properties of silicate liquids by a novel experimental approach, thermal diffusion studies.

Thermal diffusion is the phenomenon of chemical migration in response to a thermal gradient. In a substance with more than one component, chemical heterogeneity can develop in an initially homogeneous substance as a result of a diffusional mass flow consequent on heat flow. The details of this response are conditioned by the thermochemical properties and constitution of the substance. We have experimentally demonstrated that silicate liquids do undergo substantial thermal diffusion differentiation and that observations of this differentiation provide the data necessary to evaluate the form and quantitative values of silicate liquid solution parameters. This information supplements calorimetric and phase equilibrium data on silicate liquids. Silicate liquids show mixing behavior that requires models at least as complex as an asymmetric regular solution. Parameters quantitatively extracted so far include ordinary diffusion coefficients, heats of transport, and energies of mixing for SiO_2 in silicate liquid.

Additional recent application of thermal diffusion studies to magmatic systems involving coexistence of crystals with silicate melts has shown that there is a substantial potential for inducing chemical migration. Laboratory observations of cumulate maturation under the influence of thermal diffusion are in progress.

Grantee:	COLUMBIA UNIVERSITY Lamont-Doherty Geological Observatory Palisades, New York 10964
Grant:	DE-FG02-84ER13221
Title:	Seismo-Tectonics of the Eastern Aleutian Arc and Associated Volcanic Systems
Person in Charge:	K. Jacob and J. Taber

The geophysical processes of subduction and arc-magmatism are investigated by seismological methods to obtain a fundamental understanding of convergence at a plate margin and to assess seismic risk to future energy projects in an active arc-trench back arc system. We conduct a broad seismotectonic study of most of the Eastern Aleutians. In the Shumagin Islands we study in detail a 300-km long arc segment by operating a digital seismic network with 17 remote stations linked by telemetry. This segment is a seismic gap with a high probability for a great earthquake ($M > 8$) in the next two decades. The seismo-tectonic results for the Shumagin network area are integrated with results from teleseismic and other geophysical observations from the Aleutian arc outside the Shumagin seismic gap. Research topics include: the kinematics and stress orientation of the descending Pacific slab, segmentation of the slab within the Shumagin gap, velocities in the upper mantle and crust of the over-riding North American plate, seismic source and strong-motion properties, inversion of travel time residuals for velocity perturbations in the arc's magmatic root zone, seismic and eruptive activity of Pavlof volcano, and the integration of these results with geodetic deformation data to investigate plate coupling. Applications concern the geothermal energy potential of the Aleutian arc and seismic, volcanic, and tsunami hazards to off-shore oil lease-sale areas directly adjacent to the Shumagin seismic gap. Technical objectives are the sensing of wide dynamic range, seismic ground motions of small and large earthquakes for engineering applications.

Historic earthquakes (Ms > 6.9) between 1898 and 1917 have been relocated using a modified least-squares criteria. The purpose of the relocations was to improve the estimates of repeat times and thus the seismic hazards associated with specific locations long the Aleutian arc. A key finding was the location of a Ms = 7.9 event and its aftershocks in the Shumagin gap in 1917. This instrumental evidence that a great earthquake ruptured the Shumagin gap in the past almost guarantees that similar or larger events will occur there again in the future. Also, new strong ground motion records from several earthquakes ranging in magnitude from 5 to 6.4 have been recovered. Pavlof volcano eruptions in 1986 were the most violent since the Shumagin network was installed. This included stronger harmonic tremor than has been reported anywhere in the world for a volcanic eruption.

Grantee:	COLUMBIA UNIVERSITY Lamont-Doherty Geological Observatory Palisades, New York 10964
Grant:	DE-AC02-72ER04054
Title:	Study of the Time-Dependent Transmissivity of Joints
Person in Charge:	C. H. Scholz

This project involves laboratory studies of the permeability of joints in rock, taking into account both mechanical/hydraulic and chemical aspects of the problem.

A new system was built and tested for measuring flow of aqueous fluid through rock joints at high temperature and pressure. This uses two stainless steel vessels with floating pistons inside the pressure vessel that separate the active fluid from the pore pressure servo systems. These two separators are mounted on either end of the sample. This arrangement allows for the active charge of the fluid to be passed repeatedly through the sample joint at controlled rates or heads. Small fluid samples can be taken from time to time through ports in the pressure vessel that are connected to the internal vessels by capillary tubing.

Preliminary tests have been made to determine the degree to which contamination from the vessel and tubing would affect chemical analyses necessary for actual experiments planned for this apparatus. This work was curtailed partway through owing to termination of funding.

Grantee: GEO-CHEM RESEARCH ASSOCIATES
400 East Third Street
Bloomington, IN 47401

Grant: DE-FG02-87ER13802

Title: Nonlinear Phenomena at Reaction Fronts in Porous Media with Energy Applications

Person in Charge: P. J. Ortoleva

Reaction fronts in porous media play key roles in the genesis of ore deposits and petroleum reservoirs and in a variety of engineered geological systems relevant to energy exploitation. These fronts form when fluids are imposed on a medium containing minerals that react with the chemical species in the inlet fluid. Because the moving fronts involve zones sustained out of equilibrium by the continuous flow of the imposed fluid, we expect that a great variety of nonlinear, pattern-forming, and other localizing geochemical phenomena should accompany them. Our objective is to delineate and characterize these phenomena.

We will concentrate on the formation of secondary minerals during basin diagenesis and localization of metals at reaction interfaces resulting in ore-body formation. Both of these occur because transport and reaction processes interact to spatially and temporally localize mineral deposition and dissolution. This localization can lead to permeability enhancement or occlusion thereby affecting hydrocarbon reservoir quality. If the accumulating minerals are metals, as in uranium roll fronts, their localization may result in the formation of an ore body. Understanding the natural processes related to these phenomena and the resulting geochemical signatures may lead to better methods of exploration for and exploitation of these resources. Engineered reaction fronts, such as those generated by secondary/tertiary hydrocarbon recovery methods or underground high-level nuclear waste disposal, can also be studied using the methods we have developed and propose here to develop.

All the above phenomena involve the coupling of aqueous phase chemical reactions, grain growth/dissolution kinetics, and transport. Therefore, a theory capable of capturing their salient features must involve the coupling of finite rate reaction processes with transport. To our knowledge our modeling approach is the only one that correctly incorporates all these features and furthermore has led to the only computer reaction-transport code that can describe these phenomena in reasonable computational times. We shall both apply and extend our mathematical techniques developed earlier for the study of reaction fronts and optimize and generalize our existing code, REACTRAN, in a number of ways.

Grantee: HARVARD UNIVERSITY
Department of Earth and Planetary Sciences
Hoffman Laboratory
20 Oxford Street
Cambridge, MA 02138

Grant: DE-FG02-87ER13799

Title: Energetics and Thermochemical Properties of Rocks and Minerals

Person in Charge: J. B. Thomsen

One of the most fundamental properties that relate to understanding the energy related aspects of Earth processes is the knowledge of the amount of energy consumed or released by Earth materials at or near the Earth's surface as these undergo changes due to natural or man-induced phenomena.

We propose to measure and interpret the energy-related thermochemical parameters of rocks and their constituent minerals in a recently completed calorimetry lab designed specifically for this purpose. We will carry out thermochemical (and where necessary, thermogravimetric) measurements on common rock-forming minerals, mineral aggregates, and natural glasses. With a few exceptions, these data are poorly known or as yet unmeasured. An integral part of such measurements is the adequate crystallographic determination of the measured phases, since most of these are silicates of highly complex internal structures whose thermochemical properties are rarely uniquely determined by their compositions, temperature, and pressure but are also functions of a past history of incomplete internal equilibrations.

The data we will produce will be added to the increasing, but still inadequate, thermochemical data base for minerals and the more common continental and lower crustal rocks that these minerals comprise.

Grantee: UNIVERSITY OF HAWAII AT MANOA
Hawaii Institute of Geophysics
Honolulu, Hawaii 96822

Grant: DE-FG03-85ER13418

Title: Physical Characterization of Magma Samples

Person in charge: M. H. Manghnani

The project involves laboratory studies in three areas of research: 1) characterization of physical, elastic and anelastic (V_p, V_s, Q^{-1}), and electrical properties of core samples from Kilauea Iki lava lake and related rocks as a function of temperature, 2) electrical conductivity and V_p, V_s, and Q^{-1} of melts of these and related basalts as a function of pressure and temperature and fO_2, and 3) Brillouin scattering measurements on silicate melts first as a function of temperature and then as a function of temperature and pressure. The goals of the proposed research are threefold: 1) to understand how the high-temperature elastic and viscoelastic behavior and thermodynamic properties of basalts and relevant silicate melts pertaining to geothermal exploration and thermal modeling in a volcanically active area are affected by a total environmental system, 2) to investigate interrelationships between the various physical, elastic and anelastic, and thermodynamic properties of silicate melts, and 3) to develop a Brillouim scattering technique for measuring the elastic and anelastic properties of melts in a wide range of temperature and pressure. This research program provides an impetus to basic energy research needed for acquiring a better knowledge of the fundamental *in situ* high-temperature physical and viscoelastic properties of rocks and their melts relevant to geothermal exploration and to projects such as the Continental Scientific Drilling Program.

Our current efforts have focused on the elastic, anelastic, and electrical properties of melts of basaltic and related composition using ultrasonic interferometry and the four-electrode conductivity measurement system. The temperature dependence of the melt conductivity of the eight samples from Kilauea Iki samples from different depths is almost the same and follows the Arrhenius equation. Also, we have successfully tested the new high-temperature furnace for Brillouin scattering measurements. High-temperature measurements on silicate glasses are in progress. Based on the ultrasonic data to date, the temperature and frequency dependence of ultrasonic compressional velocity (V_p) and attenuation (Q_p^{-1}) measurements for various melt compositions have been interpreted in terms of viscosity, relaxation time, and structure of melt. The V_p, Q_p^{-1}, frequency, and temperature data for melts of 10 basalts have been systematized in terms of compositional and structural variations. A linear relationship between velocity and density (constant molecular weight M), similar to Birch's law, has been found. We have also found a good relationship between the measured Q_p^{-1} and viscosity value for various types of basalt melts. The composition dependence of V_p in the basalt melts studied shows that MgO plays an important role. The compressibility $\beta = (V_p^2/\rho)^{-1}$ increases signifiantly with an increase in MgO content.

Grantee: UNIVERSITY OF HOUSTON
Department of Geosciences
Houston, TX 77004

Grant: DE-FG05-87ER13771

Title: Bacterially Induced Precipitation of $CaCO_3$: An Example From Studies of Cyanobacterial Mats

Person in Charge: H. S. Chafetz

Recent investigations have indicated that bacteria are important in influencing the precipitation of $CaCO_3$ in many environments. Due to the nature of geological investigations, carbonate petrologists have overlooked the significant contributions of bacteria due to their size and the rapidity with which they commonly undergo decay. Calcium carbonates that precipitated due to the influence of bacteria undoubtedly had different physical and chemical constraints on the conditions under which they formed than either purely abiotically precipitated $CaCO_3$ or $CaCO_3$ whose precipitation was due to some other taxa. It is, therefore, important to determine the origin of cements and other related constituents, i.e., to be able to recognize bacterially influenced precipitation.

We will evaluate the role of bacteria in the lithification of cyanobacterial (blue-green algal) mats and provide criteria so that bacterially induced lithified stromatolites can be recognized in the rock record. This will involve a study of the initial lithification of modern cyanobacterial mats, laboratory experiments to try and produce "lithified" cyanobacterial mats as a result of bacterial activity, and an examination of stromatolites from the rock record to see if we can determine if they are the product, at least in part, of bacterially induced carbonate precipitation.

Grantee:	LOUISIANA STATE UNIVERSITY Diagenesis Research/Basic Research Institute Baton Rouge, LA 70803-4101
Grant:	DE-FG05-87ER13748
Title:	Ammonium Silicate Diagenesis and Its Influence on the Interpretation of Fixed-Ammonium Anomalies as an Exploration Tool
Person in Charge:	R. E. Ferrell, Jr.

One product of organic maturation that deserves more attention as an important component in clastic diagenesis is the ammonium ion (NH_4^+). Ammonium substitutes for K^+ or Na^+ in alkali sites of clay minerals, and recent studies of fixed-NH_4 concentrations in anoxic sedimentary basins indicate that anomalous NH_4^+ signatures may be preserved in other alkali silicate mineral lattices. Fixed-NH_4 is NH_4^+ incorporated in the silicate structure rather than as an exchangeable ion on the surface of a mineral. Fixed-NH_4 in clays may preserve anomalous NH_4-signatures and may help to distinguish source rock effects from alteration during hydrocarbon migration.

Ammonia (NH_3) is a product of bacterial reduction of organic matter at low temperatures 80°C), and through diagenesis, as organic matter matures, NH_3 is commonly released with methane during the catagenetic stage, provided amino acids are present in the organic source.

Since fixed-NH_4 concentrations are proportional to NH_4^+ introduced into pore fluids, e.g., from organic maturation, and presuming the rate of NH_4-fixation is geologically rapid, high fixed-NH_4 concentrations in organic rich clastic sequences may be an indicator of source rock maturity.

The research program will consist of two phases: 1) Experimental Investigation: analysis of NH_4^+ aq interaction with various clay minerals under varying Eh, pH, and temperature conditions representative of a diagenetic environment and 2) Field Investigation: an examination of natural NH_4-silicates in reducing, organic-rich environments with increasing depth of burial and organic maturity and with increasing distance from a dike. An examination of several hydrocarbon producing intervals of Gulf Coast sediments will determine whether anomalous values of fixed-NH_4 create a geochemical "halo" near a mature source rock or oil reservoir.

Grantee: UNIVERSITY OF MARYLAND
Department of Chemistry and Biochemistry
College Park, MD 20742

Grant: DE-FG05-85ER13410

Title: Study of the Salton Sea Geothermal System Using ^{10}Be Isotope and Trace Element Chemistry

Person in Charge: N. J. Valette-Silver

The aim of the proposed work is to characterize the dominant processes acting in the Salton Sea geothermal reservoir using the isotope ^{10}Be and trace elements. The use of a well proven tool such as the trace elements and of a promising new technique, ^{10}Be, constitutes a unique and potentially powerful combination never used before in a geothermal system. To make an adequate use of these indicators, we propose to study the behavior of ^{10}Be and of the selected trace elements (As, Se, Sb, Hg, V,...) in the highly saline environment of the Salton Sea. From the analysis of waters, ore deposits, sediments, and rocks, we will address the following problems:

1) we expect the aquifers in the geothermal field to have distinct chemical signature as defined by their trace element and ^{10}Be concentrations. By characterizing the aquifers in this way we will be able to identify the mixing processes occurring in the hydrothermal system.

2) we seek to estimate the ages of the rocks and sediments of the reservoir as well as the various aquifers by using ^{10}Be as a tracer and as a dating tool, and

3) we want to determine the origin of the ore deposits and, in particular, whether the metals are of sedimentary or volcanic origin.

We propose to perform this work in two steps: the first one deals with the water samples and has to be carried out during the first half of the proposal to avoid spoilage of the samples. The second one deals with the solid samples and will be carried out during the second half of the year.

Preliminary study of liquid samples from the Salton Sea geothermal field, obtained mostly from the Well Fee 5 belonging to Republic Geothermal Inc., enables us to develop and refine analytical techniques that will be used on the Salton Sea scientific drilling project samples. On the Fee-5 samples, we tested mostly our chemical separation for the ^{10}Be study and measured the isotope concentrations using the Tandem Accelerator at the University of Pennsylvania. The concentrations reached the very high value of 2×10^5 atoms/g. Analysis using INAA, ICP, and AA for major and trace elements determination were also performed in order to evaluate the effect of the very high salinity of the samples on the chemical analysis.

Grantee: MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Department of Earth, Atmospheric, and Planetary Sciences
Cambridge, Massachusetts 02139

Grant: DE-FG02-86ER13636

Title: *In Situ* Permeability Determination Using Borehole and Seismic Logging Data

Person in Charge: M. N. Toksoz, R. H. Wilkens, and C. H. A. Cheng

The purpose of this work is to study methods of determining *in situ* permeability of hydraulic conductivity of a fracture using full waveform acoustic logging (FWAL) and vertical seismic profiling (VSP) techniques. In order to test these methods, it is necessary to do control ultrasonic scale experiments in the laboratory. It is also necessary to compare physical properties of rocks from cores and from surface/borehole seismic measurements.

During the past year, we have conducted ultrasonic scale experiments of acoustic logging across a fracture. The fracture was simulated by a cut across a piece of aluminum. Fractures of various inclinations to the borehole were studied, including vertical fractures. Relative attenuation of the different borehole waves was noted. It was found that all borehole waves, P, S/psuedo-Rayleigh, and Stoneley, were attenuated across a fracture. It appeared the P and S/pseudo-Rayleigh waves were more sensitive to horizontal and sub-horizontal fractures, while the Stoneley wave was more sensitive to near vertical fractures. This work will be continued in the coming year in order to quantify the amount of attenuation with varying fracture thickness and inclination. This will provide us with a basis to develop a theoretical model.

In collaboration with Dr. Frederick Paillet of the Water Research Division of the USGS, we did a comparison of fracture permeability and hydraulic conductivity obtained from full waveform logs, flow tests, packer tests, and VSP. This comparison was performed on data collected in a fractured granitic formation at Mirror Lake, New Hampshire. It was found that the permeabilities determined from FWAL, flow tests, and packer tests are consistent with each other, while the VSP model needs a correction for fracture stiffness. More field work is planned at the same site this summer.

Grantee:	MICHIGAN STATE UNIVERSITY Department of Geological Sciences East Lansing, Michigan 48824-1115
Grant:	DE-FG02-85ER13321
Title:	The Effects of Pressure, Volatiles, and Thermal History on Chemical Heterogeneity in Magma Systems
Person in Charge:	T. A. Vogel

Drilling at Obsidian dome has provided continuous samples from both the center and edge of the dome, the conduit to the dome, and the dike that connects Obsidian dome and South Glass Creek dome. These samples provide a detailed record of ascent and emplacement of the magma at Obsidian dome. We have documented the geochemical and mineralogical variability recorded in the Obsidian dome system. Detailed comparisons between the chemical and mineralogical characteristics of the dike, conduit, and dome provide insights into shallow magma transport processes, and in particular, highlight the dynamic processes associated with the development of the conduit and the subsequent localization of the flow to feed the eruptive center.

A large chemical and mineralogical variation is present within the finely porphyritic samples in the Obsidian dome drill holes. This variation falls into two trends: a high-Ba and a low-Ba. The nature and distribution of these trends place constraints on the physical processes associated with magma chamber evacuation, dike propagation, conduit development, and magma extrusion. A comparison of the dike samples and samples from the dome and conduit provides support for a model for the development of dike-fed eruptive centers involving localized late stage flow in a plug-like conduit. Samples from the conduit margin and base of the dome provide strong evidence for comingling of magmas. These observations, coupled with the lack of evidence for mixing in the dike samples, indicate that the Obsidian dome mixing event was associated with near surface flow in the fully developed conduit. The mixing event was not associated with the initial evacuation of the magma chamber or the propagation of the dike.

We are continuing our investigation to determine whether compositional and mineralogical variations in the Inyo dike system can be related to thermal gradients established by the intrusive event. The Inyo dike system, in contrast to ash-flow sheets, provides samples that are much better constrained in terms of their flow and temperature history. That is, these samples are not complicated by eruption, transport, or deposition dynamics.

Grantee:	MICHIGAN STATE UNIVERSITY Department of Geological Sciences East Lansing, MI 48824-1115
Grant:	DE-FG02-87ER13721
Title:	Constraints on Magma Ascent, Emplacement, and Eruption: Geochemical and Mineralogical Data from Drill Core at Inyo Craters, Inyo Chain, California
Person in Charge:	T. A. Vogel

We propose to continue our investigation to determine whether compositional and mineralogical variations in the Inyo dike system can be related to thermal gradients established by the intrusive event. The Inyo dike system, in contrast to ash-flow sheets, provides samples that are much better constrained in terms of their flow and temperature history. That is, these samples are not complicated by eruption, transport, or deposition dynamics. The chemistry and mineralogy of these samples are influenced by the original conditions within the magma chamber, the pressure-temperature-composition environment in which they have intruded, and the evacuation dynamics of the magma reservoir. These conditions can be evaluated by careful documentation of the chemistry and mineralogy of the dike.

The Inyo dike system represents magma that was subjected to a very steep thermal gradient over a large depth range, with differing wall-rock conditions, and from which we can obtain unusually pristine samples. Comparison of samples from these various conditions will allow us to document the effect that these emplacement conditions have had on the magma and to separate this effect from those that occur in the magma chamber.

The proposed drilling should provide samples of the dike that has been emplaced in a wall rock that has substantially different chemical and thermal properties than the wall rock at Obsidian Dome. Careful documentation of the chemistry and mineralogy and spatial relationships in this hole should provide further constraints on the emplacement of the Inyo volcanic system. Furthermore the contrast in wall rock characteristics should allow us to further test if geothermometers and geobarometers are influenced by intrusion history.

Grantee: MICHIGAN TECHNOLOGICAL UNIVERSITY
Department of Geology and Geological Engineering
Houghton, Michigan 49931

Grant: DE-FG02-85ER13409

Title: Geothermal Alteration of Sediments in the Salton Sea Scientific Drill Hole

Person in Charge: S. D. McDowell

Hydrothermal alteration of fluvial-delatic sediments in the scientific drill hole has produced chlorite-calcite (<1980 m) and biotite (>1980 m) zone alteration similar to other wells in the geothermal system. The chlorite zone in sandstone/siltstone is characterized by the mineral assemblage calcite-chlorite-epidote-quartz-illite-albite-K-feldspar-sphene-pyrite. The biotite isograd is marked by the disappearance of calcite, an increase in epidote, and the appearance of trace quantities of biotite. At 2900 m biotite becomes noticeably more abundant, while actinolite occurs sporadically at >2480 m.

Sandstone/siltstone porosities crudely decrease through the chlorite zone from >20% to about 10% and are highly variable in the biotite zone. Mean porosities for sandstones/siltstones in the chlorite and biotite zones are $17 \pm 7/14 \pm 5$ and $8 \pm 5/13 \pm 10$, respectively. The average of all sandstones and siltstones throughout the well is 14%.

Mudstone bulk densities increase regularly from 2.02 g/cm^3 at 478 m through 2.61 g/cm^3 at 1313 m to 2.69 g/cm^3 at 2886 m, reflecting a decrease in porosity from 7 to 3 in the chlorite and biotite zones, respectively. Siltstone bulk densities increase regularly from 2.13 at 750 m through 2.45 at 1200 m to 2.71 at 2900 m. A similar increase in bulk densities of sandstone is observed. Measured permeabilities (air) for all lithologies vary linearly with bulk density from log (100 md) at 1.9 g/cm^3 to log (0.01 md) at 2.55 g/cm^3. Average permeabilities for various lithologies are 83.7 ± 197.5 md, 0.59 ± 1.04 md, and 0.02 ± 0.04 md for sandstone (13 measurements), siltstone (16) and mudstone (6), respectively. Compressional wave velocities increase with depth for all lithologies, while the curves for each lithology are distinct. Thus at 1200 m depth, velocities for sandstone, siltstone, and mudstone are, respectively, 2.8, 3.6, and 4.0 km/s. All velocities fit the standard velocity/bulk density relationship observed for sedimentary rocks.

Grantee:	NATIONAL ACADEMY OF SCIENCES NATIONAL RESEARCH COUNCIL Washington, D.C. 20418
Grant:	DE-FG01-82ER12018
Title:	Basic Energy Science Studies
Person in Charge:	T. M. Usselman

A. Studies in Geophysics *(T. M. Usselman)*

The Geophysics Study Committee of the National Research Council is conducting a series of studies dealing with timely scientific and societal aspects of geophysics and the corresponding demand on geophysical knowledge. The studies include: 1) problem-oriented studies such as demands on geophysical knowledge in connection with climatic variations, fresh water resources, mineral resources, geothermal and other energy sources, natural hazards, and environmental maintenance and 2) science-oriented studies such as geophysical data and impact of technology on geophysics. Each study is conducted by a panel selected for the specific purpose. The preliminary findings of each study are presented to the scientific community for comment at a suitable symposium. About two studies are expected to be completed each year.

B. Studies in Seismology *(T. M. Usselman)*

The research objectives of the Committee on Seismology are to influence major trends in seismology and identify related developments in other fields, conduct studies for government agencies, provide advice on U.S. government-supported seismic facilities, maintain cognizance of and provide advice on international seismological activities including seismic verification of nuclear test ban treaties, and coordinate within the National Research Council activities in engineering seismology, rock mechanics, geodesy, geodynamics, geology, and seismic verification of nuclear test ban treaties. The committee meets twice a year to discuss current topics of major importance relevant to seismology, review with government agency personnel, in particular, the actions that have resulted from recommendations of the committee and its panels, and take actions to assure a healthy science that is in a position to provide maximum benefits to the nation and to society. Panels are established to conduct ad hoc studies on topics specified by the committee. Some recent activities of the committee include providing guidance to the seismological community on networks and data handling and reviewing capabilities for monitoring underground nuclear explosions.

C. U.S. Geodynamics Committee *(P. J. Hart)*

The U.S. Geodynamics Committee (USGC) was established in 1969 to foster and encourage studies of the dynamic history of the Earth, with appropriate attention to both basic science and applications. The USGC work is based largely on the recommendations developed by its reporters (currently 22) and their associated groups. In 1976, at the request of the Geophysics Research Board, the USGC began planning U.S. research activities in solid-earth studies in the 1980s. This led to the report, *Geodynamics in the 1980s*, which emphasizes the origin and evolution of continental and oceanic crust, the continent-ocean transition, the relation of mantle dynamics to crustal dynamics, and a geodynamic framework for understanding resource systems and natural hazards. The roster of special topics of the USGC and respective reporters has been subject to continual review and revision. A major revision in 1984 included addition of 16 reporters corresponding to special topics adopted by the International Lithosphere Program. Other topics are: drilling for scientific purposes, geodynamic data, continent-ocean geodynamic transects, electrical properties of the asthenosphere, seismic networks, and sedimentary geology. Future work of the USGC includes: providing input to the International Geosphere-Biosphere Program and the proposed International Decade on Natural Hazard Reduction and addressing key topics in geodynamics, such as rates of uplift and subsidence, tectonics of the lower continental crust, geology of crustal fluids, and continental accretion.

D. Continental Scientific Drilling Committee *(W. E. Benson)*

The Continental Scientific Drilling Committee (CSDC) was established in 1980 to implement the recommendations in the USGC report, *Continental Scientific Drilling Program.* This report identified as a major goal the development of a multiagency program to maximize the scientific value of current and planned drilling activities of federal agencies and of industry through add-on experiments and supplementing these efforts with "dedicated" holes drilled for scientific purposes. The objectives of the CSDC have been accomplished through committee meetings, sponsored symposia, and issuing reports and a newsletter that inform the scientific community about plans for the national research drilling program, opportunities for scientists to become involved, and priorities for scientific objectives and targets. Between the Deep Observation and Sampling of the Earth's Continental Crust operations and DOE's geothermal program, nearly all of the CSDC's original objectives have been fulfilled and its continuing functions taken over. CSCD is therefore phasing out and will be discontinued when its final reports are published.

E. Board on Earth Sciences *(J. W. Berg, Jr.)*

The fundamental mission of the Board on Earth Sciences of the Commission on Physical Sciences, Mathematics, and Resources is to provide oversight of the solid-earth science activities within the National Research Council, to provide a review of research and public activities in the solid-earth sciences, to assess the health of the disciplines, and to identify research opportunities. This group is to take a leading role in helping to establish scientific policy bearing on larger earth science programs in and on behalf of the United States. A major charge of the Board and its committees is to assess and recommend basic research and its applications to meet national and societal needs.

The committees of the Board are: Committee on Seismology, Committee on Geological Mapping, Committee Advisory to the U.S. Geological Survey, Committee on Global and International Geology, Committee on Geodesy, Committee on Guidelines for Paleontological Collecting, Continental Scientific Drilling Committee, Steering Committee for a Workshop on Physics and Chemistry of Earth Materials, Steering Committee for a National Geographic Information Systems Symposium, Committee Advisory to the U.S. Geological Survey on Mapping Science, U.S. Geodynamics Committee, and five national committees that adhere to affiliated bodies of the International Council of Scientific Unions: USNC/Geochemistry, USNC/Geology, USNC/International Geographical Union, USNC/International Union on Geodesy and Geophysics, and USNC/International Union for Quaternary Research.

Grantee:	UNIVERSITY OF NEVADA-RENO Seismological Laboratory Reno, NV 89557-0047
Grant:	DE-FG08-86ER13628
Title:	Shallow-Crustal Magma Zones in and South of Long Valley Caldera
Person in Charge:	W. A. Peppin

The occurrence of an abundance of earthquakes in and south of Long Valley caldera, near Mammoth Lakes, CA and the implementation of a dense network of seismic stations have led to a library of hundreds of thousands of seismic traces. We have discovered quite a few novel features on seismic records that appear directly or indirectly related to shallow-crustal anomalous zones in and south of the caldera, which in previous work might reasonably be identified as magma bodies. This work complements other DOE and USGS programs, wherein intense efforts have been made to study the subsurface structure under the caldera, partly in an effort to determine the best site for the proposed DOE deep drill hole within the caldera. We find evidence in two studies for the presence of shallow-crustal anomalies that may well be magma bodies, one is within the caldera and the other is near the south end of what is the mapped trace of Hilton Creek fault, some 10 km south of the caldera. This evidence comprises more than 1,000 anomalous seismic phases, the origination of which has so far defied explanation in terms of commonly observed phenomenology, such as phase conversions across flat-lying interfaces and the source radiation pattern.

We have studied observations of a pre-S arrival for earthquakes traveling from SE to NW through the part of the caldera identified as having a magma zone. Two preliminary models are presented that can satisfy the fact of observed constancy of time interval between this pre-S arrival and S, in the distance range 30 to 90 km. One of these involves an S to P to S conversion within the caldera within a shallow anomaly placed at the location of the main magma zone. The other involves an S to P conversion across a planar zone striking N45E and dipping 45° to the SE at a location to the NW of the caldera. Instrumentation is being placed in the field to determine the particle motion, apparent velocity, and direction of approach of this phase and to provide constraint and perhaps elimination of these models.

The three-component wideband digital data taken from the 1978 Wheeler Crest earthquake aftershocks have been analyzed. A very strong pre-S arrival, which shows on the vertical component most strongly, has been interpreted as a reflection from a shallow-crustal anomaly near the south end of Hilton Creek fault. We specifically find that no explanation for the phase in terms of flat-lying interfaces and reflections, conversions, or reverberations therefrom can explain these observations. Taken together with other evidence, the strongest of which is that the same regions have been remarkably aseismic while surrounding regions have produced many thousands of earthquakes, there is indication of some kind of crustal anomaly in this vicinity, with the above explanation consistent with reflection from a very sharp, localized interface with roughly spherical shape.

Grantee: CITY UNIVERSITY OF NEW YORK, BROOKLYN COLLEGE
Department of Geology
Brooklyn, NY 11210

Grant: DE-FG02-87ER13692

Title: Deep Burial Diagenesis of Carbonate Reservoirs

Person in Charge: G. M. Friedman

The purpose of this research program is to investigate deep burial diagenesis in carbonate rocks with emphasis on the evolution of rock textures, mineralogy, and porosity with depth. Specific investigative problems include the differential behavior of dolostones and limestones under deep burial, the role of fracture in porosity formation at depth, the relationship of experimentally induced rock compaction textures versus those in a geological situation, and the persistence of porosity under deep burial conditions. The latter is particularly important, since it may provide limitations on depths to which potential hydrocarbon production zones can be expected.

Samples for study were obtained from wells in the Anadarko basin, and the Delaware basin, extending to depths of 30,000 ft. Sequential samples of both dolostones and limestones were selected downhole in order to study diagenetic changes with depth. The samples chosen came from basins where there was adequate control on thermal and burial history. Experimental compaction tests aided in extending and duplicating information gained from geological situations.

From the beginning, this investigation was being conducted along two parallel lines: experimental compaction tests at various temperatures and pressures of natural carbonate sediments to study the evolution of porosity and textures as observed in deeply buried carbonate strata and study of carbonate rocks from boreholes extending to depth of 20,000 to 30,000 ft.

As this study evolved a third line of investigation became important, explained as follows: textural characteristics resulting from deep-burial diagenesis may be observed in strata currently exposed on surface; studies employing various techniques suggested that strata now at the present land surface were heated to temperatures that imply former great depth of burial and subsequent uplift and erosion to bring these formerly deeply buried strata to the present land surface.

Grantee:	STATE UNIVERSITY OF NEW YORK Albany, New York 12222
Grant:	DE-AC02-83ER13013
Title:	Thermal Evolution of Sedimentary Basins
Person in Charge:	T. M. Harrison

Our research objective is to assess the usefulness of $^{40}Ar/^{39}Ar$ age spectrum analyses of detrital microcline in providing thermochronological information necessary for reconstructing the thermal evolution of sedimentary basins. Detrital microclines preserve a record of thermal events in the temperature range $\sim$ 100°C to 200°C, depending on length of heating and several mineralogical variables. The utility of this approach has been previously demonstrated on deep drill core samples from a variety of active basins (San Joaquin Valley, California; Albuquerque basin, New Mexico; North Sea graben). Our activities in 1986 were on two fronts: the application of microcline thermochronology (MTC) to an old basin that is no longer at peak temperature conditions and the development of microanalysis techniques to allow intra-crystal and single-crystal measurement.

The most useful application of MTC is to older basins that have experienced retrograde temperature histories. Both economic assessment and geodynamic analysis of basins are complicated in cases where peak temperatures and heating durations are not known. We have investigated drill core samples from the Anadarko basin, Oklahoma. Individual microcline-bearing clasts in cores from depths of 2.17, 3.27, 3.34, 3.57 and 4.40 km provided to us by the Oklahoma Geological Survey yield $^{40}Ar/^{39}Ar$ age spectra showing a clear correlation for the Pennsylvanian-Permian Granite Wash between depth and radiogenic ^{40}Ar ($^{40}Ar^*$) loss, consistent with the expectation that the deeper parts of the Anadarko basin have experienced the higher temperatures. A less expected result is that the initial ages in the five age spectra converge at $\sim$ 100 m.y., indicating that these samples were hot enough to cause diffusive loss of $^{40}Ar^*$ from the microcline lattice until as late as Albian times. Activation energies for this process are very similar to some of those involved in producing fluid hydrocarbons from organic matter. Therefore, we suggest that although there is good evidence of petroleum generation in the Anadarko basin by the end of the Permian, progressively larger volumes of source rock may have resided within the oil window in Triassic to Early Cretaceous times as the thick sediments of the basin warmed by conduction. Plateau ages indicate that temperatures as high as 180°C were obtained during the Mesozoic in rocks now lying at a depth of about 4 km. The coherence of the age spectra strongly suggests abrupt cooling of the basin beginning 100 m.y. ago.

To avoid this general problem of analyzing aggregates of heterogeneous provenance and kinetic properties, we have developed techniques for analysis of single crystals of K-feldspar while maintaining temperature control needed for kinetic analysis. We have mated a miniaturized double vacuum furnace/extraction line with a VG 1200S mass spectrometer, yielding a sensitivity and background that allow $\sim$ 50 μm spot analyses to be performed on single crystals.

Grantee:	STATE UNIVERSITY OF NEW YORK AT PLATTSBURGH Center for Earth & Environmental Science Plattsburgh, NY 12901
Grant:	DE-FG02-87ER13747
Title:	Depositional and Diagenetic History of the Edgecliff Reefs (Middle Devonian Formation of New York and Ontario)
Person in Charge:	T. H. Wolosz

Reefs of the Edgecliff member of the Onondaga formation (Middle Devonian) are poorly understood in terms of their depositional and diagenetic history despite their proven history as natural gas reservoirs. The current model for Edgecliff deposition is one of reef growth on a subsiding carbonate ramp. This model fails to explain a number of aspects of Onondaga deposition and a new model is proposed. The new model depicts reef growth in a cool-water, tectonically active arm of the Appalachian basin which can be subdivided into three distinct environmental zones. These zones are: an eastern shallowing zone, a central zone of rapid subsidence, and an eastern transgressive zone. Patterns of reef development based upon both biotic and physical criteria for identifying changes in depth related water turbulence levels are proposed as a test for this model.

A second aspect of this research will concern a preliminary investigation of the diagenetic history of these reefs. A possible geographic trend in porosity development/preservation will be evaluated using a combination of field mapping and both standard and cathodoluminescence microscopy techniques. This aspect of the proposed research will act as a springboard for future study of Edgecliff reef diagenesis.

Grantee:	STATE UNIVERSITY OF NEW YORK AT STONY BROOK Research Foundation of SUNY P. O. Box 9 Albany, NY 12201
Grant:	DE-FG02-87ER13416
Title:	Geochemistry and Origin of Regional Dolomites
Person in Charge:	G. N. Hanson

The goal of this project is to develop geochemical approaches for testing models describing the geochemistry and dynamics of fluid systems responsible for the development of regional dolomites, which are major reservoirs for petroleum. The Mississippian Burlington-Keokuk formations of Iowa, Illinois, and Missouri, in which we have developed a detailed calcite cement and dolomite zonal stratigraphy, have been used for developing these approaches. C, O, Sr, Pb, and Nd isotopes and a range of trace elements (REE, Pb, Zn, Ba, Li, Sr, Mg, Fe, and Mn) are or will be used to characterize the various generations of dolomite and calcite. Quantitative approaches are being developed to predict how the isotope values and trace element abundances of the carbonates will vary depending on the extent and mechanism of fluid-rock interaction and the composition of the fluid. Approaches that will allow one to determine how and when dolomites and their porosity formed will help in evaluating the potential of a given carbonate sequence as a petroleum reservoir.

Grantee:	UNIVERSITY OF NORTH CAROLINA Department of Geology Chapel Hill, North Carolina 27514
Grant:	DE-FG02-85ER13414
Title:	Activity-Composition Relationships in Silicate Melts
Person in Charge:	A. F. Glazner

The purpose of this investigation is to gain insight into the relationship between the composition of magma and its thermochemical properties. These studies are useful for understanding the energy balance in a cooling magma body and for using samples of crystallized magma to infer the pressure and temperature conditions of crystallization. A secondary goal of the project has been to determine one-atmosphere phase relationships in mixed magmas.

We recently completed a set of 95 experiments on the one-atmosphere phase equilibria of basalt-rhyolite mixtures. Starting materials were an alkali basalt from Pisgah crater, CA, and a high-silica rhyolite from the Bishop tuff, Owens Valley, CA. These materials were chosen because the compositional trend of the mixtures mimics many continental calc-alkaline suites. It was found magnesian olivine is the stable liquidus phase in mixtures containing up to 63 wt% SiO_2. This result suggests that olivine can crystallize directly from natural silicic andesites and supports the conclusion reached by some investigators that olivine in silicic andesites is a phenocryst phase and not a xenocryst.

Also, comparison of effects of crystal fractionation and magma mixing on calculated residual liquid densities has shown that hybridization of basaltic magmas is more efficient than crystal fractionation in reducing magma density. This has led to the development of a general model for the role of hybridization and mean crustal density in the buoyant rise of basaltic magmas in regions undergoing crustal extension. When applied to the Basin and Range province of the western United States, this model can explain why the proportion of basalt erupted has increased with time, why the amount of contamination suffered by basalts has decreased with time, and why major silicic volcanic centers (e.g., Long Valley) are located in areas of low crustal density.

Although augite coronas commonly occur around quartz crystals in basalts and andesites, the origin of these coronas is not well understood. We have successfully duplicated this textural relationship by adding quartz grains to basalt-rhyolite mixtures. Scanning electron microscopy of natural augite coronas in basalt suggests that augite nucleates and grows at an interface between basaltic liquid and a rhyolitic liquid zone around the quartz that originates either as a product of quartz dissolution or as rhyolite glass adhering to the entrained quartz grain.

Grantee: UNIVERSITY OF OKLAHOMA
School of Geology and Geophysics
Norman, Oklahoma 73019

Grant: DE-FG05-85ER113412

Title: A Study of the Source Material, Mechanisms of Generation, and Migration of Oils in the Anadarko Basin, Oklahoma

Person in Charge: R. P. Philip

The major objectives of this research are designed to study the origin and migration pathways of oils in the Anadarko basin, Oklahoma. Despite the large quantities of oil and gas produced from this basin, a great deal of uncertainty remains concerning the source(s) of the major oil accumulations. The organic geochemical approach being used in the study makes extensive use of the biomarker concepts for unraveling source relationships and migration pathways. Migration mechanisms of crude oils is an area that is not well understood at this time. If relationships can be established between specific families of oils and their suspected source rocks in this basin, it will provide an opportunity to study both the mechanisms of primary and secondary migration and the effects of migration on crude oil composition.

The work has diversified into a number of different areas. The major subdivisions are: specific oil/source rock correlations in well defined areas of the basin, use of hydrocarbon and porphyrin biomarkers to further our understanding on the origin of oil seeps occurring in the Ordovician Oil Creek sandstone, and study the effects of biodegradation on biomarkers and asphaltenes in various oil seeps and biodegraded oils such that parameters can be derived that will be of use in correlation of altered and unaltered oils with their suspected source rocks.

To date our study in the Pauls Valley area of the Anadarko basin has shown that 85% of the oils in this region are derived from a common source, in all probability the Woodford shale. The remaining oils are derived from the Viola limestone. This study is now being refined by examining additional groups of biomarkers to confirm our preliminary findings. A study of the oil seeps in the Ordovician Oil Creek sandstone has shown that the porphyrins are virtually unaltered as a result of biodegradation. Other classes of biomarkers such as steranes and hopanes have been extensively altered. The extent of alteration appears to vary with depth and to correlate with porosity and the ability of oxygen bearing water to penetrate the sandstone.

The overall aim of this work is to develop, define, and evaluate new and existing geochemical parameters that can be used in the continued search for new sources of hydrocarbons. Organic geochemistry has developed very rapidly in the last few years, and with the continuing development of analytical equipment and our knowledge of the fate of organic matter in the sedimentary environment, geochemistry will become an even more important exploration tool in the next few years.

Grantee: PRINCETON UNIVERSITY
Department of Geology and Geophysical Sciences
Princeton, New Jersey 08544

Grant: DE-FG02-85ER13437

Title: Silicate, Aluminosilicate and Borosilicate Melts: Thermochemical Studies by High Temperature Calorimetry

Person in Charge: A. Navrotsky

High temperature solution calorimetry is used to determine heats of mixing in aluminosilicate and borosilicate glasses and melts. The results of calorimetric and NMR studies along the join $NaAlSi_3O_8$-$NaBSI_3O_8$ are being prepared for publications. Densities and glass transition temperatures along the joins $NaAlSi_3O_8$-$LiAlSi_3O_8$ and $KAlSi_3O_8$-$LiAlSi_3O_8$ are being measured to complement calorimetric and conductivity studies of the mixed alkali effect in these glasses.

Enthalpies of solution of glasses in the basalt-analog system anorthite-diopside-forsterite are measured using a twin Calvet-type oxide-melt solution calorimeter at 702°C with $2PbO \cdot B_2O_3$ flux. Initial results for the joins at 0, 10 and 20 wt% forsterite indicate that the enthalpy of solution is small (± 2 kJ/mol in magnitude) except for anorthite-rich glasses. Above $\sim$ 75 wt% anorthite the enthalpy of solution becomes increasingly exothermic with anorthite content, reaching a value of roughly -13 kJ/mol at pure anorthite glass.

The calculation of enthalpies of mixing relative to the glass (or liquid) components An, Di and Fo requires knowledge of the heat of fusion (or vitrification) of Fo, which is at present a poorly constrained quantity. Because the heat of solution changes little for compositions in a region defined by 0-20 wt% Fo and $<$ 75 wt% An, the heat of mixing of any two compositions within that region (i.e., analog magmas) is small and is slightly exothermic (0 to -3 kJ/mol). Recent basaltic magma mixing models have presumed that there is no significant enthalpy of mixing. The validity of this approximation should be clarified by the present data and future work on direct measurement of enthalpies of fusion in the system An-Di-Fo.

The Setaram transposed-temperature-drop calorimeter is being used to study the joins and Ab-An, Di-An, $Ab_{0.5}Di_{0.5}$-An, Di-Fo. From these studies at 1500°C we are obtaining both values of the heats of fusion of end-members and constraints on the magnitudes of heats of mixing directly in the molten state.

The data and models developed in this work are correlated to the structure and physical properties of silicate melts and have potential applications in such diverse fields as geochemistry, magma energy generation, ceramic science, nuclear waste disposal, and reactor safety.

Grantee: PURDUE UNIVERSITY
Department of Earth and Atmospheric Sciences
West Lafayette, IN 47907

Grant: DE-FG02-87ER13784

Title: Midcontinent Rift System Scientific Drilling Workshop

Person in Charge: W. J. Hinze

The Scientific Advisory Committee of Deep Observation and Sampling of the Earth's Continental Crust, Inc., has expressed interest in receiving a pre-proposal regarding scientific drilling into the midcontinent rift system (MRS). This interest reflects the significance of this Precambrian tectonic feature, which extends over a length of 2000 km in the midcontinent of the United States, in the evolution of North America and its potential role as a frontier hydrocarbon province. Before submitting a pre-proposal it is important for interested geoscientists to meet to prioritize potential drill sites and to critically define scientific objectives of each site. This investigation is particularly important to DOE because the MRS is one of the last remaining frontier hydrocarbon provinces of the conterminous United States that has potential for major production levels. Furthermore, information derived from this major continental rift system will be useful in a generic way in evaluating the geological evolution and hydrocarbon potential of other continental rifts. The funding request of this proposal is limited to providing monies for partial travel support of workshop participants and the preparation of the workshop report and related pre-proposal.

Grantee: SOUTH DAKOTA SCHOOL OF MINES AND TECHNOLOGY
Rapid City, South Dakota 57701-3995

Grant: DE-FG01-84ER13259

Title: Thermally Induced Chemical Migration: A Natural Analog Approach

Person in Charge: J. J. Papike

The major objective of this research is to gain a quantitative understanding of chemical migration in the geologic environment over a range of temperatures and pressures and in diverse geologic media. Contact metamorphic occurrences serve as geologic analogs for the underground storage of nuclear waste, with the igneous intrusion providing the heat and trace element source, and the country rock, the medium through which migration takes place. The specific sites for this study are pegmatite/wallrock interaction zones in the Black Hills, South Dakota. This type of study provides information on chemical migration over geologic times, a time span that cannot be duplicated in laboratory experiments or with presently available calculation procedures.

The fluid transport of relatively incompatible elements (Li, Rb, Cs) out of the rare-element pegmatite system and subsequent interaction between that fluid and amphibolite result in the stabilization of holmquistite-bearing assemblages (lithium-containing amphiboles). In the amphibolite adjacent to the Edison pegmatite, Black Hills, South Dakota, three amphibolite assemblages resulting from fluid-country rock interaction can be distinguished: 1) biotite alteration assemblage, 2) hornblende-holmquistite alteration assemblage, and 3) hornblende-plagioclase assemblage.

Holmquistite occurs only in assemblages 1) and 2) in which it co-exists with and partially replaces hornblende. In coexisting holmquistite-hornblende pairs, the $(Al+Fe^{3+}+2Ti^{4+})$ value is greater and $(Fe^{2+}+Mn)/(Fe^{2+}+Mn+Mg)$ is less in holmquistite relative to coexisting hornblende. By analogy to calcic and Fe-Mg amphiboles, a wide compositional gap exists between calcic and lithium amphiboles at temperatures of alteration zone formation.

The alteration of the amphibolite appears to be the result of Li and K metasomatic alteration by alkali-rich pegmatite-derived aqueous fluids and retrograde metamorphism by the aqueous fluids resulting in the instability of plagioclase and ilmenite and the formation of epidote and sphene. The fluid had a low boron concentration and log f_{H_2O}/f_{HF} was approximately 5.35 at 365°C. The conditions at which the alteration occurred were between 510 and 350°C at 3–4 kbar. Field and textural evidence cannot discriminate between a single or multiple fluid/amphibolite interaction model.

Grantee:	UNIVERSITY OF SOUTHERN CALIFORNIA Department of Geological Sciences Los Angeles, California 90089-0741
Grant:	DE-FG03-85ER13336
Title:	Continental Scientific Drilling Program: The Seismology of Continental Thermal Regimes
Person in Charge:	K. Aki

This program was started as an involvement in two major geothermal projects; namely, the Hot Dry Rock Geothermal Energy Project of Los Alamos National Laboratory and the Magma Energy Project of Sandia National Laboratories. The theory and methods developed for interpretation of various seismic experiments conducted at Fenton Hill, New Mexico, and Kilauea Iki, Hawaii, however, found a variety of applications to other geothermal areas and volcanoes, and our research has been evolving into what might be called volcanic seismology.

In this program we are applying the methods of passive seismology using natural seismic sources occurring in geothermal areas as well as active seismology using artificial sources to the candidate sites for the CSDP in order to delineate the geothermal and mechanical properties as well as the mass and energy transport mechanism of the geothermal system.

During the past year, we made considerable progress in 1) interpretation of long-period events observed at Mt. St. Helens and the Fenton Hill hot dry rock site in terms of seismic radiation from a fluid-filled crack, 2) interpretation of teleseismic data collected in and near the Valles caldera in terms of a model with irregular topography, caldera fill, and magma chamber, 3) interpretation of VSP data from the Oroville fault zone by ray-tracing and polarization calculation for P, SV, and SH waves in heterogeneous anisotropic media containing aligned cracks, and 4) developing a new powerful method for calculating seismic motions in media with irregular topography and interfaces by the superposition of Gaussian Beams. The above four areas will be our building blocks with which we shall construct the interpretation method for seismology in the continental thermal regime. Our goal is to develop a computer package for calculating synthetic seismograms for three-dimensionally heterogeneous anisotropic media with irregularly shaped topography and discontinuities. In parallel with the development of interpretation methods, we shall acquire seismological data from the CSDP candidate sites in continental thermal regime including Mt. Katmai, Long Valley-Inyo-Mono Lake, Valles caldera, Fenton Hill hot dry rock site, and Mt. St. Helens. We shall collect both the records of seismic events occurring naturally and the data obtained by the use of artificial sources.

Grantee:	STANFORD UNIVERSITY Stanford, California 94305
Grant:	DE-FG03-86ER13601
Title:	Porosity with Fluids: Origin and Effects on Physical Properties of Crustal Rocks
Person in Charge:	A. M. Nur

During the past year we have investigated a range of rock physics problems related to the characterization of reservoirs and the crust and to the exploration for and production from hydrocarbon reservoirs. Laboratory studies of the relationships among compaction, acoustic properties, and clay content in sand-clay mixtures were carried out on Ottawa sand, smectite powder, and their mixtures. In pure sand under pressure, porosity and velocity show approximately elastic behavior. In contrast, pure clay is permanently compacted. In sand-clay mixtures both porosity reduction and velocity changes with pressure are dominated by clay content. The results can be applied to sonic log and seismic interpretation.

We undertook a systematic study to identify the causes and understand what controls the magnitude of large decreases with temperature of velocities in heavy oil sands. One of our most striking results is that compressional velocities Vp in natural hydrocarbons decrease very much with temperature (e.g., 15% to 30% per 100°C). Furthermore, results for pure alkanes and alkenes reveal a systematic relation between Vp, temperature, and the inverse of the molecular weight of these hydrocarbons. These results suggest that it should be possible to obtain information from seismic velocities about the type for hydrocarbon present in rock and that efforts to monitor thermal EOR fronts *in situ*, including hot water and steam floods, could be highly successful.

Measurements were made of the dielectric constant (E') of tight gas sandstones as a function of water saturation (S_w). At low saturation ($S_w < 5\%$) E' shows little hysteresis between saturation and desaturation. At high saturation the adsorption of water vapor leads to the development of thin gas pockets in the center of the partially saturated pore space leading to large capacitance and high measured values of E'. Upon drainage no such thin gas pockets develop, thus leading to the large observed hysteresis. These results are useful for characterizing gas bearing reservoirs and cores.

Also, the maximum entropy method was used to infer the crack geometrical characteristics in rocks from measurements of compressibility, electrical conductivity, and permeability. Using this approach the crack size distribution in Westerly granite was determined from laboratory measurements of elastic and transport coefficients. The predicted size distribution is comparable with the distribution estimated from direct observations of cracks with a scanning electron microscope.

We developed a model for the coupling of pore pressure in the Earth's crust to stress, temperature, and tectonic strains. We applied the model to estimate the development of pore-pressure in a rock mass subjected to lateral compressive strains. We found that rocks in such settings exhibit rapid buildup of substantial fluid overpressures. Such overpressures are probably very important in facilitating deformation of rocks in accretionary wedges, mountain building, and crustal mechanics in general.

Grantee:	STANFORD UNIVERSITY Department of Applied Earth Sciences Stanford, California 94305
Grant:	DE-FG03-85ER13319
Title:	Mechanisms of Shallow Dike Emplacement and Phreatic Eruptions at Inyo Craters, Long Valley, California.
Person in Charge:	D. D. Pollard

The objective of our work has been to study the origin and sequence of development of a set of normal fault scarps, fissures, and associated phreatic craters (including the Inyo craters), which lie at the south end of the Inyo volcanic chain in eastern California. The eruptions that formed the Inyo craters were among the last in a sequence of activity that took place in the Inyo chain 550–650 years ago. The faults and fissures are spacially associated with the craters and lie roughly along the trend of the most recent eruptions, suggesting that their origin is related to intrusive activity along the Inyo chain. As such, the fissures, faults, and craters may represent a type of surface deformation and phreatic activity that precedes eruptions in the Long Valley area. Our early work led us to conclude that the Inyo craters formed above a north-south trending dike, whose thickness is at least a few tens of meters and whose top is within a few hundred meters of the surface.

Additional modeling of elastic surface deformation above a shallow dike has been done to determine the dependency of the locations of elastic strain maxima at the surface on the driving pressure distribution of the dike. The results of these models support our earlier conclusion that the dike top is $\sim$ 500 m deep or less and that the dike is vertical or dips steeply to the east. Physical models of surface deformation suggest that faults and fissures may form within a narrower region above a dike top than would be predicted by the theoretical models. A sequence of fissuring and fault growth also has been documented using the physical models whereby deformation begins with growth of fissures at the surface, parallel to the dike, in two regions on opposite sides of the dike plane. Normal faults are produced when fissures at the surface connect with extensional fractures that form near the dike top in the subsurface.

Additional mapping in the Inyo craters area has delineated the extent of phreatic deposits from these eruptions. Preliminary ballistic analysis of blocks thrown from the phreatic craters indicates that the ejection velocities of these blocks did not exceed several tens of meters per second. We hypothesize that the erupted debris originated at least partly from the walls of fractures above and along the sides of the dike. We also hypothesize that heat from the dike raised the temperature of ground water that was vigorously convected upward through vertical fractures to produce the eruptions. Additional studies of the phreatic deposits and analytical studies of heat transfer will be used to test these hypotheses.

Grantee: TEXAS A&M UNIVERSITY
Department of Geophysics and
Center for Tectonophysics
College Station, TEX 77843

Grant: DE-FG05-86ER13165

Title: Stress-Induced Seismic Anisotropy

Person in Charge: R. L. Carlson

Particle motions detected on arrays of 3-component digital seismographs and on borehole instruments used in vertical seismic profiling and oblique seismic experiments indicate *in situ* elastic anisotropy. The observed anisotropy is thought to arise from alignments of cracks that, in turn, are caused by tectonic stresses. Such interpretations are supported by theoretical and numerical models and by a few experiments conducted at low stress levels, but the phenomenon of stress-induced elastic anisotropy in rocks has not been thoroughly investigated.

We are undertaking a series of laboratory experiments with the aim of ascertaining the effects of deviatoric stress on rocks containing natural microcracks. More specifically, our objectives are: 1) to relate the dynamic elastic stiffness tensor to the stress tensor for different stress fields, 2) to determine how the elastic stiffness coefficients are affected by the level of stress, and 3) to replicate field observations in the laboratory under known stress conditions.

The materials used in these experiments will be Westerly granite and Maryland diabase. Specimens will be machined to form cubes 15 cm on a side, and suitably oriented P- and S-wave ceramic transducers will be mounted on the faces, edges, and corners of the cubes. Dynamic elastic constants will be calculated from measured P- and S-wave velocities. Stresses up to 40 MPa will be applied using flat jacks. The free faces of the cubes will be instrumented with strain gauges to monitor the uniformity of the applied stresses. Replication of field experiments will be done using transducers mounted on the free faces of the specimens.

We are in the process of refining the experimental design and assembling the apparatus, some of which must be fabricated. Samples of Westerly granite to be used in the experiments will be selected in May 1987 and the task of characterizing the rocks will begin immediately thereafter.

Grantee:	TEXAS A&M UNIVERSITY Center for Tectonophysics College Station,Texas 77843
Grant:	DE-FG05-86ER13228
Title:	Mechanical Properties of Rocks at High Temperatures and Pressures
Person in Charge:	M. Friedman

The recovery of geothermal energy requires stable boreholes at elevated temperatures and relatively modest effective pressures in the presence of hot aqueous fluids and differential stress and often in fractured rock masses. Previously, we investigated the influences of effective pressures to 200 MPa and temperatures to partial melting. During this year we have investigated: why the strengths of rocks decrease with increasing temperature in the presence of water, frictional strengths of rocks at high temperatures, slip in biotite single crystals, and the stability of boreholes in fractured rock.

Testing Westerly granite in extension, we find strength decreases markedly, wet and dry, between 600 and 800°C, with water much enhancing the temperature effect. Thermal intragranular and grain boundary cracking (the latter particularly conspicuous in wet specimens) are primarily responsible for the weakening. That is, the coalescence of precurive microfractures into macrofractures (tensile or shear) is facilitated by thermal cracks. Using Sioux quartzite up to 500°C, we find strengths are insensitive to temperature and strain rate. Nonlinear elastic behavior occurs at 500°C with a sharp increase in inelastic work. Fracture surfaces indicate a consistent direction of overall fracture propagation across a specimen. However, propagation directions are randomly oriented as inferred from grain-scale fracture-surface markings.

In studying frictional strength of rock surfaces at temperature, we find that, although the effects of chemically reactive fluids are not yet well understood, Byerlee's empirical relation between frictional strength (shearing resistance) and normal stress is a good enough approximation for igneous rocks under conditions of concern to the borehole stability problem, regardless of composition, temperature, and loading rate. Also, single biotite crystals oriented for basal slip deform by dislocation glide at confining pressures as low as 100 MPa. Transitional behavior between frictional sliding and slip occurs at about 50 MPa.

For a vertical borehole in fractured rock cut by a fracture dipping β degrees, we find that, for $\beta < 90°$, borehole stability depends on the coefficient of sliding friction, μ, and the ratio, R, of mean normal stress to maximum shear stress. Results include: 1) for a constant value of μ, the unstable range of β decreases and ultimately disappears as R increases, 2) R decreases as pore pressure increases, which leads to an increase in the size of the unstable range of β, and conversely, decreases in pore pressure tend to stabilize the fracture and the borehole, and 3) increasing borehole pressure (above pore pressure) decreases R, which increases the size of the unstable range of β and thus has a destabilizing effect.

Grantee:	TEXAS A&M UNIVERSITY Center for Tectonophysics College Station, Texas 77843
Grant:	DE-FG05-87ER13711
Title:	Anisotropic Yielding of Rocks at High Temperatures and Pressures
Person in Charge:	A. K. Kronenberg and J. E. Russell

The exploration and development of sources of geothermal energy associated with buried magma chambers and regions of high heat flow require drilling to depths of up to 10 km at temperatures ranging from ambient surface temperatures to those of partial melting. Successful drilling to these depths within steepened geothermal gradients depends upon rock strengths sufficient to support the stress fields generated around the borehole at depth. Previous experimental studies, directed towards determining the strengths and ductilities of rocks under conditions appropriate to the borehole environment, have provided useful constraints on the conditions for which borehole failure may be anticipated for massive, relatively isotropic rocks. However, predictions of borehole stability in such strongly foliated rocks as slates, schists, and gneisses cannot be made using isotropic failure envelopes.

One of the outstanding problems remaining in the prediction of borehole stability in crystalline rocks is the influence of fabric anisotropy on yielding. We have initiated a study of the mechanical behavior of foliated rocks using anisotropic yield criteria with the view to predicting their behavior in the stress field surrounding a borehole at temperatures and pressures representative of the borehole environment. Our approach is to perform a suite of experiments designed to determine the full anisotropy of yielding for Westerly granite (presumed to be nearly isotropic), a layered gneiss, and a strongly foliated quartz-mica schist, followed by modeling their behavior in the vicinity of a borehole.

While the three dimensional fracture and flow properties of rocks at elevated temperatures and pressures have, with few exceptions, not been explored experimentally, the theoretical framework describing anisotropic yielding has been clearly formulated and will guide our experimental program. Deformation mechanisms will be investigated using both optical and electron microscopy and models developed, based upon these observations, in an effort to understand how various fabric elements influence mechanical behavior.

The results of these studies will be used to establish the means of predicting the mechanical response of schists, slates (using published results), and gneisses to the stress fields surrounding boreholes over a wide range of temperatures and pressures that may be encountered in geothermal source regions.

Grantee:	TEXAS A&M UNIVERSITY Department of Geology College Station, TX 77843
Grant:	DE-FG05-87ER13767
Title:	Sedimentologic and Diagenetic History of the Mission Canyon Formation (Mississippian) and Stratigraphic Equivalents, SW Montana and East-Central Idaho and Determination of Rare Earth Element Abundances in Diagenetic Carbonates
Person in Charge:	S. L. Dorobek

This is a study of the sedimentologic and diagenetic history of the Mississippian Mission Canyon formation and its stratigraphic equivalents in southwestern Montana and east-central Idaho. Sedimentologic studies will concentrate on documentation of the platform-to-basin transition through the use of detailed logs of measured stratigraphic sections. Definition of facies geometry and thickness distribution may prove useful for future exploration for hydrocarbon reservoirs in these rocks. Additionally, this study will examine the relative effects of sea level fluctuation, regional subsidence, and sedimentation rates and how these parameters influenced overall platform evolution.

Laboratory analyses of integranular cements, fracture-filling cements, and diagenetic replacement minerals will allow documentation of the diagenetic history of the Mission Canyon formation and its stratigraphic equivalents. Special emphasis will be placed on defining the sources and migration pathways of pore waters involved in diagenesis. Analyses of diagenetic phases will involve standard petrography, cathodoluminescence and epifluorescence petrography, electron microprobe analyses, stable isotope analyses, x-ray diffraction studies, and instrumental neutron activation analyses.

A relatively new approach to this study will be the determination of rare earth element (REE) abundances in various diagenetic phases. Preliminary REE data from the Mission Canyon formation suggest that the REE may be extremely useful indicators of the types of pore fluids involved in diagenesis.

This study will provide important information on a widespread carbonate sequence in the Northern Rockies, which is a proven hydrocarbon reservoir and potable groundwater aquifer in many other parts of the Northern Rockies.

Grantee:	UNIVERSITY OF TEXAS AT ARLINGTON Department of Geology Arlington, Texas 76019
Grant:	DE-FG05-85ER13413
Title:	Volcanological Investigation of the Banco Bonito Eruption (c. 150,000 yr) and Subsurface Geology of the Ring Fracture Zone, Valles Caldera, New Mexico.
Person in Charge:	S. Self and J. A. Wolff

The eruptive units studied in this project are the products of the youngest volcanic event from the Valles caldera in the Jemez Mountains volcanic field of north-central New Mexico. The major aims of the study are to characterize the eruptions, to investigate the geochemistry and petrogenesis of the magma, and to explore the subvent stratigraphy by examination of lithic (accessory) clasts in pyroclastic deposits.

These young eruption products from the Valles caldera have been informally named the El Cajete series (ECS). Detailed documentation of the three units of the ECS, the El Cajete pumice deposits, the Battleship Rock ignimbrite, and the Banco Bonito lava flow, has enabled the physical emplacement processes associated with this eruption to be evaluated. An important finding arose from consideration of incompatible trace element abundances in the ECS and comparison with data from the Bandelier tuffs and other Valles caldera rhyolites. Geochemical dissimilarities between successive caldera-related rhyolites indicate that they are not products of a single, long-lived magma chamber but instead represent several discrete rhyolitic magma batches generated over the last 2 m.y. beneath the Valles caldera. Geochemically, ECS magma closely resembles pre-caldera dacitic rocks, while petrographic relations suggest melt production by fusion of pre-existing igneous rocks.

These results must have important implications to geothermal energy considerations of the Valles system, because previously it has been considered that the Valles hydrothermal system is generated by a long-term heat source such as an "active" magma body of sub-batholitic proportions. Evidence is now pointing to the fact that the magma system may be much less steady-state than hitherto realized, with the implication that activity of the hydrothermal system may also be more pulse-like. The active hydrothermal system of the Valles is in the western part of the caldera and may, in fact, be operating on residual thermal energy supplied by magma of the ECS. Long-range CSDP plans to drill into the Valles caldera should be preceded by further comprehensive studies on other Valles rhyolites.

Grantee: UNIVERSITY OF TULSA
Tulsa, Oklahoma 74104

Grant: DE-FG05-85ER12317

Title: Stability of Natural Gas in the Deep Subsurface

Person in Charge: C. Barker and N. Takach

Investigations of the stability of natural gas in the deep subsurface have continued using a combined experimental and theoretical approach. Fluid inclusions provide uncontaminated samples of deep gases but most minerals commonly have more than one population of inclusions. To avoid combining gases from multiple populations we have analyzed gases in individual fluid inclusions using a microcomputer-controlled, rapid scanning, quadrupole mass spectrometer. Mineral samples are heated in vacuum and as each inclusion bursts the released gas is analyzed in 25 ms. Up to 144 inclusions can be analyzed in 2 hours using approximately 10 mg of sample. Dynamic range is close to 1 part in 10,000. In the last year the old electron multiplier was replaced to give increased sensitivity and stability. Additions to the computer software have made it possible to select data for particular size ranges of inclusions. Large inclusions are more likely to have geological complications due to necking and leaking, while small inclusions are analytically more difficult because they are more influenced by instrument noise. The middle-to-large size range generally gives the most consistent compositional data. Size information has been added to the graphics. Considerable time was spent examining individual burst shapes for each component. This showed that water behaves like any other gas and adsorption is not a problem. While many single bursts occur, occasionally the release is more complex with successive bursts coming before the previous one has pumped down. Presumably planes of secondaries or cleavage surfaces are "unzipping." Calibration has continued using both pure gas mixtures and inclusions that have one dominant component. The latter approach has the advantage of calibrating under conditions identical to those used in analysis.

Study of samples from the deep Smackover formation, Mississippi, has continued and fluid inclusions in calcite cements from 19,000 to 23,500 feet have been analyzed. These show very variable H_2S, CH_4, and CO_2 contents depending on details of the local mineralogy. In continuing to evaluate the method a wide range of samples from different geological environments have been studied. While most of these have been quartz or calcites, other minerals also work well. Preliminary studies of the VC-1 core hole, Valles caldera, New Mexico, showed dominantly water in the fracture-filling cements but higher sulfur content in the rhyolite glasses, including some inclusions that were dominated by sulfur dioxide. These appeared to be in the phenocrysts.

The analytical studies have been supported by thermodynamic calculations of gas composition in deep reservoirs ($\leq 40,000$ ft). We have used the computer program developed over the past few years that finds the minimum free energy in multi-component (up to 70), multi-phase (up to 30) systems for various reservoir mineralogies. Calculations have been made for carbonate and sandstone reservoirs and a wide range of geologic conditions. In general, the measured gas compositions are within the range of those calculated by the computer program.

Grantee: UNIVERSITY OF UTAH RESEARCH INSTITUTE
Earth Science Laboratory
Salt Lake City, Utah 84108

Grant: DE-FG02-87ER13476

Title: Logging and Hydrothermal Alteration Studies of Hole VC-1, Valles Caldera, New Mexico

Person in Charge: D. L. Nielson and J. B. Hulen

Paleozoic and Precambrian rocks intersected deep in Continental Scientific Drilling Program corehole VC-1, immediately southwest of Valles caldera, are extensively disrupted to form a spectacular breccia sequence. These breccias, of both tectonic and hydrothermal origin, were formed in the Jemez fault zone, near the intersection of this major regional structure with the Valles caldera's ring-fracture zone. We have investigated these breccias by: detailed logging of the VC-1 core, with particular emphasis on fracturing and brecciation as well as hydrothermal alteration mineralogy and zoning; equally detailed petrographic examination and determination of bulk and clay-fraction mineralogy by x-ray diffraction analysis; and fluid-inclusion studies of hydrothermal quartz deposited both prior to and during brecciation. Results of these studies, when considered along with the local geologic history, yield the probable depth of hydrothermal brecciation, the contemporaneous state of stress, and the temperature prevailing when the breccias were formed. Our work on deep VC-1 breccias indicates that they were generated after about 1.5 Ma at a depth of about 515 m at temperatures in excess of 275°C. The pressure required to initiate hydrofracturing was about 6 MPa. Temperatures during brecciation were considerably in excess of the 161°C temperature currently prevailing in the breccia zone. Our work on the VC-1 core has shown that hydraulic fracturing and hydrothermal brecciation are very likely to have enhanced structural permeability in recently and presently active hydrothermal systems of the Valles caldera.

Grantee:	UNIVERSITY OF UTAH RESEARCH INSTITUTE Earth Science Laboratory Salt Lake City, Utah 84108
Grant:	DE-FG05-87ER13555
Title:	Caldera Processes, Hydrothermal Dynamics and Ore Deposition in the Sulphur Springs Vapor-Dominated Zone, Valles Caldera, New Mexico (VC-2A)
Persons in Charge:	D. L. Nielson and J. B. Hulen

VC-2A is the second Continental Scientific Drilling Program corehole in the Valles caldera, but the first to be drilled in the high-temperature interior of the caldera's active geothermal system. Situated at Sulphur Springs, within the hottest and most active zone of surface thermal discharge in the caldera, VC-2A was drilled primarily to investigate the vapor-dominated portion of the Valles geothermal system. Initial results indicate that the hole penetrated through this vapor cap into the underlying liquid-dominated regime below a depth of 450 m (TD = 528 m).

In collaboration with investigators from Los Alamos National Laboratory, we have logged the VC-2A core in detail, analyzed samples at nominally 6 m intervals for bulk and clay-fraction mineralogy by x-ray diffraction. Preliminary fluid-inclusion studies and petrographic examination are in progress. We are combining the results of these studies with those from our previous investigations of the caldera subsurface using drill cuttings from deep geothermal wells to refine our current models of the evolution of the Valles caldera complex and associated hydrothermal systems.

VC-2A penetrated an intracaldera ash-flow tuff sequence readily recognizable from previous work and including the 1.45–1.12 Ma Bandelier tuff. However, this sequence is intensely altered and locally hosts unique, sub-ore grade molybdenite mineralization. Preliminary fluid-inclusion studies indicate that the molybdenite was deposited from dilute solutions at temperatures near 200°C.

The VC-2A molybdenum mineralization will be summarized in a joint UURI/LANL article to be published shortly in *Geology*. A final report will be prepared upon completion of in-progress fluid-inclusion, petrographic, and alteration studies.

Grantee: UNIVERSITY OF WASHINGTON
Geophysics Program
Seattle, Washington 98195

Grant: DE-FG06-86ER13472

Title: Two- and Three-Dimensional
Magnetotelluric Inversion

Person in Charge: J. R. Booker

Our objective is to interpret magnetotelluric (MT) data when the electrical properties of the Earth vary laterally as well as vertically. Since most real MT data is significantly affected by lateral structure, understanding the multi-dimensional inverse problem is critical to reliable use of MT in exploring for thermal and hydrocarbon energy resources. Our approach uses the fact that the Frechet derivative of MT data with respect to vertical conductivity structure is closely related in the one and higher dimensional cases. They are the same except that the electric field that must be used in calculating the Frechet derivative is the true electric field existing in the laterally varying structure. This suggests an efficient iterative inversion scheme. At each step, the data at each site are inverted as though they were one-dimensional, except that the Frechet derivatives use the electric field from a forward calculation using a laterally varying model based on all the one-dimensional inversions at the previous step. This process should converge to a laterally varying model that fits the data. Understanding this convergence and subsequent appraisal of the model are our major tasks.

We have developed a very stable one-dimensional inversion that produces models that have the least possible structure. The minimization of structure is important as it eliminates spurious structures whose significance may be difficult to assess. We have adapted the one-dimensional inversion code to allow minimization of a norm of the laplacian of two- and three-dimensional models. We have embedded the adapted code within a main program for inverting two-dimensional data. Initial tests inverting two-dimensional data show success in finding models that fit the data and resemble the structures that produced the data.

We have written a two-dimensional (finite difference) forward modeling program that is used at each iteration of the two-dimensional inversion program to find the electric and magnetic fields that would be inducted in the conductivity model of that iteration. We plan to modify this to take advantage of new highly efficient iterative methods (incomplete factorization) of solving the resultant equation for the forward problem.

Grantee: WASHINGTON STATE UNIVERSITY
Geology Department
Pullman, WA 99164--2812

Grant: DE-FG06-87ER13796

Title: Geologic Spatial Analysis

Person in Charge: R. L. Thiessen

Washington State University, in cooperation with Pacific Northwest Laboratory, is generating a package of geologic spatial analysis (GSA) computer programs designed to determine crustal fracture geometries. These geometries are based on analysis of digital data bases developed from topography, lineaments, faults, and joints observed in the field, earthquake foci, gravity, magnetics, and borehole data. These GSA techniques center on radical new digital analysis techniques that determine if structures in three-dimensional space are controlled by the same planar fracture and are, therefore, coplanar. The unique power of GSA is this three-dimensionality; older techniques looked at orientations or surface traces but rarely both.

The main goals of this research project are to develop an integrated GSA program package and to use the techniques to identify crustal fracture planes at Department of Energy sites. Sites to be studied include the Morgantown Energy Technology Center's unconventional gas recovery and deep source gas exploration areas (Eastern Gas Shales and Western Washington Conductivity Anomaly); CSDP sites (Long Valley, Valles Caldera, Salton Sea, Geysers, and Yellowstone); and potential nuclear repository localities (Yucca Mountain, Nevada; Deaf Smith, Texas; and Hanford, Washington). Examination of additional energy-related sites, such as the San Andreas fault system, Mt. St. Helens, and Hawaii, is also proposed. Each of these locations is a prime research and development site because of the extensive digital data bases that are being generated, the concentrated supporting geological studies, and the crucial needs for determining and identifying fracture systems.

Grantee: UNIVERSITY OF WISCONSIN
Department of Geology and Geophysics
Madison, Wisconsin 53706

Grant: DE-FG02-84ER13184

Title: Thermal Stress Microfracturing of Granite

Person in Charge: H. F. Wang

We have developed an experimental capability to quantify thermally induced microfractures in rock. These microfractures can affect fluid transport and mechanical properties important in several energy technologies and geologic processes. We measured crack porosity and crack compressibility after one-inch diameter granite cores were heated to temperatures between 20 and 350°C while subjected to a confining pressure of 55 MPa. We also counted the cracks, sorting them by grain boundary and intragranular types and by mineral pair occurrence. The four granites tested were Westerly (RI), Illinois, Stripa, and Climax.

A relation in which the logarithm of the crack porosity is a linear function of temperature provides a good fit to the crack strain data for each granite. Crack compressibility indicates the dependence of crack porosity on burial depth. The crack compressibilities for the Westerly, Stripa, and Illinois samples show large, distinct peaks below 30 or 40 MPa confining pressure.

We distinguished between intragranular and grain boundary cracks and we determined the mineralogy of cracked grain boundaries as a function of the maximum temperature, using the scanning electron microscope (SEM). The ratio of cracked grain boundaries to total grain boundaries of each type was tabulated along a series of traverse lines. This ratio, termed normalized linear crack density (NLCD), has the advantage of removing grain size differences between samples. Combining the NLCD data for all four granites shows that crack densities increase modestly for samples heated to temperatures of 200°C and below but sharply for those heated to 300°C. This petrographic result closely matches the crack porosity data. The SEM observations further reveal that grain boundary cracks consistently account for 60% and intragranular cracks for 40% of the total crack population at all temperatures.

Thermal expansion and thermal anisotropy mismatches produce thermal stress heterogeneity on a grain-to-grain scale. The grain boundary NLCD from most significant to least is in the sequence: 1) quartz-quartz, 2) biotite/muscovite/chlorite-quartz/feldspar, 3) quartz-feldspar, and 4) feldspar-feldspar. These results imply that the thermal expansion contrast between two quartz grains is generally higher than that between adjacent feldspar grains.

Grantee:	UNIVERSITY OF WISCONSIN Department of Geology and Geophysics Madison, Wisconsin 53706
Grant:	DE-FG02-86ER13593
Title:	Deformation and Stress Modeling of Recent Magmatic Tectonics at Long Valley, California
Person in Charge:	H. F. Wang

The research program is to develop deformation and stress models for the south moat region of the Long Valley caldera as part of the thermal regimes portion of the Continental Scientific Drilling Program. Ground deformation and seismicity observed from 1975 to the present support the existence of a major body of magma within the central part of the Long Valley caldera, California. Although geodetic data indicating significant surface deformation have been collected from 1975 to present, we use the data of 1975–1982, as this period is the only one that contains both: significant uplift data (in excess of 0.4 m) and sufficient horizontal displacement data throughout the caldera. Constraints on the source geometry are obtained from deformation modeling of uplift and trilateration data. The deformation data are analyzed with elasticity theory, which incorporates an ellipsoidal magma chamber, the Hilton Creek fault, and the South Moat fault. The best fit to the uplift plus horizontal deformation data indicate a nearly spherically shaped source within the central part of the caldera at a depth about 9.5 km. However, significant deviations of some horizontal displacement data from the model suggest movements along structural faults are probably more complicated than the constant dislocations assumed.

Corresponding to the deformation data, the predicted perturbing stress field using a spherical model is mild. Stresses due to a narrow prolate ellipsoidal model, which produces about the same uplift as the spherical source model, leads to a horizontal tensile stress that is about one order of magnitude higher in the region directly above the source. For an assumed radius of 5 km in the spherical model, tangential stress at the surface of the magma chamber has a maximum tension near the bottom of the South Moat fault. It is possible that the 1983 earthquake swarms were triggered by the perturbing stress field plus shallow magma intrusions at the bottom of the South Moat fault. The crack opening location for magma injection is at the top of the source for the prolate ellipsoidal model. Hence we emphasize that stress is of importance as a means of discriminating between different magma source models. The stresses calculated from alternative deformation models may provide useful information for locating stress measurements in drill holes in Long Valley. Also, the stress field predicted by the best model may be useful for understanding seismicity and possible crack opening locations for magma injection.

Grantee:	WOODS HOLE OCEANOGRAHIC INSTITUTION Woods Hole, Massachusetts 02543
Grant:	DE-FG02-86ER13466
Title:	Organic Geochemistry of Outer Continental Margin and Deep Ocean Sediments
Person in Charge:	J. W. Farrington and J. K. Whelan

The objective of this program is to develop a better understanding of the processes of hydrocarbon generation and migration in coastal and offshore sedimentary basins as an aid in predicting favorable exploration areas for petroleum. Research this year has concentrated on applying our expanded analytical capabilities for the C_{15+} compounds. These data are being fitted into the overall geological and geochemical framework as provided by collaboration with other laboratories and our previous light hydrocarbon (C_1-C_{15}) and thermal distillation-pyrolysis data.

Detailed studies to determine C_{15+} profiles are in progress for the Alaskan North Slope Ikpikpuk and Seabee wells. Both wells become overmature with respect to both oil and gas generation in the deepest sections. Therefore, the sediment extracts are being examined for consistent changes in potential maturation indicators, such as relative ratios of naphthalenes, biphenyls, and phenanthrenes that may be useful in complementing and supplementing biomarkers as indicators of maturation such as hopanoids and steranes. Downhole profiles of these compounds are also being compared to those of other compounds, such as n-alkanes, pristane, and phytane as well as to those of the light hydrocarbons (C_1-C_{15}) and thermal distillation pyrolysis parameters determined in earlier stages of the work and described in previous reports. The goal of this work is to provide basic data on the strengths and limitations of the various biomarkers and other parameters in elucidating maturation and migration phenomena in basins, such as those in the Alaskan North Slope area.

Collaborative work with Dr. Arif Yukler has been carried out in modeling the time-temperature history of oil and gas generation for the Alaskan North Slope Ikpikpuk well. The initial results agree well with independently determined geological and geochemical parameters. Further work was completed on determining the characteristics of deep overmature Alaskan North Slope sediments with respect to gas generation. Pyrolyzable methane was measured as an approximate upper limit on remaining gas (methane) generation potential and compared with sorbed (generated) methane actually present in the same sediments. These studies show that even in highly overmature sediments (up to Vitrinite Reflectance 4%) the ratio of pyrolyzable to sorbed methane remains constant at about 100. Therefore, care has to be taken that sorbed methane present in deep overmature formations is not "artifact" gas generated during drilling. Collaborative work on isotopic and compositional characteristics of the gas was carried out with Dr. Eckhardt Farber of Germany to determine that sorbed gas present in one deep Seabee sample was typical of high maturity gas, rather than artifact gas. A new pyrolysis technique, thermogravimetric Fourier transform infrared spectroscopy, was applied to sediments from the Seabee well. Initial results show that this technique is valuable in characterizing high maturity sediments typical of the gas generation zone.

Grantee: UNIVERSITY OF WYOMING
Department of Geology and Geophysics
Laramie, WY 82071

Grant: DE-FG02-87ER13805

Title: Techniques for the Delineation of Liquid Hydrocarbon Resources Using Maturation and Enhanced Reservoir Porosity Models

Person in Charge: R. C. Surdam and H. P. Heasler

The solution of two problems is paramount in delineating liquid hydrocarbon targets. First, the maturation history of potential oil source rocks must be discerned. Factors that affect the maturation history include the temporal variation of terrestrial heat flow, sediment thermal properties, the burial history of the sediments, and the chemical kinetic properties of the hydrocarbon source rock. Second, the potential for reservoirs to accept the expelled hydrocarbons must be estimated. Factors that affect the ability of a reservoir to become charged with hydrocarbons include the depositional character of the reservoir rocks, early and late diagenesis of the reservoir rock, and the timing of intense diagenesis in relation to hydrocarbon expulsion from oil source rocks.

We are evaluating many of these critical factors that affect the delineation of liquid hydrocarbon targets. In general, we will consider three foreland basis of Wyoming (Bighorn, Powder River, and Wind River) in order to supply geologic constraints for our models. We will then develop and integrate thermal, maturation, and diagenetic models. Using our developed models constrained by field and laboratory data, we will construct a general scenario for the temporal maturation of liquid hydrocarbons in relation to enhanced reservoir porosity for Wyoming foreland basins.

Grantee: YALE UNIVERSITY
Department of Geological & Geophysics
New Haven, Connecticut 06511

Grant: DE-AS02-76ER10455

Title: Opening Mode Crack Growth in Rock

Person in Charge: R. B. Gordon

This research is a study of how the tensile fracture characteristics of rock are determined by microstructure. The data are intended to be used in the interpretation of fractures in rock in the field, particularly where the passage of fluids through the rock is of interest. Measurements of fracture energies were made earlier in the project on a set of different types of rocks having a wide range of fracture characteristics; the focus of the research is now to show how the fracture energy and the distance that a crack must advance before attaining steady state propagation are determined by the microstructure of the rock. The relation of fracture characteristics to other physical properties is also being investigated. In the study of crack propagation, polished specimens are split while on the stage of an optical microscope and the progress of the crack is followed as successively greater loads are applied. Thin sections of the rock samples are made after the fracture experiments and used to determine the proportion of the different minerals traversed by the crack relative to the volume fractions of minerals present in the microstructure of the rock.

Marble, granites, diabase, and basalt are now being examined to determine the mean crack density (the ratio of total crack length to the length of the rupture path), mean branching frequency, process zone width, fraction of the fracture pattern developed on preexisting cracks, and ratio of intergranular to transgranular cracking. Three different processes of crack pattern development are observed: continuous extension of the original crack, coalescence of crack segments, and secondary crack fill-in. There is a good correlation between these modes of rupture and the above crack pattern characteristics; when the crack density and branching frequency are low, coalescence and fill-in are not observed during the rupture process.

An extended set of rebound hardness measurements has been made on the rocks used in the fracture research and on their constituent minerals. The structural changes in the rock produced by the indentation process are also observed. Development of a characteristic crack pattern is the dominant process of indentation so it is expected that there will be a correlation between rock hardness and the weighted average hardnesses of the constituent minerals. The results confirm this but show deviations in some of the rocks that are determined by the rock structure. Rocks with weak grain boundaries are softer than expected; those with strong grain boundaries are harder.

GEOSCIENCES RESEARCH (ERDA/DOE)
HISTORICAL SUMMARY
(OPERATING FUNDS — THOUSANDS)

ON-SITE	FY 1978	FY 1979	FY 1980	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987
ANL	$ 100	$ 140	$ 240	$ 310	$ 330	$ 330	$ 360	$ 360	$ 355	$ 340
LANL	810	1,084	1,420	1,500	1,375	1,684	2,343	2,289	2,263	2,603
LBL	660	735	995	1,075	1,180	1,405	1,485	1,596	1,632	2,162
LLNL	250	630	910	1,060	1,110	1,280	1,815	1,898	1,521	1,837
ORNL	180	240	280	380	430	430	470	480	492	690
PNL	280	450	565	580	520	520	578	595	605	725
SNL/A	500	800	1,165	1,310	1,546	1,682	2,087	1,861	2,256	2,462
ON-SITE TOTALS	$2,780	$4,079	$5,575	$ 6,215	$ 6,491	$ 7,331	$ 9,138	$ 9,079	$ 9,360	$10,819
TOTAL OFF-SITE	$1,152	$1,895	$2,509	$ 3,030	$ 3,141	$ 4,523	$ 3,309	$ 4,253	$ 3,507	$ 4,449
TOTAL OPERATING	$3,932	$5,974	$8,084	$ 9,245	$ 9,632	$11,854	$12,447	$13,339	$12,867	$15,268
TOTAL EQUIPMENT	—	$ 355	$ 560	$ 923	$ 900	$ 890	$ 960	$ 1,100	$ 1,094	$ 1,150
TOTAL GEOSCIENCES	$3,932	$6,329	$8,644	$10,168	$10,532	$12,744	$13,407	$14,439	$13,951	$16,418

GEOSCIENCES RESEARCH (ERDA/DOE)
HISTORICAL SUMMARY/OFF-SITE
(OPERATING FUNDS — THOUSANDS)

INSTITUTION (PI)	FY 1978	FY 1979	FY 1980	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987
U/ALASKA (AKASOFU)	—	$ 85	$ 84	$108	$113	$117	$120	$126	$126	$128
U/ALASKA (PULPAU)	59	113	87	70	—	—	—	—	—	—
U/ARIZONA (HILL)	—	—	91	96	99	101	90	121	—	101
U/ARIZONA (NORTON)	—	—	—	66	60	48	—	—	—	—
*ARIZONA STATE (FINK)	—	—	—	—	—	—	—	22	23	11
ARIZONA STATE (NAVROTSKY)	—	—	35	62	66	123	—	—	—	—
ASPEN INSTITUTE (ROBERTS)	48	57	71	—	—	—	—	—	—	—
BECHTEL (HARPER)	—	—	—	—	—	—	—	—	25	—
*BROWN U (HERMANCE)	—	95	140	164	165	333	—	166	—	150
*CAL TECH (AHRENS)	—	—	—	—	—	72	81	160	—	160
*CAL TECH (STOLPER)	—	—	—	—	—	—	—	50	98	—
U/CALIFORNIA-B (HELGESON)	—	—	—	—	—	204	—	120	120	135
U/CALIFORNIA-B (REYNOLDS)	148	127	168	144	150	165	196	233	200	200
U/CALIFORNIA-D (Mac GREGOR)	71	61	23	—	—	—	—	—	—	—
U/CALIFORNIA-LA (ANDERSON)	—	—	—	—	—	—	60	74	—	23
U/CALIFORNIA-LA (BOEHLER)	—	—	—	46	NFX	60	66	75	—	—
U/CALIFORNIA-LA (KENNEDY)	60	72	72	—	—	—	—	—	—	—
U/CALIFORNIA-LA (ERNST)	—	—	—	—	—	—	—	—	—	64
U/CALIFORNIA-LA (WARREN)	50	103	107	121	NFX	—	—	—	—	—
*U/CALIFORNIA-R (Mc KIBBEN)	—	—	—	—	—	—	—	50	—	40
U/CALIFORNIA-SD (CHAVE)	—	—	—	—	—	—	—	—	—	120
U/CALIFORNIA-SD (CRAIG)	—	—	—	—	—	—	35	41	41	42
U/CHICAGO (ANDERSON)	—	—	64	NFX	38	98	NFX	46	—	—
U/COLORADO-B (SPETZLER)	—	—	—	—	—	—	—	—	—	95
COLUMBIA U (ENGELDER)	75	100	140	150	156	289	—	150	75	—
COLUMBIA U (JACOB)	256	274	312	318	318	337	359	360	360	360
COLUMBIA U (WALKER)	—	—	—	—	—	—	73	79	106	—
DOSECC, INC. (RALEIGH)	—	—	—	—	—	—	—	6	—	—
GEO CHEM RES ASSOC (ORTOLEVA)	—	—	—	—	—	—	—	—	—	50
HARVARD U (THOMPSON)	—	—	—	—	—	372	—	115	—	18
U/HAWAII (MANGHNANI)	—	—	—	—	88	96	99	200	—	100
U/HOUSTON (CHAFETZ)	—	—	—	—	—	—	—	—	—	69
HEADQUARTERS SERVICES	—	—	—	—	6	1	3	15	5	3

GEOSCIENCES RESEARCH (ERDA/DOE)
HISTORICAL SUMMARY/OFF-SITE
(OPERATING FUNDS — THOUSANDS)
(CONTINUED)

INSTITUTION (PI)	FY 1978	FY 1979	FY 1980	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987
LOUISIANA STATE (FERRELL)	—	—	—	—	—	—	—	—	—	60
U/MARYLAND (VALETTE-SILVER)	—	—	—	—	—	—	—	43	—	—
U/MINNESOTA (JOHNSON)	—	—	—	68	57	NFX	—	—	—	—
MIT (AKI)	113	142	152	160	151	158	147	—	—	—
MIT (SIMMONS)	100	100	90	100	106	106	110	80	80	—
MIT (TOKSOZ)	—	—	—	—	—	—	—	—	142	—
*MICHIGAN STATE (VOGEL)	—	—	—	—	—	—	—	31	NFX	34
*MICHIGAN TECH (McDOWELL)	—	—	—	—	—	—	—	50	—	—
NAS/NRC (HART)	9	44	116	168	282	—	200	187	124	202
NATL CTR ATM RES (HERRING)	—	—	—	—	—	—	—	—	—	10
NATL SCIENCE FDN (WRIGHT)	—	—	—	—	—	—	—	—	—	200
*U/NEVADA (PEPPIN)	—	—	—	—	—	—	—	—	143	—
*U/NEVADA (RYALL)	—	—	—	—	75	87	95	—	—	—
*U/OKLAHOMA (PHILP)	—	—	—	—	—	—	—	—	28	—
CUNY-B (FRIEDMAN)	—	—	—	—	—	—	—	95	86	100
CUNY-Q (SCHREIBER)	—	—	—	83	81	49	—	116	—	—
SUNY-A (DEWEY)	—	—	—	86	—	—	—	—	—	—
SUNY-A (HARRISON)	—	—	—	—	39	136	—	58	60	54
SUNY-P (WOLOSZ)	—	—	—	—	—	—	—	—	—	72
SUNY-SB (HANSON)	—	—	—	—	—	112	118	120	120	128
SUNY-SB (PAPIKE)	—	51	59	65	—	—	—	—	—	—
U/N. CAROLINA (GLAZNER)	—	—	—	—	—	—	—	38	39	—
OHIO STATE UNIV (ADLER)	—	—	—	—	—	—	—	—	—	50
U/OKLAHOMA (PHILP)	—	—	—	—	—	—	—	84	88	106
U/OREGON (WEILL)	—	—	—	—	—	103	94	—	—	—
OREGON STATE (FEHLER)	—	—	—	—	38	—	—	—	—	—
PENN STATE (MARTIN)	—	—	62	83	NFX	—	—	—	—	—
PENN STATE (GIVEN)	—	—	—	—	—	—	100	—	NFX	—
PORDUE UNIV (HINZE)	—	—	—	—	—	—	—	—	—	8
PRINCETON U (NAVROTSKY)	—	—	—	—	—	—	—	100	—	85
RPI (FRIEDMAN)	—	—	—	91	99	150	—	—	—	—
RICE (AVE LALLEMENT)	—	—	—	—	—	120	121	—	—	—

GEOSCIENCES RESEARCH (ERDA/DOE)
HISTORICAL SUMMARY/OFF-SITE
(OPERATING FUNDS — THOUSANDS)
(CONTINUED)

INSTITUTION (PI)	FY 1978	FY 1979	FY 1980	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987
*S. DAKOTA M&T (PAPIKE)	—	—	—	—	67	100	130	150	99	100
*U/S. CALIFORNIA (AKI)	—	—	—	—	—	—	—	150	150	156
U/S. FLORIDA (SACKETT)	—	—	—	34	—	—	—	—	—	—
SMU (BLACKWELL)	—	—	—	54	70	—	—	—	—	—
STANFORD U (LIOU)	—	—	—	—	34	45	NFX	—	—	—
STANFORD U (NUR)	104	147	140	140	125	160	172	172	165	165
STANFORD U (PARKS)	—	—	—	—	57	56	56	—	—	—
*STANFORD U (POLLARD)	—	—	—	—	—	—	—	39	42	44
U/ROCHESTER (GOVE)	—	—	—	—	—	—	—	—	—	8
*U/TEXAS-AR (SELF)	—	—	—	—	—	—	—	43	NFX	80
U/TEXAS-AU (BARKER)	—	—	—	—	—	54	—	—	—	—
TEXAS A&M (CARLSON)	—	—	—	—	—	—	—	—	98	—
TEXAS A&M (CARTER)	—	—	—	—	—	—	70	—	—	—
TEXAS A&M (DOROBEK)	—	—	—	—	—	—	—	—	—	62
TEXAS A&M (FRIEDMAN)	—	63	208	202	200	201	93	100	194	—
TEXAS A&M (GILBERT)	—	—	—	—	—	—	—	—	98	88
TEXAS A&M (KRONENBERG)	—	—	—	—	—	—	—	—	—	117
U/TULSA (BARKER)	—	60	NFX	75	71	75	80	80	81	133
USGS (HAAS)	54	54	—	—	—	—	—	—	—	—
USGS (MORGAN)	—	—	—	—	—	—	—	—	—	35
*UURI (NIELSON)	—	—	—	—	—	—	—	—	114	—
U/WASHINGTON (BOOKER)	—	—	—	—	—	—	—	—	27	30
U/WISCONSIN (WANG)	—	—	57	38	—	—	48	62	97	84
U/WYOMING (SURDAM)	—	—	—	—	—	—	—	—	—	65
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WOODS HOLE (WHELAN/FARRINGTON)	—	—	—	—	—	—	—	223	223	226
WOODS HOLE (HUNT)	—	102	141	139	150	190	208	—	—	—
*WOODWARD-CLYDE (BURDICK)	—	—	—	—	100	100	100	40	—	—
XDATA (DINES)	—	—	—	—	54	66	—	—	—	—
YALE U (GORDON)	—	46	4	35	26	39	184	—	—	—
OTHER	5	—	96	64	—	—	—	—	—	—
OFF—SITE TOTALS:	$1,152	$1,896	$2,509	$3,030	$3,141	$4,523	$3,309	$4,260	$3,507	$4,463

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