Summaries of Physical Research in the Geosciences

August 1979
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FOREWORD

The Department of Energy supports research in the geosciences in order to provide a sound underlay of fundamental knowledge in those areas of the earth, atmospheric, and solar/terrestrial sciences which relate to DOE's many missions. The Division of Engineering, Mathematical and Geosciences, which is a part of the Office of Basic Energy Sciences and comes under the Director of Energy Research, supports under its Geosciences program major DOE laboratories, industry, universities and other governmental agencies. Such support provides for payment of salaries, purchase of equipment and other materials, an allowance for overhead costs, and is formalized by a contract between the Department and the organization performing the work.

The summaries in this document, prepared by the investigators, describe the work performed during 1978, include the scope of the work to be performed in 1979 and provide information regarding some of the research planned for 1980. The Division of Engineering, Mathematics, and Geoscience Program, part of the Office of Energy Research, supports under its Geoscience Program, research in geology, petrology, geophysics, geochemistry, hydrology, solar-terrestrial relationships, aeronomy, seismology and natural resource analysis, including the various subdivisions and interdisciplinary relationships, as well as their relationship to the Department's technological needs.
DESCRIPTIVE STATEMENT
BASIC ENERGY SCIENCES
GEOSCIENCES
RESEARCH CATEGORIES

The following outline of research categories in the Department of Energy (DOE), Office of Energy Research (OER), Basic Energy Sciences (BES), Division of Engineering, Mathematical and Geosciences (EMG) program in the Geosciences is intended to be illustrative rather than exhaustive. Categorization will evolve with time from this FY 1979 basis. Individual research efforts at DOE, university, college, corporate, not-for-profit and other Federal agency laboratories supported by this program frequently will have components in more than one of the categories or sub-categories listed.

Research supported by this program may be directed toward: a specific energy technology, national security, conservation or environment and safety objective of DOE; providing geoscience and geoscience-related information of relevance to more than one DOE objective; or development of a broad, basic understanding of geoscience materials and processes necessary for the attainment of long-term DOE objectives. In general, individual research efforts supported by this research will involve elements of all three types of research.

1. Geology, Geophysics, and Earth Dynamics
   a. Large-Scale Earth Movements: Research related to physical aspects of large-scale plate motion, mountain building and regional scale uplift and subsidence.
   b. Evolution of Geologic Structures: Research bearing on history and development of geologic structures (e.g., folds, faults, landslides, and volcanoes) on a local or subregional scale (subsets of 1.a.).
   c. Properties of Earth Materials: Research on physical properties of rocks and minerals determined in the laboratory or field (in situ) by direct or indirect techniques.
   d. Rock Flow, Fracture, and Failure: Research related to response of minerals, rocks and rock units to natural or artificially induced stress. Includes the range of strain rates from those appropriate to drilling to viscoelastic response.
   e. Continental Drilling for Scientific Purposes: Research on advanced technology, and services concerned with utilization of shallow (<300 m), intermediate (300-1,000 m) and deep (1,000-9,000 m) drill holes in the U.S. 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 of the drill hole as an active experimental facility for study of crustal materials and processes. DOE focus on drilling through an active hydrothermal system (or systems) into a magma chamber or into high-temperature igneous rocks. Includes research aspects of drilling technology development for such hostile environments. Part of a multiagency (USGS, NSF, DOE, DOD) coordinated program.
2. **Geochemistry**

   a. **Geothermal Fluids:** Research related to thermodynamic, physical, and transport properties of natural geothermal fluids and their synthetic analogues. Emphasis is on generic rather than site-specific studies.

   b. **Static Rock-Water Interactions:** Laboratory-based 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. Includes research on origin and development of coal, petroleum, and gas.

   d. **Geochemical Migration:** Research on chemical migration in materials of the earth's crust where emphasis is on generic rather than specific understanding which may (ultimately) lead to predictive capability. Focus is on experimental and theoretical studies of chemical transport induced by pressure, temperature, and composition gradients within, between and by a phase or phases. Part of a multiagency (DOE, NSF, USGS) joint program.

3. **Energy Resource Recognition, Evaluation, and Utilization**

   a. **Resource Definition and Utilization:** Research with a principal goal of developing new and advanced physically, chemically, and mathematically based techniques 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 origin, migration, emplacement, and crystallization of natural silicate liquids or their synthetic analogues. Emphasis is on studies related to energy extraction from such liquids.

   d. **Information Compilation, Evaluation, and Dissemination:** Research activities which are principally oriented toward the evaluation of existing geoscience data to identify significant gaps, and includes the necessary compilation and dissemination activities.

4. **Hydrologic and Marine Sciences**

   a. **Ground Water Hydrology:** Research related to chemical and physical principles underlying the flow of water through porous and permeable rocks near the earth's surface.

   b. **Fresh Water Systems:** Research on the chemistry, physics, and dynamics of fresh water systems including streams, rivers, and lakes.
c. **Oceanography:** Research involving materials and processes of the marine environment. Principal emphasis on geological, geophysical, and geochemical research related to rocks and sediments beneath the water column.

5. **Solar-Terrestrial/Atmospheric Interactions**

a. **Magnetospheric Physics and Chemistry:** Research directed toward development of a fundamental understanding of interactions of the solar wind with the terrestrial magnetic field. Research related to 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 on the earth. Includes long-term effects of solar radiation on climate.

d. **Meteorology and Climatology:** Inter-relationships of weather and climate with energy systems and vice versa.
PART I

GEOSCIENCES

ON-SITE
Scope of Work

Argonne National Laboratory Geosciences is concerned with measurement of thermochemical properties of minerals and brines, and with elucidation of mechanisms whereby trace elements migrate through rocks. Results should contribute to the advancement of technological efforts in geothermal energy exploitation and in radioactive waste disposal.

A. Thermochemistry of Geothermal Materials (C. E. Johnson/P. O'Hare)

This program is devoted to determination of thermochemical properties of well-characterized minerals and prototypic brines. Systems studied are selected with the aim of utilizing data for development of predictive schemes. Properties measured are standard enthalpies of formation and heat capacities in the 300-700 K range and under pressures up to 500 bars. Fluorine bomb-, solution-, and drop-calorimetric techniques are methods employed. Current research interest is on sulfide minerals (e.g., stibnite and chalcopyrite), selected synthetic zeolites (e.g., chabazite and zeolite A), and synthetic brines. Information gained should prove useful in exploitation of both vapor dominated hot-dry-rock and hot water (brine) dominated geothermal systems.

B. Trace-Element Transport in Geologic Media (M. G. Seitz/R. A. Coutre)

Trace elements that migrate in rocks can produce uranium ores or, in other settings, they can upset man's schemes to extract geothermal energy or to dispose of wastes generated with energy. Our goal is to understand fundamental mechanisms that underlie transport by flowing groundwater of trace elements in rocks. We investigate trace-element migration that is either controlled by an ion-exchange reaction or by precipitation and dissolution reactions.

In hydrothermal-infiltration experiments, groundwater solutions are pumped through columns of rocks or minerals. Trace elements introduced into solution streams are eluted through columns to determine migration behavior relative to flowing solutions.

A result of experiments performed in FY 1979 is that kaolinite, nominally $\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$, has an affinity for Cs$^+$ in the presence of Na$^+$ that decreases with temperature from 25 to 212°C (and, hence, cesium is more mobile in kaolinite at higher temperature). Nearly linear relationships were found between the logarithm of the distribution coefficient and the reciprocal of temperature, and between the logarithm of the Cs$^+$/Na$^+$ selectivity coefficient and the reciprocal of temperature. The standard
change of entropy for the exchange reaction is equal to the difference in standard entropies of Cs\(^+\) and Na\(^+\).

The result, applied to nuclear-waste disposal, suggests that, because of nuclear-decay heating, transport of certain nuclides could be substantially faster through a clay backfill in a nuclear-waste repository than previously expected. The adsorption isotherm is nonlinear at trace concentration of iodate \((10^{-4} \text{ M})\) with fraction adsorbed greater at lower concentration. Yet adsorption is sufficient even at concentrations higher than \(10^{-4} \text{ M}\) so that only 200 metric tons (200 Mg) of hematite could adsorb about 98% of an annual yield of 2000 moles of iodate resulting from reprocessing 1500 metric tons of nuclear fuel. Thus, iron oxide might constitute an effective barrier to migration of iodate.
Objective is to conduct research in remote sensing and to develop data analysis methodology and instrumentation required to meet DOE's needs for data relating to geoscience and the environment.

A. Remote Sensing and Geophysical Data Set Correlation (H. P. Foote, G. M. Petrie)

Geological remote sensing is most effective when it can be combined with other kinds of geological and geophysical data. Data correlation methodologies are developed to effectively acquire, process, and utilize combinations of remote sensing and geophysical data sets. These techniques will be based on conversion of remote sensing and geophysical data into compatible digital data sets which can be analyzed on high-speed digital computer systems and displayed on computer graphics devices.

B. Image Enhancement and Classification (H. P. Foote)

Computer and analog processing techniques are being developed for enhancing and analyzing multispectral satellite and aerial remote sensing data. These techniques include spectral analysis, image enhancement, noise filtering, pattern recognition, texture analysis and geographic transformations.

C. Instrumentation Development (H. P. Foote, G. A. Sandness)

PNL develops aerial imaging systems for specific remote sensing applications. These systems include both optical, mechanical and photographic systems which can be configured with various sensors or film. Also, an interactive digital system is being developed to conduct data analysis required to produce final remote sensing data products.

D. Simulation of Solid Earth Processes (G. A. Sandness, W. M. Phillips)

Advanced data analysis methodologies are used by PNL geoscientists to better understand large-scale geologic processes in the Pacific Northwest Region. These studies will provide data needed to develop an initial simulation model of tectonic processes.
Scope of Work

Insolation and aeronomy programs at Battelle Observatory are concerned with measurement and characterization of ground-based solar flux (insolation) and nighttime, upper-atmospheric, optical emissions (auroras). The insolation program is directed toward spectral resolution studies of direct and diffuse solar radiation and high spatial resolution measurements of the diffuse component of solar radiation. Data acquired will have direct applicability to solar power site evaluations, photovoltaic and photo-biological programs, and it will provide basis for a quantification of insolation modification by clouds and aerosols.

Since insolation studies and auroral emissions studies share a common instrument, and to a certain extent data handling techniques, much development proceeded in parallel. Aeronomy focused on use of nighttime optical emissions as a diagnostic tool for investigation of state of the upper atmosphere and the plasmasphere-magnetosphere interaction region. It is important to obtain understanding of Earth’s magnetosphere because it influences not only radiation belts but helps protect the ozone layer, significantly affects radio communications, and it has been recently suggested that there exists a close but subtle relationship between the state of the magnetosphere and terrestrial weather.

A. Insolation Studies (J. J. Michalsky, E. W. Kleckner)

1. Analysis

Analysis of insolation data proceeds at several levels. The fundamental objective is to provide carefully calibrated spectral data in the 300-1100 nm range to potential users. Data are to be archived at the National Climatic Center in Asheville, North Carolina. Direct solar measurements through seven filters are taken at five-minute intervals throughout each day, and all-sky scans are made every half hour. Routine data collection also includes higher spatial resolution solar-zenith and solar almucantar scans at half-hour intervals. On clear days, data provided by these latter measurements as well as direct measurements will be used to derive aerosol properties including average size, size distribution, index of refraction and, quantity.

2. Experiment

Principal goal is to measure and calibrate solar radiation both direct and diffuse at seven specific wavelengths. A Mobile Automatic
Scanning Photometer was developed. It is a dual-purpose instrument which makes nighttime observations as well.

The instrument measures insolation in spectral bands centered at 395.0 nm, 470.0 nm, 570.0 nm, 680.0 nm, 785.0 nm, 900.0 nm, and 1010.0 nm. Field of view of the solar photometer is 1.5°. Basic data yield both direct and diffuse measurements of radiation. The detection mode allows a basic stability in the measurement of +2% and the instrument module is portable and suitable for remote siting.

B. Aeronomy (L. L. Smith, E. W. Kleckner)

1. Analysis

A recently completed analysis program included correlating nights when observations of plasma densities, temperatures and spectral energies were obtained by the ISS-II, AEC, AED and ESRO-4 satellites simultaneously when ground observations of auroral optical emissions were obtained by the MASP units at Battelle Observatory, Richland, Washington, and at Hinsdale, Montana. A high spatial coincidence was found between the ground-based observed equatorward boundary of the diffuse 6300A auroral emission with the equatorward boundary of satellite-observed soft particle precipitation and the F region electron density trough poleward cliff. If diffuse aurora is indeed the ionospheric counterpart of the plasma sheet Earthward boundary, the 6300A diffuse boundary may afford a means of monitoring convection characteristics of the spectrally soft, near-Earth, plasma sheet boundary over large spans of time and activity.

2. Observations

a. Battelle Observatory

Beginning in September 1967, all-sky photometric observations of the emissions [OII] 5577A, N₂ + 4278A and Hβ 4861, and continuums 5350, 6080, and 7150A have been taken routinely on all cloudless, moonless nights from Battelle Observatory, Richland, Washington. Observing technique consists of scanning the night sky in a series of almucantars at elevations 10°, 15°, 20°, 30°, and 50°. Since the photometric field of view is approximately 5°, these scans adequately cover the entire circle of view.

b. Global Program

Because most detailed investigations are done at single stations, understanding emission patterns tends to be regional. Synthesis that might be provided by simultaneous global observations is lacking.

What is needed is a set of simple, reliable, identical optical instruments dispersed over the globe. Battelle developed such an instrument called the Mobile Automatic Scanning Photometer (MASP). The same all-sky scanning technique presently used at
Battelle Observatory is implemented on the MASP. The main thrust of the aeronomy observational program is siting, calibrating and operating MASP units as a part of the "Global Patterns" programs. Four MASP units are now in operation, one at Battelle Observatory, one at Hinsdale, Montana, one at Boulder, Colorado, and one at Ft. Providence, Northwest Territory, Canada.

Battelle Observatory is a member of the International Magnetospheric Study (IMS). Three MASP units have been constructed and installed, and provide data from Iron Mountain, Michigan, LeDuc, Alberta, Canada, and Albany, New York. Funds have been received to build two additional units. The IMS program organized a data center in Boulder, Colorado, at which each member reports observations and can also retrieve observations other members report pertinent to this research.

C. Carbon Dioxide (G. M. Stokes, R. A. Stokes)

1. Background

Earth's atmosphere now contains $85 \times 10^9$ more carbon, as CO$_2$, than in 1860, mostly as a result of burning fossil fuels. Because of the CO$_2$ content, Earth's average surface temperature is 35 K higher than the bolometric temperature as seen from space.

A critical input to models which predict either results of CO$_2$ increase and/or exchange of CO$_2$ between various reservoirs is a value of the "Pre-industrial" atmospheric carbon dioxide abundance. The current program is designed to obtain a pre-industrial CO$_2$ abundance from a hitherto unexploited source of data, measurements of the near-infrared solar spectrum accumulated since the mid-1890's for astronomical purposes.

2. Analysis

In the past year research focused on: evaluating required accuracy of any technique designed to contribute to the historical study of the carbon cycle, organizing new and existing data for analysis, and determining abundances. Accuracy requirements for carbon dioxide abundance studies were estimated in several ways. In particular, over and above any long-term change in CO$_2$, is an annual variation in CO$_2$ concentration. At Mauna Loa, this variation amounts to approximately 1% of the total CO$_2$ abundance.

The first two areas of concern in analysis of data have been line identification and continuum placement. Using a line identification scheme contained in the REDUCER data reduction package, developed by Kitt Peak National Observatory, as a starting point, a method that automatically gives wavelengths of lines found in a digitized spectrum was developed. This scheme is extremely important since the spectral region chosen for analysis, the 1 to 2.5 micron region, contains well in excess of 10,000 lines, more than 7,000 of which originate in the Earth's atmosphere. The second step in analysis is placement of the solar continuum that is the reference level against which strength of
Scope of Work

Principal goal is to develop predictive capability based on a physical understanding of rate, extent, and mechanisms of migration of selected elements in the Earth's crust. Elements, trace metals, and nuclear waste products were chosen for this study because their migration behavior impacts man in resource exploration and development and environmental effects of waste disposal.

A. Structure and Mechanisms of Interaction of Transition Metal-Organic Complexes with Soil (J. A. Franz)

The basic experimental approach involves preparation of organic complexes of Zr, Nb, Ni, Co, Tc(IV), and Tc(V) and using these species in batch and column experiments to determine their adsorption coefficients for different soils.

B. Investigation of Mechanisms that Control Concentration of Radionuclides in Geologic Solutions (Dhanpat Rai and R. G. Strickert)

Goals are to determine effects of various factors (such as pH, Eh, complexing and competing ligands, tracer concentration, oxidation state of the element, solid phases) in controlling concentration of elements in solutions in equilibrium with different geomedia. We are evaluating role of pH, Eh, Al, Fe, and Pu compounds in controlling Pu concentrations in PuO$_2$ contaminated soils.
Scope of Work

The Geosciences Program at Lawrence Berkeley Laboratory consists of eight projects. These projects are broadly based fundamental studies that support development of geothermal energy, hot water energy storage, stimulated recovery of oil, isolation of radioactive wastes, and uranium resource evaluation and recovery. Studies include formulation of theoretical concepts, development of new instrumentation, experimental measurements, and simulation of processes using computer models.

A. Reservoir Dynamics (P. A. Witherspoon and C. F. Tsang)

Purpose is to understand physics and chemistry of mass and energy transport in hydrological systems and to isolate and study critical phenomena in these systems through development of computer models.

1. Reservoir Dynamics Related to Geothermal Energy

Several problems of a fundamental nature in development of geothermal energy are addressed.

a. Pressure of Reinjection into Geothermal Reservoirs

Transient pressures in reservoirs for isothermal systems are well-known. The present work studies thermal effects. An analytical as well as a numerical approach will be taken. This will give understanding of effect of temperature-dependent viscosity and density. It may suggest new methods of monitoring thermal front movements in a reservoir.

b. Nonisothermal Flow in a Porous Medium with Fractures

Work will incorporate discrete fractures (and the well bore) into a numerical model "CCC". This model presently studies nonisothermal flow through porous media.

c. Incorporation of Variable Flow Rate and Variable Injection Temperature into the Numerical Model "CCC"

Presently "CCC" allows only constant flow rates and constant injection temperatures as inputs. This new work will increase utility of the model to treat variable conditions typical of real situations.
2. **Reservoir Dynamics Related to Thermal Energy Storage in Aquifers**

   Careful study will be made on thermal dispersion due to geological heterogeneity. This effect has been generally ignored. Numerical studies to explore effects of heterogeneities will be made to understand its implications.

3. **Reservoir Dynamics Related to Nuclear Waste Geological Storage**

   One important factor to consider for geological isolation of nuclear waste is the fluid movement in fractures and porous medium around the waste repository. A study will be made of the temperature field and induced fluid flow on a global scale due to presence of the repository containing nuclear waste. Semianalytic, as well as numerical methods, will be used. Effects of a simple connecting fracture will be calculated.


   Objectives are to measure desired physical properties under simulated subsurface environmental conditions and to develop models which will predict properties, and their changes, with changes in environmental conditions. Properties needed include porosity, permeability, electrical resistivity factors, compressional and shear wave velocities, bulk, pore, and matrix compressibilities, and thermal properties including conductivity, diffusivity, thermal expansions and the vaporization-condensation-capillary (heat-pipe) effect. These properties are currently being measured on a variety of rock-fluid systems at elevated temperatures and pressures but new apparatus has been designed and is soon to be constructed to extend the range to 400°C temperature and 1250 bars pressure. Most properties will be measured concurrently or sequentially on the same test specimen in order to facilitate correlation of data.

   Models have been developed which permit prediction of thermal behavior of rock-fluid systems. Only a minimum amount of data such as porosity, approximate mineral composition, median grain size and sorting, and fluid content, are required to predict base thermal conductivity. Models and correlations are then available to predict thermal conductivity with changing conditions of temperature, pressure and fluid saturation. With an oxide analysis of the rock, specific heats may be estimated with considerable accuracy. These values combined with thermal conductivities and densities allow estimation of thermal diffusivities for use in transient heat-flow calculations.

   Similar models and correlations are being developed for other properties such as permeability, electrical properties, and sonic velocities.

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

   Theoretical and experimental studies of solution thermodynamics of strong aqueous electrolytes over a wide temperature range provides essential
information for technical utilization of many geothermal resources. Theoretical work successfully dealt with complex mixtures at room temperature, simple systems over wide temperatures, moderately weak electrolytes involving dissociation equilibria, and moderately soluble electrolytes. Future work will continue using existing volumetric and thermodynamic data for modeling. The recently constructed flow calorimeter and densimeter are yielding heat capacities and densities up to about 300°C and 1 kbar on systems previously unreported, in addition to extending existing data to higher temperatures and pressures. Results will be integrated with theoretical work to develop equations allowing prediction of properties at temperatures and compositions other than those measured.

After tests with NaCl have been completed, measurements will proceed to other pure components important in geothermal fluids, KCl, CaCl₂, MgCl₂, Na₂SO₄, MgSO₄, etc., and then to mixtures. The aim is to determine important parameters over the range to 300°C and 1 kbar and to verify accuracy of our equations for mixed electrolytes. With experimental data becoming available it will be possible to extend modeling calculations, of the type so successful for NaCl at high temperatures, to other salts as to mixtures.

D. Rock Water Interactions (J. A. Apps)

Objective of this project is to quantify rates of dissolution and precipitation of common rock forming minerals between 25° and 400°, and to determine impact of such reactions on rock composition and permeability during groundwater transport. In accomplishing this objective, insight will be gained regarding controlling mechanisms of these processes.

Work currently proceeds with measurement of solution of low albite over the temperature range cited, and in solutions of different initial compositions. With completion of solubility studies on albite, chlorite, tremolite, and epidote will also be investigated by analogous techniques, over the same temperature range.

Mineral dissolution rates will be related to rock geometry through measurement of dissolution of rock wafers containing the minerals studied. Measurements will be made using both "open" and "closed" conditions. Aqueous solution compositions will be monitored continuously during open system operation using specially designed autoclaves and autoanalyzers. Aqueous species present in solution will be computed from experimentally measured solution compositions using available distribution codes, and results compared with reactions using individual minerals.

Inert tracers will also be incorporated in the aqueous phase and monitored to determine uptake by rock as a function of time. This information will be used to compute rock porosity and pore tortuosity. Experimental results will be related to theoretical models describing advective transport through porous or fractured rocks, chemical diffusion into the rock matrix from fractures or highly permeable beds, and surface rate controlled chemical precipitation or dissolution of minerals.
E. Thermodynamic Properties of Silicate Liquids (I. S. E. Carmichael)

This project is a continuing experimental investigation to measure physical and thermodynamic properties of silicate liquids. In almost all cases measurements detailed below are in the stable liquid region, at temperatures considerably above the glass region.

Experiments on densities and thermal expansivities are virtually complete in the temperature range 1000° to 1500°C, although obtaining values for FeO proved experimentally difficult in view of the propensity of this component to oxidize at high temperatures. From these data molar volumes of SiO$_2$, TiO$_2$, Al$_2$O$_3$, FeO, MgO, CaO, Na$_2$O and K$_2$O have been calculated at various temperatures, and within the experimental errors, there is no compositional dependence of these partial quantities. However, by analyzing a quite different set of experimental data for the excess partial molar free energies of liquid components, there is a small positive excess volume for these components in the pressure range 1 to 12,000 bars.

Experiments are now underway to measure compressibility of silicate liquids over a range of temperatures and compositions using an ultrasonic technique.

Design of an apparatus to measure compressibilities at elevated pressures will be initiated.

It is planned to design a drop calorimeter to operate up to 2000°C to determine heats of fusion of the dozen or so common minerals that crystallize from magmas.

It is proposed to measure migration of a number of elements in a silicate liquid with an imposed thermal gradient. From these measurements will come both sign and magnitude of the Soret coefficient.

F. Chemical Transport in Natural Systems (C. L. Carnahan)

The project consists of two parallel lines of investigation: (1) Experimental and theoretical studies of solute-solid interactions in two sorptive systems, and (2) a numerical modeling study of chemical transport in dispersion-dominated flow systems. Studies of solute-solid phase interactions are directed toward definition of the time-dependent behavior of sorption processes, and definition of final equilibrium states, in the sorption of cesium ions on two solid phases, a smectite clay and pure silica. Batch experiments are being performed with $^{137}$Cs tracer and each solid phase; the smectite is in the homoionic sodium form in each experiment. At each of three temperatures in the range 15° to 100°C, concentrations of $^{137}$Cs tracer in solution will be measured during approach to sorptive equilibrium with each solid phase; final equilibrium states will define a sorption isotherm for each solid phase at each temperature. Six to eight equilibrium points are required for each isotherm, and approximately six to eight intermediate points are required for definition of kinetic behavior for three equilibrium points in each isotherm. Kinetic data will be analyzed to derive rate laws controlling sorption processes in systems studied and their temperature dependence. The equilibrium sorption
isotherms will be used to derive heats of adsorption as functions of extent of sorption. Concurrently with the experimental work, theoretical studies of the effects of nonequilibrium sorption and nonlinear sorption isotherms on concentrations of transported chemical species are being conducted. The results of the experimental and theoretical studies will provide information needed for the formulation of a generalized nonequilibrium, nonlinear source term for use in numerical preparation of an operative computer code to simulate chemical transport in nonsteady groundwater flow systems in the presence of strong dispersion. The code will incorporate nonequilibrium, nonlinear source terms for the transported solute.

G. Characterization of Mineral Hosts Using Spectrometric Techniques: NQR Spectroscopy (S. M. Klainer)

Initial research is expected to begin in FY 1980. Aluminum-27 has been selected as the probe nucleus, and the plagioclase mineral suite has been chosen as the system for study. This will permit the NQR approach to be fully and fairly evaluated using samples which have been well-characterized by other methods. It will also permit those areas to be defined when NQR best supplements existing data.

In parallel to the NQR studies on aluminum-27, two other tasks will be initiated. Calculations will be made on suitability of NQR to measure uranium-235, neptunium-237, plutonium-239, and cesium-133. Secondly, NQR spectrometers presently available will be continuously upgraded. First they will be made compatible with probe nuclei of interest, and then emphasis will be placed on attaining greater sensitivity, better data handling and interpretation, the measurement of ultra small samples and operation in the remote mode.

H. National Geothermal Information Resource (S. L. Phillips)

Objective is a single, comprehensive data base of basic properties of aqueous solutions for geothermal energy utilization. Compilation, critical evaluation, and correlation constitute a data book of recommended values for research and modeling, including identification of areas where data are either lacking or are inadequate, and recommendations for research to provide needed data. Scope covers thermodynamic and transport properties of the following aqueous solutions: (1) substances which on dissolving in water significantly change basic properties of the solution, for example NaCl, KCl, CO3; (2) substances which cause scaling, corrosion, or erosion when present in brines. Carbonates, silicates and H2S are examples of these substances.

We completed a data base containing over 1000 references on basic properties of aqueous solutions, and a report on viscosity of NaCl solutions to 150°C and 30 MPa. We also completed: entropy, heat capacity, thermal conductivity, density, solubility, and electrical conductivity on NaCl solutions. Tables of data with a correlation equation are available for each property to 350°C, and at either vapor saturation pressures or high pressures.

We will complete a compilation and correlation of the major scale-forming substances, silicate, carbonate, and sulfide.
I. Feasibility of Shear Wave Vibrators for Deep Crustal Studies in Geothermal Environments (H. Frank Morrison)

The occurrence of large shear wave reflection coefficients at the boundaries of low shear rigidity regions in the earth suggests the use of shear wave reflection surveys as a means of detecting and mapping such zones. The purpose of this project is to evaluate the means of using horizontal (shear) vibrators for deep crustal seismic profiling in geothermal environments. There are two main goals:

1. To evaluate the effects of low-shear velocity regions on the source radiation pattern and develop techniques of mapping geothermal targets using shear wave reflections.

2. To enhance the transfer of seismic energy into the earth and to beam it directionally.

These goals are being accomplished through numerical two-dimensional modeling to establish whether multiple shear wave resources can be beamed at an angle, scale modeling to investigate three-dimensional inhomogeneities and analytical studies to determine means of optimizing shear wave energy transfer into the earth.

A time domain finite element program and a frequency domain integral equation program have been used to model radiation patterns and scattering for single and multiple SH line sources over homogeneous and layered half-spaces. Off vertical axis sounding has been accomplished using multiple sources serially phased in time. A comparison of seismic responses for P and SH wave sources demonstrates that an improvement in the detectability of structurally simple low shear velocity zones is possible using shear wave sources.

The radiation impedance and radiation pattern for a torsional shear vibrator has been analytically calculated for homogeneous and layered half-spaces, for both damped and undamped models. The radiation impedance provides information concerning the thickness and shear wave velocity of the weathered layer. This information may be used to make a dynamic weathered layer correction during the course of a vibrator survey, and in selecting source locations for optimum vibrator-earth coupling. Work has begun on the analytic solution for the radiation impedance and radiation pattern for horizontally and vertically vibrating sources over layered visco-elastic media.

During the forthcoming year the numerical analysis will be extended to include beaming of seismic radiation in the presence of complex two-dimensional structures. Seismograms will be generated in an effort to determine methods of optimizing data reduction of scattered reflections using a multiple source. Scale modeling will be used to study radiation patterns, beam forming, and scattering from simple three-dimensional inhomogeneities. The radiation impedance and radiation pattern from beamed multiple source arrays may also be investigated analytically.
Scope of Work

Geosciences at LLL is organized to study physical and chemical properties and responses of earth materials that are important to DOE programs and initiatives. All of these efforts make use of experimental work, novel diagnostic techniques, and computer modeling. The common objective of this integrated program, from a scientific viewpoint, is to develop models that can be used to predict and understand the behavior of the earth, both near-and far-field.

Current effort is divided among studies of (1) basic rock mechanics, (2) determination of seismic Q with depth in the earth, (3) kinetics and transport in aqueous solutions, and (4) information dissemination and data management of Department of Energy drilling activities. Within existing programs special attention will be paid to thermomechanical properties of rocks as they relate to the formation of rock melt (basic rock mechanics), and development of two-dimensional computational models to predict thermo-mechanical response of rock (basic rock mechanics), and development of a mathematical code to permit calculation of both thermodynamic and kinetic effects in aqueous solutions (kinetics and transport in aqueous solutions). In coming years we will expand these current efforts to include (5) studies of diffusivities of atoms in minerals using a unique radioisotope tagging scheme, (6) development of laboratory, field, and computational tools to utilize remote techniques to infer geophysical parameters so as to achieve capability to image geologic structure underground, (7) studies of uranium distribution and mobilization in granitic intrusives to understand mobility of uranium decay chain species in natural rocks, (8) an investigation of thermodynamic and transport properties of silicate melts, and (9) research into production of natural mineral forms capable of incorporating constituents of the waste from nuclear fuel.

As part of our involvement in the Continental Drilling for Scientific Program purposes we will continue to set-up the information unit on Department of Energy drilling activities, we will plan and direct geophysical modeling of a site, we will plan and direct the effort to measure physical and chemical properties on recovered core, work closely with Sandia Laboratories and bring our expertise on hydrothermal systems to bear on the magma drilling program. Along with the Los Alamos Scientific Laboratory and Sandia Laboratories, we will participate in the programs to obtain in situ data.

Fundamental efforts in basic rock mechanics, silicate melt geochemistry and geophysics, and rock mechanics modeling will be directed toward understanding processes involved in disposal of radioactive waste by in situ rock melting.
Basic Rock Mechanics studies are aimed at developing a better understanding of effect of the rate of explosive energy release on rock fracturing. Effect of confining pressure on fracture damage, measuring effect of intermediate-rate loading on fracture propagation and energy deposition, development of the computer program which calculates block motion, and on ultrasonic identification of the spatial distribution and form of rock fractures, are parts of this program.

1. **Effect of Confining Pressure on Explosive-Induced Fracture**

   Small explosive charges have been detonated in blocks of porous sandstone held at 50 MPa, 25 MPa and 0.1 MPa confining pressure. A program to measure fracture damage using the scanning electron microscope and density changes using x-ray radiography, and then to compare these measurements with computer predictions near completion. Implications for gas stimulation by explosive fracturing are that, in a porous material, computer predictions of fracture damage are reliable, but that compaction effects near a conventional explosive probably dominate, thus inhibiting rather than enhancing permeability.

2. **Effect of Intermediate Rate Loading on Borehole Emanating Fractures**

   Adverse compaction effects near a borehole can be avoided and fracture surface production maximized if multiple fractures, as opposed to single fracture, can be driven through the compaction zone and into the surrounding damaged, but not densified region. Preliminary experiments, done on our intermediate strain-rate loading apparatus, verified that such multiple fractures can indeed be driven from a borehole into the surrounding medium if borehole pressurization rate is controlled. Work is in progress to modify equipment so that constitutive equations relating pressure strain-rates, and fracture production can be obtained.

3. **Discrete-Interacting Blocks Computer Model**

   This computer program is in the final phases of development, with test problems being run. The first application will be to calculate oil-shale retort block-motion and study the mechanical properties of granular geologic materials. In the first phases of planning is a modification to allow calculations of thermally generated deformation of an underground nuclear waste repository in jointed rock.

4. **Ultrasonic Analysis of Crack Structures**

   Broad-band, ultrasonic or sonic, analysis can possibly be used to indicate properties of joints of fractured rock, such as spacing, orientation, and density. These in turn can be correlated with properties such as bulk strength and permeability. A study is underway to develop basic techniques in the laboratory using samples of granular rock salt.
5. Thermomechanical Rock Properties (H. C. Heard)

For the rock melt process to be acceptable as a method of radioactive waste disposal, growth with time of the molten rock-waste mixture must be well understood and totally predictable. During the growth phase the stress field in the surrounding rock will be thermally perturbed and lead to localized failure near the melt-solid rock boundary as a result of fracture or plastic flow. Later, during cooling recrystallization the stress field will again be disturbed. In order that these processes be modeled successfully, a knowledge of rock properties is required over the entire temperature range to be encountered. Experiments would be devised to measure physical and mechanical properties required to construct a computational model in several possible host rocks. We will investigate constitutive behavior of host rock and of host rock-waste mixture at realistic conditions up to hypersolidus temperatures. We plan to measure uniaxial stress behavior and thermal expansion under pressure (0.1 to 150 MPa) and at high temperature (25°C to 1000°C). Pore H₂O pressures in equilibrium with the material would be independently controlled and could range up to 150 MPa. We would also measure overall deformation behavior as a function of time through creep (constant stress), constant strain rate, or stress relaxation loading.


In order to proceed to demonstrate feasibility of the rock melt concept for disposal of radioactive waste, we must be able to reliably predict quantitatively physical as well as geochemical phenomenology. The concept was initially developed utilizing a one-dimensional heat conduction code assuming isothermal melting of the rock. This has proved useful in predicting maximum melt radius and temperatures outside the melt with time; however, a more detailed model is needed to assess and incorporate effects such as convective heat transfer, effects of both thermal stresses and those due to expansion of melt, more realistic melting and mixing of waste and rock, etc.

The present capability for modeling thermo-mechanical processes associated with conventional high level waste disposal is applicable to predicting temperatures, stresses, and displacements with two- or three-dimensional finite element codes in continuous, isotropic rock bodies where temperatures do not exceed 100°C. We will extend our current capabilities to include discontinuities, anisotropy, plastic flow, failure with crack propagation, and migration of water, both gaseous and liquid in fractures. The upper temperature limit of the model studies would include complete melting of rock, and include viscous effects including convection within the rock melt itself.

The model then should be two-dimensional, not only to account for difference in initial geometries of the cavity into which melt is added, but also to model changes in geometry during melting.
B. Rock-Fluid Systems (A. G. Duba)

Seismic velocity and electrical conductivity measurements are important field tools which may delineate structure and extent of natural rock-fluid systems. We studied the relationship between electrical conductivity as a function of fluid content and composition in the laboratory and at elevated pressure and temperature in a portable field test device. In addition, we developed a new technique for measuring electrical conductivity of rocks which we later developed into a new core characterization tool. Laboratory equipment to measure velocity, permeability, and conductivity simultaneously under simulated in situ pressure and temperature conditions was built and debugged.

The apparatus can produce pressures to 200 MPa (2 kbar) and temperatures to 400°C. It can accommodate rock cores up to 100 mm long by 25 mm in diameter. Pore pressure can be varied independently of confining pressure. Measurement of electrical conductivity, acoustic velocities, and permeability can be performed simultaneously. Experimental parameters are controlled by a microprocessor.

C. Seismic Q in the Earth (J. M. Mills, F. E. Followill)

A unique suite of seismic and geologic data gathered through the LLL seismic net is being used to calculate interval velocity and seismic Q between reflectors in the Earth's mantle for the Basin and Range Province. This will allow detailed knowledge of a particularly interesting part of the upper mantle, from the viewpoint of plate tectonics as applied to North America. There is strong application to treaty verification of foreign nuclear testing.

D. Aqueous Geochemistry (D. G. Miller, T. J. Wolery)

Diffusion in the multicomponent brine and ground water systems is complicated, and simple approximations do not yield cross term effects between flows of different salts. Therefore, experimental work is required to characterize representative binary and ternary systems to provide a basis for improved estimation procedures based on irreversible thermodynamics. Included will be aqueous $\text{SrCl}_2$, $\text{CsCl}$, $\text{NaI}$, $\text{MgCl}_2$, and their mixtures with $\text{NaCl}$.

Modeling of reactions in geochemical systems requires a thermodynamic data base, which includes free energies of formation of minerals and ionic species. Also needed are activity coefficients of species dissolved in groundwaters or brines because of their strong departures from ideality. One portion of this study is measurement of activities in representative aqueous systems. The other is critical review of existing theoretical or empirical expressions for describing activities in multicomponent aqueous systems. This includes incorporating results into chemical equilibrium and kinetics codes.

Many aqueous geochemical processes are slow so that chemical equilibrium calculations are particularly suitable. Therefore, what kinetic effects there are will be dominated by a few slow reactions. Thus, the
mathematical description should include combined thermodynamic and kinetic portions. We will develop a code to permit such calculations.

E. Diffusion in Earth Materials (R. H. Condit, A. J. Piwinski)

We will use a novel technique for radiotracer diffusion, developed at LLL, to study ionic diffusivity in silicate minerals relevant to processes in the earth's crust and mantle. The technique uses rare but stable isotopes which are used in diffusion experiments and then are selectively made radioactive afterward. Oxygen-18 is made radioactive by ion bombardment to produce $^{18}$F ($t_{1/2} = 1.8h$). Autoradiography is used to locate the tracer and measure concentrations. $^{30}$Si will be used similarly. We will initiate studies with measurements in olivine, a major mantle constituent which has been relatively well characterized. Measurements would then extend to pyroxenes, feldspars, and other materials. These measurements would be first concerned with single crystal diffusion, then grain boundary and interface diffusion, and finally with liquid-solid interface problems of material transport.

F. Underground Imaging (A. G. Duba, R. J. Lytle)

The goal is to develop laboratory, field, and computational tools for remote identification of geophysical parameters of interest to DOE programs. The ultimate success of such DOE programs as geologic storage of radioactive waste, in situ recovery technologies, enhanced oil and gas recovery, geothermal energy, and seismic monitoring and verification may depend on our ability to predict material properties based on geophysical measurements made some distance away. Adaptation and development of methods for predicting physical properties from geophysical measurements will depend on accuracy of modeling and interpretation techniques, as well as capability of field and laboratory geophysical measurements. We will develop equipment necessary to measure, and provide modeling and computational tools necessary to interpret, geophysical data to remotely assess subsurface material properties.

G. Continental Drilling for Scientific Purposes Program (CDSP)

LLL involvement in the CDSP Program will consist of two components. The first is a service role for the entire program.

1. Information and Data Management Systems (N. W. Howard)

The information and Data Management project will provide data bank and information services for the CDSP program. Included will be subsurface data as well as core and sample data information on programmatic drilling by Federal agencies and new wells drilled by industry that offer opportunity for cooperative efforts and a computerized data bank for drill hole data acquired in CDSP projects. Information will be disseminated to the scientific community on plans and drilling activities in a timely manner.
2. **Subsurface Processes (P. W. Kasameyer)**

We will plan and direct geophysical modeling of a site before drilling to aid in site selection, during drilling, and after drilling to characterize the site utilizing our present capability in obtaining and reducing geophysical data. We will work closely with Sandia Laboratories to gain scientific understanding of a complete magma/hydrothermal system. We will participate jointly with Los Alamos and Sandia Laboratories to obtain in situ data.

H. **Natural Uranium and Daughter Product Mobility (K. G. Knauss)**

In addition to salt and basalt storage, consideration is being made to storage of radioactive wastes in granite bodies. However, little consideration has been given to mobility of uranium and/or its daughter products in granite either on short or long time scales. Techniques exist to study mobility of natural uranium and its decay series members since time of crystallization. Understanding uranium mobility may be critical to storage of radioactive wastes because long-term activity will be entirely determined by the uranium decay series, once $^{239}$Pu has decayed. An examination will be made of granitic intrusives which remained "closed" systems and retained uranium as well as intrusives in which large scale mobilization occurred. Uranium distribution as well as processes and time scales for uranium mobilization will be determined. Methods used include (1) fission track techniques to determine age, thermal history, and present uranium distributions; (2) disequilibrium techniques (low-level gamma and alpha spectrometry) to study mobilization due to weathering, and (3) U-Pb systematics to determine total amount of uranium liberated by all processes since crystallization.

I. **Transport and Thermodynamic Properties of Silicate Melts (A. J. Piwinski)**

Technical feasibility of rock melt waste disposal rests on our ability to predict behavior of the molten mass with time. In particular, thermodynamic and transport properties of molten rock-waste mixtures are critical parameters in understanding mixing of waste with rock, convective processes, and thermal energy distribution within the molten rock mass. We will determine transport and thermodynamic properties of silicate melts over expected temperature, pressure, and concentration ranges for candidate host rocks. Reasonable boundary conditions: pressure - 150 kPa to 50 MPa, temperature - 900°C to 1700°C, activity of water - zero to unity. Specific properties of the melt which will be examined include viscosity, thermal conductivity, enthalpy, diffusion, electrical conductivity, and thermal expansion.

J. **Geochemical Studies of Mineral Waste Forms (R. W. Taylor, J. D. Tewhey)**

In the rock melt process the geochemical form of the waste components in the resolidified silicate matrix will determine their availability to intruding groundwater, and natural mineral forms could provide a significant barrier to leaching. We will study the final chemical form of important waste components in several promising host rock types over the range of concentrations and conditions expected. Leachability will also be studied.
The study will also extend into the range of higher waste concentrations appropriate to conventional isolation. Natural examples of candidate host minerals for waste components will be selected and studied. Initial work will be done at atmospheric pressure utilizing simulated reactor waste mixed with rock, heated to melting and slowly cooled, and sampled periodically during cooling. Samples will be characterized utilizing optical microscopy and x-ray diffraction. Mixtures will range in waste concentration from very low values to ~20 percent. Later studies will be done under steam pressure with very slow cooling.
Scope of Work

Multidisciplinary Geology and Geophysics basic research at LASL advances fundamental understanding required for nuclear waste isolation, geothermal energy exploration and development, and coal use. Waste isolation studies provide rock models to evaluate long-term stability and integrity of repositories. Geothermal research focuses on understanding structure, tectonics, and evolution of potential geothermal resources, and properties of reservoirs. Coal work concerns characterization of accessory minerals and determination of occurrence and distribution of minor and trace elements, especially sulfur. Rock physics research supports engineering of waste isolation facilities by exploring the brittle-ductile transition in granite, basalt, and tuff, and determining effects of water on ductile and brittle deformation of silicates. Geothermal support includes seismic profiling, radiative heat transfer measurements, numerical modeling, equation-of-state research on rocks and minerals, field geology, trace elements and isotopic analyses of geothermal waters, and electron microprobe, x-ray diffraction and petrographic examinations of deep hole rock samples. We study minor and trace accessory phases in coal by electron microanalysis, x-ray diffraction, and petrographic techniques.

Focus for geochemistry research is experimental and theoretical study of phase equilibria to define solution-mineral kinetics at elevated temperature and pressure. Experimental work models natural reservoir rock-fluid reactions in open and closed systems. Thermochemical measurements provide thermodynamic properties of minerals such as heats of formation and heat capacities. In mineral synthesis we fabricate pure and well-characterized mineral-like materials. Many of these experiments use geochemical computer calculations.

A. Basic Geosciences

1. Igneous Processes (J. C. Eichelberger, G. Heiken, F. Goff)

Origin, evolution, and cooling history of igneous rocks associated with young volcanic fields are important factors that determine energy reserves of geothermal fields. Expanding research provides information concerning evolution of several major volcanic fields.

One goal of petrologic work is to predict presence of large magma reservoirs in the crust from petrology of surface lavas.

We determine volcanic hazards in several western states in support of terminal nuclear waste storage. Work consists of three parts: (1) a worst case scenario predicting disruptive events near potential waste
vaults, (2) prediction of high risk zones in the western U.S., and (3) development and evaluation of calculation procedures to determine volcanic risks.

We study evolution of shallow magma reservoirs by examining petrology and geology of surface rocks exposed by erosion. Calculations show that reservoirs which mix during replenishment of magma from below and in which there is a high initial density contrast between intruding magma and reservoir magma, must lie very close to the surface. These shallow reservoirs may be significant geothermal targets.

2. **Rio Grande Rift** (W. S. Baldridge, J. Bridwell)

We perform research on petrology and chemistry of young (5 m.y.) basaltic rocks from the Rio Grande Rift. Results allow determination of the depth at which magmas originate and mechanisms by which they evolve in shallow reservoirs during ascent. Correlation of basalt chemistry with structural setting provides insight into regions of magma genesis beneath continental rifts. Ages and compositions of older (30 to 5 m.y. old) volcanic rocks permit correlation of disconnected enclosing sedimentary units. Since these sediments deposit in response to tectonic movements, age data provide better understanding of structural evolution. Time dependency of magma composition constrains changes in depth, amount of partial melting, and mechanisms by which magmas evolve in shallow crustal reservoirs.

Mafic and ultramafic inclusions (xenoliths) represent direct samples of lower crust and upper mantle. Compositions of coexisting mineral phases yield temperature and pressure (depth) estimates for latest equilibration. These data permit calculation of geothermal gradient, and place compositional and physical constraints on geophysical models.

We use integrated numerical models to investigate hypotheses for lithosphere Cenozoic thinning and evolution of continental rifts. Models use data from heat flow, petrology, age dating, and mantle rheologies to predict temperatures, effective shear stress, viscosity variations, and velocity fields. We examine long-term density-driven asthenospheric circulation and lithospheric thinning with resulting crustal uplift. Response of a hot buoyant diapir beneath the rift during dynamic thinning predicts velocities and topography of the free surface.

3. **Mantle Petrology** (J. Smyth)

A computer program casts analyses of rocks (real or hypothetical) into a suite of "normative" minerals appropriate for a 30 kbar (=100 km depth) environment. It includes hypothetical Mars mantle compositions. We use the algorithm to predict mineral assemblages and partial melt compositions in the mantle of Mars. The program also defines critical deep planet depths which require experimental petrologic investigations, especially in iron-rich compositions postulated for the interior of Mars.

We plan a multidisciplinary research program to study and to understand an entire geothermal system associated with a young silicic magma body located near a major continental rift. We will examine the Jemez Mountains caldera located on the Rio Grande Rift in northern New Mexico. Due to a unique combination of existing deep drilling operations and abundant geologic and geophysical data, such a goal is attainable in the Jemez Mountains.

We established a core sample repository to provide a center for preparation, care and distribution of deep drilling samples along with basic lithologic and historical data for each sample.


C. Coal Research (R. Raymond, Jr., R. Gooley)

Immediate goals are to: (1) develop a homogeneous, stable standard for organic sulfur determination in coal using the electron probe microanalyses; (1) use a recently developed method of organic sulfur determination to measure abundances and distribution of this environmentally troublesome element; (2) determine how common elements such as Na, Mg, Al, Si, S, K, Ca, Ti, and Fe occur throughout macerals on a submicron scale. Longer range objectives are to: (2) define mineralogical site of trace elements and inorganic minerals in coal with depositional environments; (3) determine chemical and mineralogical effects (e.g., trace element concentrations, mineral alterations) in laboratory simulations of in situ coal gasification (and possibly liquefaction) processes.

We use electron probe microanalysis and scanning electron microscopy to determine occurrences and distributions of minor and trace elements in coal. Sulfur data yield information on its origin in coals, and on organic molecular structure variations between different maceral types. The latter is especially important in understanding gasification and liquefaction reaction mechanisms.

D. Rock Physics

1. Mechanical Properties (J. Blacic, P. Halleck, R. Riecker, J. Bridwell, T. Shankland)

Rock physics research supports HDR-GTE, evaluates long-term stability and integrity of nuclear waste repositories, defines structure and tectonics of the Rio Grande Rift, applies geophysical techniques to site selection, in situ properties, and samples from the Continental Drilling project.
We study deformation mechanisms in silicates. This work within a range of T, P, and strain rate conditions, determines regions in which fracture, dislocation motion, kink banding and recrystallization predominate. For example, study of flow properties of the common crustal mineral group clinopyroxenes improves understanding of crustal rock response to tectonic forces in rift zones. We use numerical models of non-Newtonian thermal creep to scale experimental observations to field problems.

We study complicated chemo-mechanical effects of water on rock deformation. Water stress corrosion of silicates is poorly understood but it affects a wide range of tectonic and applied rock physics problems.

We perform experiments to determine extent of rock cracking due to thermal stress. We employ these data in calculations of efficiency and lifetime of the LASL hot dry rock system.

Mechanical response of rock under pressures to 2 kbar and temperatures to 500°C becomes increasingly important as mines and drill holes reach deeper. For example, we begin study of sandstone response to cyclic loading under these conditions for application to compressed air energy storage. We fabricate large testing machines for work on 2-inch diameter samples under brittle, ductile, and transition conditions.

Ultimately, a geothermal resource depends on conduction of heat into near-surface rocks. Current work confirms that radiative heat transport accounts for nearly half of the total thermal conductivity in many earth minerals.

2. **Transport Properties** (T. J. Shankland)

We examine electrical and thermal transport properties in rocks and minerals to understand better behavior of nuclear waste rock media and emplacement of crustal and upper mantle heat sources. Concurrent studies of elastic properties complement this work and help to develop equations-of-state for increased understanding of deep earth processes.

3. **Equation-Of-State** (J. Shaner, R. McQueen)

We measure thermodynamic properties of rocks and minerals of geophysical interest at pressures and temperatures similar to those existing throughout the earth. We determine isotherms in static high pressure x-ray cells to more than 100 kbar. We also generate simultaneous high pressures and temperatures using shock waves; peak states simulate earth core conditions. Experiments yield Hugoniot pressure-density curves. Interpretations of the Hugoniots yield improved understanding of deep earth compositions.

We also measure shock wave velocities in rocks at high pressure and temperature. These measurements complement longitudinal and shear wave velocities determined seismically, and they also place constraints on deep earth compositions.

Seismology supports discovery of geologic sources of energy and assesses hazards from natural and induced earthquakes.

A permanent network of approximately 20 stations records background seismicity throughout northern New Mexico at a magnitude threshold near $M_L = 1$. Continuous recording of these stations provides epicenter maps; earthquake focal depths, magnitudes, and mechanisms; and velocity and Poisson's ratio information for regional earth structure.

Portable seismographs augment network stations for determining seismic risk. We use these data to determine magnitude vs. frequency of occurrence, likelihood of damaging ground accelerations, structural vibration response to ground motions, and may provide information for earthquake prediction.

We use seismic monitoring to identify earthquakes induced by DOE programs. Observations of background seismicity contribute to understanding of the regional tectonic framework against which the cause of each earthquake may be judged. Additional evidence of casualty comes from spectral analyses and from time correlation with suspect activities such as injection or withdrawal of fluids in the LASL hot dry rock geothermal demonstration and the salt dome storage of the strategic petroleum reserve.

We use experimental and theoretical refraction seismology to infer models of earth structure, focusing in areas of geothermal and mineral resources. We employ data from portable seismic stations and from numerical calculations to create crust and upper mantle models of rock velocities and densities in two dimensions. The models provide estimates of in situ temperature and pressure conditions, and of structural evolution.

Gravity, Geomagnetic and Surface Wave Observations, programs which are in early stages of development, help delineate structural features and transition zones. Four contiguous physiographic provinces in northern New Mexico require a broad spectrum of geophysical interpretation to reduce ambiguity of observations.

Portable seismic arrays and deep well geophone packages are essential instrumentation for studying special problem areas. Data acquired demonstrate significance of aftershocks of nuclear weapon tests and earthquakes, and of acoustic emissions in the hot dry rock geothermal reservoir.

Although most techniques employed were proven elsewhere, we pioneer application to geothermal resource exploration and development.

F. Geochemistry

1. Experimental Geochemistry (R. Vidale, R. Charles)

We react rocks with initially pure water, sodium chloride solutions, or sodium carbonate solutions in closed reaction vessels and in circulating systems. We use closed systems to determine the final
equilibrium assemblage of rock and solution whereas circulation systems attempt to model intermediate, transient, mineral assemblages coexisting with solution. One circulation system now operating can model effect of an increment of cool water entering a rock fracture and proceeding up a temperature gradient, for example, along a natural or man-made fracture. These experiments provide mass transport and rock-water interaction data needed to model chemical and physical behavior through time of a hot rock geothermal reservoir.

2. **Thermochemistry of Minerals (C. Holley)**

   We determine enthalpies and entropies of formation of minerals (Synthetic Mineral Standards) for use in calculations of multi-component equilibria in geothermal systems.

   We determine enthalpies of formation by measuring heats of solution of minerals, and their component oxides. We do this in a molten oxide solvent in a calorimeter. With auxiliary data, we calculate enthalpies of formation. Entropies of formation are calculated from measured values of mineral heat capacities.

3. **Synthetic Minerals (C. C. Herrick)**

   We prepare synthetic minerals for equation-of-state research, thermodynamic property determinations, single crystal experiments, and surface transport and nuclear waste migration investigations.

4. **Geochemical Calculations (C. C. Herrick)**

   We use computer modeling when the number of experimental variables is too great for individual measurements, experimental conditions lie in inaccessible depths (pressures), and to refine and extend current theory. We expand the data base of an existing mass transfer code (PATHCALC) for nuclear waste applications, interpret the skull melting process using a complex equilibrium code (SOLGASMIX), and predict material integrity using a finite element code (TSAAS).
Contractor: LOS ALAMOS SCIENTIFIC LABORATORY
University of California
Los Alamos, New Mexico 87545

Contract: W-7405-ENG-36

Title: II. Solar-Terrestrial Physics

Person in Charge: G. A. Keyworth

Scope of Work

The solar wind, solar corona, earth's bow shock and magnetopause provide a unique plasma in which any spacecraft approaches a truly nonperturbing diagnostic probe. The solar wind is also the medium through which disturbances propagate and, thereby, couples near-earth environment to solar variations. Scope of this project is to analyze and interpret existing satellite data to yield information and understanding of: (1) nature and long-term effects of sun-earth coupling through the solar wind, (2) processes that determine heavy ion abundances and charge states in the solar wind, (3) evolution and saturation of heat flux regulating mechanisms as well as ion beam and anisotropy-driven instabilities, and (4) sources of free energy in particle velocity distribution in earth's magnetically confined upper atmosphere. Relations to DOE's missions include applications to: (a) plasma physics and MHD problems relevant to fusion energy technology, (b) understanding long-term solar wind and earth climate variability, and (c) future space-based energy technologies.


We made progress in understanding kinetic phenomena which actively regulate the internal state of the interplanetary plasma near earth. Significant results are: (1) solar wind heat flux near earth does not depend on local temperature gradient, but is limited by combined action of proton-electron Coulomb collisions and wave-electron interactions. A general form for a heat transport closure relation for the Vlasov moment equation characterizes solar wind electron parameter variations near earth, (2) general ion velocity distributions measured in the high-speed solar wind are linearly unstable yet belong to a special class of nonlinear plasma equilibrium.
Scope of Work

Objectives of this program are twofold: (1) to apply physical chemical methods to study of speciation, equilibria, and thermodynamics of systems identified as important to development of hydrothermal resources and (2) to provide phase equilibria and crystal growth data for P-T-X conditions simulating crystallization of magma systems in the upper crust of the earth. Aqueous processes upon which we focus are: ionization of water, ionization and polymerization of silicic acid, fluorosilicate equilibria, carbonate ionization equilibria and solubility of silica in concentrated brines. Methods most commonly used are: potentiometric, isopiestic, and phase equilibrium. In addition, we will model common igneous rocks (e.g., gabbros, basalts, granites, and rhyolites) using chemically simplified bulk compositions in the system SiO₂-Al₂O₃-MgO-FeO-CaO-Na₂O-K₂O-0₂-H₂O. After obtaining data on model systems small concentrations of components of special interest can be added to observe their specific effects. A variety of analytical techniques is used to identify and characterize experimental products. Routine phase identification will be made with standard petrographic and x-ray diffraction techniques. Chemical characterization of constituents requires use of electron and ion microbeam techniques.

A. Carbonic Acid Ionization Equilibrium (R. H. Busey, C. S. Patterson, R. E. Mesmer)

Carbon dioxide is present under considerable pressure in many hydrothermal brines and its ionization reactions are likely pH controlling. The flowing potentiometric cell has been reactivated to study the first ionization equilibria of carbonic acid at temperatures from 50° to 300°C and in NaCl solutions of ionic strength 0.2, 0.5, 1.0, 3.0, and 5.0 m. Precise analysis of the CO₂-HCO₃⁻ content of solutions caused considerable difficulty. In 1.0 m NaCl the logarithm of the equilibrium quotient has values -5.900, -5.912, -6.111, -6.390, -6.709, and -6.986 at 50°, 100°, 150°, 200°, 250°, and 295°C respectively. Effect of salt is to shift equilibrium toward greater ionization with increasing salt concentration, e.g., at 150°C log Q = -6.111 in 1 m NaCl and log Q = -5.919 in 5 m NaCl. We also determined pressure coefficient of ionization equilibrium under all conditions of salt concentration and temperature except at 300°C. Work is now in progress on the second ionization equilibrium. These data on ionization reactions will make possible accurate calculation of pH of natural brines and calculation of solubility of CaCO₃ and other phases in such brines.
B. Thermodynamics of Geothermal Brines (H. F. Holmes and R. E. Mesmer)

Using the isopiestic method (in a BES project "Aqueous Chemistry and Thermodynamics at Elevated Temperatures and Pressures"), we determined information needed to calculate activities of all major components in geothermal brines in the Salton Sea field (NaCl, KCl, and CaCl₂). Measurements extended to 200°C and can be extrapolated to 250°C or 300°C. We now have values for γ°NaCl, γ°KCl, and γ°CaCl₂ in pure salt solutions and interaction coefficients εK-Ca at temperature from the value at 25°C. Now activity coefficients of these components can be calculated with an uncertainty of a few percent.

C. Phase Equilibria and Crystal Growth in Magmatic Systems (M. T. Naney)

Laboratory apparatus was assembled to perform 1 atm high temperature experiments to 1400°C. Initial 1 atm experiments to determine the liquidus temperature of six iron- and magnesium-free synthetic rock compositions (two rhyolitic, four basaltic) were performed. The liquidus phase for both granitic compositions is plagioclase, and olivine is the liquidus phase for basaltic compositions. Engineering specifications have been written for purchase of a pressure vessel and gas intensifier system. This apparatus will permit experimentation at pressures to 414 MPa and temperatures to 1400°C simultaneously.

D. Kinetics of Silica Deposition from Brines (E. G. Bohlmann and P. Berlinski)

Supersaturated brines were passed through columns packed with several forms of silica (crystalline α quartz, polycrystalline α quartz, and porous Vycor). Also, silica deposition on ThO₂ microspheres and titanium powder was studied under controlled conditions of supersaturation, pH, temperature, and salinity. Residence time was varied by adjustments of flow rate and column length. Silica contents of input and effluent solutions were determined colorimetrically by a molybdate method.

We observed: (1) essentially identical deposition behavior was observed once the substrate was thoroughly coated with amorphous silica and the BET surface area of the coated particles was taken into account; (2) reaction rate is not diffusion limited in columns; (3) silica deposits for a solution containing only monomeric Si(OH)₄; (4) deposition on all surfaces examined was spontaneously nucleated; (5) dependence on supersaturation concentration, hydroxide ion concentration and temperature were determined.
Scope of Work

The Magma Energy Research Project assesses scientific feasibility of extracting energy directly from buried magma sources. This resource has potential to provide high quality thermal energy or gaseous fuels. The project is divided into four major research tasks:

A. Magma Source Location and Definition,
B. Magma Source Tapping,
C. Magma Characterization and Material Compatibility, and
D. Energy Extraction

Definition and characterization of magma chambers also provide information on heat sources for geothermal systems and may provide insight into location of mineral resources. Consequently, background from magma energy research provides preliminary studies on drilling and magma-hydrothermal geoscience for the Continental Drilling Program.

A. Magma Source Location and Definition

A series of geophysical sensing experiments were performed in 1976 on Kilauea Iki Lava Lake where a defied body of molten rock exists.

The 1976 experiments were:

(1) Dipole-Dipole Electromagnetic Induction Experiments (Frischknect, Zablocki),
(2) Very Low Frequency Radio Wave Methods (Zablocki, Anderson),
(3) Galvanic Four-Electrode Resistivity Soundings (Zablocki, B. Smith),
(4) Audio-Frequency Magnetotelluric Profiling and Sounding (Bostick, S. Smith, Boehl),
(5) Passive Monitoring of Seismic Noise (Aki, Chouet, Colp),
(6) Teleseismic Measurements (Aki, Chouet),
(7) Small-Scale Seismic Refraction Experiments using Artificial Charges (Aki, Chouet)

Analyses of these experiments showed that passive seismic and VLF electromagnetic measurements agreed within 25-50 m in definition of the edge of the molten lens. Geophysics measurements did not define vertical extent of the
molten lens. However, a combination of results from seismic, magnetotelluric and electromagnetic measurements has been combined with drilling data and information from other lava lakes to develop a model of the vertical lake structure.

To better interpret results of geophysical measurements, a series of six holes was drilled in the lava lake during December 1978 through January 1979. Preliminary results from drilling and associated experiments are:

1. The crust consists of an upper 41 m zone of two-phase convection with a sharp temperature discontinuity at the bottom of the two-phase zone. Depth of this discontinuity can vary by 2 m depending on rainfall and time of day. Upper crust permeability measured at 0.3 Darcy agrees with that obtained in heat transfer calculations.

A conduction zone at least 12 m thick lies below the 41 m region.

2. Temperature profiles in the 12 m thick conduction zone had a curvature that can be explained in terms of a moving solidification front, conduction solution. Recent temperature profiles show the predicted curvature has reversed suggesting that solidification is almost complete.

3. A zone of melt stringers is encountered at depths of 45-50 m. Below 50 m, the formation becomes plastic and appears to contain a high viscosity melt with solids. A core sample at 62 m, 1052°C contained 40% olivine crystals.

4. A hole drilled through the frozen edge showed the lake depth to be 95 m whereas depth estimates from topographic maps were 70 ± 3 m.

Analyses of data have just started but information on hydrothermal circulation, mechanism of freezing of molten rock bodies, and characterization of magma bodies by heat flow measurements were obtained.

B. Magma Source Tapping

Magma source drilling and well completion studies include borehole stability studies and limited drilling technology development in support of the lava lake geoscience experiments.

Borehole stability studies are currently focused on measurements of strength of igneous rocks to 1000°C and 4 kbar at the Center for Tectonophysics at Texas A&M University. Strengths of granodiorite and andesite samples decrease as temperature increases, but brittle fracture occurs even at high temperature. Results imply the rock will be drillable with conventional methods up to partial melting and that the borehole may or may not remain open depending on the stress distribution. Spalling at 2-3 km at temperatures of 700-1000°C is possible.

Four penetration concepts developed for drilling into the lava lake were evaluated during experiments at Kilauea Iki. The concepts included: a penetrometer to push through soft rock into liquid, jet core and jet drag bits that use high velocity jets of water to freeze a foam structure ahead.
of the cutting surface and an insulated drill-string-drag bit concept that would operate at the temperature of the formation. Prototype designs were evaluated in laboratory testing but were not fully evaluated at the lava lake since a low viscosity melt was not encountered. However, both the jet bits successfully drilled through 4 m of liquid stringers and plastic rock where conventional drilling had failed. Extensive torque, load and speed data were obtained to aid in the design of new drilling concepts.

C. Magma Characterization and Material Compatibility

The internally heated 4 kbar pressure Magma Simulation Facility is completed. Studies initiated to measure chemical and physical properties of molten rock containing dissolved volatiles and to study compatibility of metals with simulated volatile-containing magma. The facility can maintain large volume samples (~750 cm$^3$) at uniform temperatures to 1500°C and pressures to 4 kbar. A variety of electrical sensors are present for property evaluation. Initial experiments underway include measurements of viscosity and electrical conductivity of simulated magmas.

A comprehensive thermodynamic study of volcanic gas collection data has been completed. This study provides a data base of 100 corrected volcanic gas analyses for samples collected in close association with active lava at temperatures in excess of 950°C. Thermodynamic modeling studies are also underway for C-O-H-S-C1-N magmatic gases at pressures and temperatures up to 5 kbar and 1400°C. Results apply in simulating magmatic environments for materials development research. This thermodynamic base and methodology has been used to show the organohalogenes noted in the 1977 Kilauea eruption came from decomposing plant matter and were not evolved from the magma source. The calculations also identify conditions conducive to generation of abiogenic methane, a possible new fuel resource.

Compatibility of some pure metals with molten basaltic lava (Kilauea - 1971) was determined at 1150°C. A cover gas was used to simulate oxygen and sulfur fugacities calculated to exist in actual lavas. Exposures were made for 96 hours during which extensive reaction was observed for Fe, Ni, W, Pd, Rh, Ti, Zr, Nb, and V; moderate reaction was observed for Cr, Co, and Ta; and virtually no reaction was noted for Mo, Re, and Pt. Metals undergoing extensive corrosion reacted to form sulfides (Fe, Ni, Pd, Rh), oxides (W), oxides and sulfides (Nb, V) or oxides, sulfides and silicates (Ti, Zr). Reaction mechanisms are being determined and compared to predictions based on thermodynamic stability diagrams. Future work will concern binary alloys and commercial superalloys.

D. Energy Extraction

Two methods of energy extraction being considered include generation of steam for subsequent conversion to electricity and generation of gaseous fuels ($H_2$, $CH_4$, $CO$, etc.) by decomposition of water-biomass systems.

Previous laboratory experiments in basalt at 1450°C-1650°C under isothermal conditions gave heat extraction rates of 180-300 Kw/m$^2$. During the 1977 eruption of Kilauea, heat transfer measurements made in a 1090°C
Eddy of the lava river gave heat transfer rates decreasing from 200 Kw/m² to an asymptotic value in the range of 5-10 Kw/m². Measurements made in the conduction region of the lava lake through a cased hole gave heat extraction rates of 10-20 Kw/m². The unexpected high values are believed due in part to water circulation on the outside of the well casing, thereby suggesting energy extraction from the conduction zone above a magma body may be feasible.

A long tube heat exchanger, 0.010 m dia. x 12 m long, was assembled and used to evaluate the thermal and hydrodynamics in a system with significant hydrostatic head variation as might be experienced in extracting energy from magma sources. Operation with stable conditions was obtained at hydrostatic pressure variations up to 190 kPa, water flow rates of 0.06 to 0.6 l/s and heat flux rates from 0 to 50 Kw/m². Results indicate that a closed loop exchanger concept is a technically feasible method of energy extraction from high energy density fields.

Thermodynamic calculations of the generation of gases from water and cellulosic material in contact with basaltic magma bodies indicate gases at 600°C and 100 MPa would contain 1-10% CH₄, 1-2% H₂ and about 0.1% CO. Hydrogen generation is enhanced by higher temperatures and water reduction by the ferrous materials in the melt.

E. Continental Drilling Program

The Continental Drilling Program requires completion of diagnostic wells that penetrate through hydrothermal regions into magma for scientific studies on sources and heating systems of geothermal resources. A workshop of geoscientists, geoinstrumentation experts and drilling engineers was held to define potential drilling environments and to assess state-of-the-art drilling and instrumentation technology as it applies to continental drilling.

Studies in conjunction with the Magma Energy Research Program, other BES-sponsored geoscience workshops and other geothermal programs at Sandia continue to develop a plan for deep drilling, instrumentation and geosciences of the magma-hydrothermal region.

PART II

GEOSCIENCES

OFF-SITE
Contractor: UNIVERSITY OF ALASKA
Geophysical Institute
Fairbanks, Alaska 99701

Contract: EY-76-S-06-2229 005

Title: A Study of the Magnetic Field Annihilation Process in the Magnetosphere and Some Applications (Electric Currents in the Trans-Alaska Pipeline Induced by Auroral Activity)

Person in Charge: Syun-Ichi Akasofu

Scope of Work

The magnetic field annihilation process is believed to be one of the basic processes in cosmic electrodynamics, releasing a considerable amount of energy in terms of kinetic energy of plasma particles. The magnetospheric substorm is known to be such a process and takes place around the earth, where in situ satellite measurements of plasma quantities are possible. Therefore, it is logical to study the magnetospheric substorm as a first step toward a better understanding of the annihilation process in other situations, such as solar flares, flaring of stars, Mercury, Jupiter etc.

We have just begun to understand the magnetospheric substorm as a response of the magnetosphere to an increased efficiency of the solar wind-magnetosphere dynamo. In order to match an increased input power generated by the dynamo, the magnetosphere tends to short-circuit a significant part of the generated current from the current sheet in the magnetotail to the ionosphere where the Joule dissipation can take place.

We are currently investigating basic plasma processes which are responsible for short-circuiting the magnetotail current to the ionosphere by a numerical computational method. We are also attempting to understand solar flares in terms of the power generation in the photospheric level, the resulting formation of a current sheet in the lower corona, short-circuiting the current to the chromosphere.

We are also interested in energy related geophysical problems in the Arctic region. We are helping corrosion engineers of the Alyeska Pipeline Company in monitoring amount of aurora-induced electric current in the trans-Alaska oil pipeline, in locating where induced current leaves the pipe and in estimating the expected amount of corrosion. Amount of induced current is typically of the order of a few hundred amperes during medium magnetic activity. During an intense storm, current exceeds one thousand amperes.

Aurora induces also electric currents in power transmission lines. As a result, serious fluctuations of power can occur. We are working closely with the local powerline company in monitoring induced current and in examining performance of a transformer when (quasi) dc currents are induced in power transmission line.
Scope of Work

The Aleutian-Alaska arc system is the result of convergence of two lithospheric plates, where the Pacific plate subducts beneath the American plate. It is the only such system in the United States, as are its associated features such as deep sea trench, shallow thrust zone with high potential for large, tsunamigenic earthquakes, Benioff seismic zone and overlying chain of andesitic volcanoes. A short-period seismic network is operated on the Alaska Peninsula, a portion of the arc system. The net is part of a seismic monitoring system operated by different agencies under various grants, that covers an approximately 1000 km section of the eastern portion of the arc structure. Data from this network are being used to study, comprehensively, seismotectonics and associated volcanism. Data also provide for assessment of seismic and volcanic hazards in an area of high potential for both fossil and geothermal energy sources.
Scope of Work

Our task is to discover the most feasible physical mechanisms by which variable solar activity affects earth's weather and climate. Our first task is to describe the most important relationships in sufficient detail that an attempt can be made to construct a physical model to explain them.

Numerous solar parameters have been used by our colleagues and us to investigate short-term sun-weather effects. Using size of low-pressure troughs integrated over the northern hemisphere as one meteorological parameter, we found that various solar signals give different responses. If the solar signal is such as to increase electromagnetic radiation received by Earth, e.g., a solar flare, cyclonic activity increases. However, flares are characteristically followed by geomagnetic storms, within a few days, and the geomagnetic storm is associated with a sharp decrease in cyclonic activity. Thus when a large flaring region on the sun approaches the central meridian of the sun, earth's cyclonic activity increases, but shortly after when the region passes by the central meridian and magnetic storms occur, cyclonic activity declined to a minimum.
Contractor:  BROWN UNIVERSITY
Geophysical Laboratory
Department of Geological Sciences
Providence, Rhode Island 02912

Contract:  DE-AC02-79ER10401

Title:  Application of Natural Electromagnetic Field Methods
(Magnetotellurics/Geomagnetic Variations) to Exploring for
Energy Resources: Development of a Broad-Band Data
Acquisition/Processing Facility

Person in Charge:  John F. Hermance

Scope of Work

Geophysics is playing a central role in meeting the challenge of the
emerging energy crisis both in the exploration for new resources and in
re-evaluation of already discovered resources. Among geophysical methods
available, increased use is being made of natural electro-magnetic methods, such
as magnetotellurics and geomagnetic variations, which in principle have positive
advantages in delineating sub-surface structural features associated with
distribution of potential energy resources (oil, gas, geothermal, uranium) along
with evaluating possible sites for deep containment of nuclear waste.

We are assembling a magnetotelluric field system for the purpose of
improving precision with which one can estimate electromagnetic parameters of
the earth. Moreover, we plan on performing on-site computer processing of the
raw data using a small mini-computer. The system is designed on the basis of
achieving (a) higher data quality, (b) wider frequency band coverage ($10^4$ sec
to $10^3$ Hz), (c) on-site data processing, (d) computer generated graphical
displays of data parameter on maps of the survey area while the field system is
on-site, (e) minimal turn-around time from making the measurement to final data
analysis. We are encouraging other research groups to consider using our
facility as part of their own on-going research programs.
Scope of Work

This laboratory conducts research in rare gas mass spectrometry where the broad objective is to read the natural record which isotopes of the rare gases comprise as trace constituents of natural gases, rocks, and meteorites. A new program is to design, construct, and operate apparatus which will analyze elemental and isotopic composition of rare gases from fluid sources in the field, at or near the sampling site. Long-range scientific goals are to search for additional manifestations of primordial gases and to see how they relate to convection patterns within the earth. Rare gases from steam wells and other geothermal energy sources will also be examined with particular interest in assaying proportions of recycled atmospheric gas versus radiogenic gas. While instrumentation for field studies on fluids is being fabricated, we are working with volcanic xenoliths and megacrysts and suboceanic volcanic basalts to determine what information the rare gases can provide about their genetic relationships and about the out-gassing sequence of magmas. We have also observed interesting isotopic and elemental patterns in these volcanic samples, and are trying to determine from these patterns the primordial and radiogenic rare gas components of the mantle.

We also study isotopic inhomogeneities, such as we observe in the carbonaceous chondrites. It is likely that they originate because of incomplete isotopic mixing of fractions with different histories of nucleosynthesis.

There is currently emphasis in our work on the carbonaceous, acid-resistant residues in chondritic meteorites which, although they represent less than one percent by weight of the stones, carry virtually all planetary gases trapped in these objects. Very markedly anomalous isotopic patterns for argon, krypton, and xenon are observable in these residues after the bulk of the gases has been released by selective chemical treatments. In collaboration with cosmochemists at NASA's Ames Laboratory we try to locate trapping sites for these gases in fine-grained residues by various means--chemical treatments, colloidal techniques, and density separations.
Scope of Work

In general, effects of pressure on rock microstructure and interaction of acoustic waves with rock microstructure are extremely important in several shallow crustal problems of geophysical significance (e.g., fluid transport properties in geothermal area, earthquake prediction). More specifically, delineation of the statistical interrelationships of rock properties will help develop a useable geophysical understanding of the mechanisms involved in such problems. Toward this end, we are pursuing four separate, but related lines of investigation:

1. Correlation of elastic moduli-pressure behavior with observed petrography.
2. Statistical parameterization of observed rock microstructure for use as a modeling parameter.
3. Inversion of elastic moduli data into crack spectra.
4. Relation of measured permeability to both observed and calculated rock microstructure.

Preliminary results of these studies indicate that several phenomenological correlations exist and continued work is developing a greater physical understanding of them. From this, laws for statistically averaging effects of finite densities of real rock microstructure on bulk rock properties can be established.
Scope of Work

The pressure volume temperature equation-of-state has been measured with high precision for NaCl at hydrostatic pressures up to 32 kbar and temperatures up to 500°C. The measurement is a differential length change measurement between a one-inch long single crystal of NaCl and a tungsten carbide standard using a simple electrical contact piezometer. Length change of tungsten carbide is small compared to that of NaCl and high accuracy is obtained.

Results show a lower compression of NaCl at room temperature than the frequently used Decker equation. At high temperature good agreement with Decker is obtained. The zero pressure bulk modulus and its pressure derivatives agree with ultrasonic measurements.

The pressure dependence of the Grüneisen parameter of quartz, quartzite and fluorite have been determined up to 35 kbars using a pressure pulse method. Hydrostatic pressure in the sample is abruptly increased and \((\partial T/\partial P)_S\) is measured as a function of pressure. The Grüneisen parameter is then calculated from the thermodynamic relationship \(\gamma = K_s/T (\partial T/\partial P)_S\) where \(K_s\) is the adiabatic bulk modulus. Difference between isothermal and adiabatic bulk modulus is very small for quartz and fluorite and we use isothermal compression data to 30 kbar for our calculation.

The relationship between \(\gamma\) and volume can be expressed by \(q = -(\partial n\gamma / \partial n V)_T\). Values of \(q\) of .64, .99 and 4.3 were obtained for quartz, quartzite and fluorite respectively.

Similar measurements of \((\partial T/\partial P)_S\) were made on sodium and potassium at room temperature (297°K). For both metals a large decrease in the value of \((\partial T/\partial P)_S\) is observed as the pressure increases. Values of \(q\) of .8 ± .1 for sodium and 1.4 ± .3 for potassium are obtained.
Contractor: COLUMBIA UNIVERSITY
Lamont-Doherty Geological Observatory
Palisades, New York 10964

Contract: EY-76-S-02-3134 B

Title: A Comprehensive Study of the Seismotectonics of the Eastern Aleutian Arc and Associated Volcanic Systems

Persons in Charge: J. Davies, K. Jacob, L. Sykes

Scope of Work

This comprehensive study of the seismotectonics of the eastern Aleutian arc is aimed at providing a solid data base and a detailed understanding of the basic tectonic processes in an active arc and its associated volcanic systems. The emphasis is on using information contained in seismicity and seismic waves to (1) delineate major modes and structures associated with subduction of the Pacific plate beneath the arc; (2) understand associated deformation within the arc-trench gap; and (3) monitor magmatic and eruptive activity of several volcanoes along the arc with regard to assessing their potential for geothermal energy. For these purposes we operate a telemetered seismic array in the Shumagin Islands segment of the eastern Aleutian arc (15 stations), a dense array on Pavlof Volcano (12 stations), a small array (3 stations) near Dutch Harbor which also monitors two volcanoes (Makushin and Akutan), and a single station on St. Paul, in the Pribilof Islands. Results from companion studies using mean-sea-level measurements, geodetic leveling, and geologic surveys of raised terraces and beaches are used together with collected seismic information (i.e. fault plane solutions, stress drop determinations) to obtain a detailed picture of state and variability of strains and stresses across the arc. Latest results suggest that the arc segment near the Shumagin Islands is in a state of high compressive stress, particularly near the down-dip end (40 km depth) of the major thrust zone which usually ruptures during large (M >7) earthquakes. This high stress appears to be transmitted to the volcanic arc, and may be responsible for the rather high level of eruptive activity of volcanoes within this arc segment. Seismic data also have direct application to identifying shallow tectonic structures in fore-arc and back-arc basins which may be important for seismic engineering purposes in connection with petroleum exploration in the coastal region of the Alaska Peninsula and the adjacent continental shelf.
Scope of Work

Permeability of jointed Barre granite, Cheshire quartzite and fused silica was measured at pressures up to 3 kilobars. Jointed samples were split cylinders with surfaces prepared to various roughnesses by grinding with 120-grit, 310-grit, or 600-grit polishing compounds. A profile meter shows that surfaces prepared with the same grit vary between the rougher granite and smoother fused silica. Joint permeability and joint aperture change with pressure and are sensitive to initial surface roughness. The granite joint is more permeable than the fused silica joint. For closed joints (aperture <30 µm) the parallel plate model for fluid permeability \(k \propto d^2\) breaks down. Once a joint is subject to pressures in excess of 1 kbar, pore pressures high enough to lower the effective pressure to less than 0.5 kbar are necessary to open the joint appreciably.

Permeability is not a simple function of difference between confining pressure \(P_c\) and internal pore pressure \(P_f\). At a particular \(P_c\), the volume flow rate, \(q\), is proportional to \((P_c - P_f)^{-n}\). Increasing surface roughness of the joint decreases the volume of \(n\).

Using apparent cross-sectional area of the joint based on joint closure measurements, the apparent joint permeability is a function of both joint aperture and pore pressure. Changes in pore pressure affect changes in aperture and permeability that conform with a power law between fracture permeability and aperture.
Scope of Work

We are developing and applying several seismic methods for determining structure of geothermal energy source regions, such as magma reservoirs and conduits in a volcano or a hydrofractured crack of a hot dry rock geothermal system. We are taking a dual approach based on active and passive experiments.

In the active experiment, we use an artificial source such as a buried explosion and study seismic velocity, attenuation and scattering under different conditions of liquid pressure in the system. Theoretical work is done on scattering, reflection and attenuation of seismic waves by a finite crack filled with viscous fluid. Results are used in interpreting seismic data obtained at the Kilauea Iki Volcano, Hawaii and at the Fenton Hill Hot Dry Rock Geothermal Site, Los Alamos, New Mexico, for defining location, shape, and size of fluid-filled cracks. At Kilauea Iki, we found a thinner and more viscous magma lens than previously thought. At the Fenton Hill, we found evidence suggesting that the crack may be a complex system of multiple cracks.

In the passive experiment, we use seismic signals generated from the geothermal energy source region to determine physical parameters of the geothermal system. Theoretical work includes seismic motion due to magma transport through cracks and synthetic seismograms for a tensile crack source in a layered half-space. These results were used to interpret volcanic tremor data from Kilauea Volcano and seismic events from Kilauea Iki and Fenton Hill. We found, for example, that source parameters of Iki events agree with the explanation that they represent a process of columnar joint formation.

A new method for determining frequency dependence of seismic attenuation has been developed. The method applies to an area with some microearthquake activity, and is based on combined use of direct body waves and coda waves. This method is being interfaced to our microprocessor system connected to a network of digital event recorders.
Scope of Work

Many physical properties of rocks (such as hydraulic permeability, compressibility, electrical conductivity, and velocities of sound waves) are controlled largely by cracks present. We developed methods with which to characterize microcracks in rocks. We use the scanning electron microscope and petrographic microscope to determine morphology, spatial and temporal relationships, and degree of sealing. Energy dispersive systems and the electron microprobe are used to determine elemental composition of host grains, crack sealing minerals, and small grains dispersed along sealed cracks. Differential strain analysis (DSA) yields information about open microcracks - orientation of sets of cracks, distribution of linear and volumetric crack porosity with respect to closure pressure of individual cracks.

We are examining microcracks in suites of rocks from two geothermal areas, Coso and Raft River. We are also collecting samples for study of microcracks in coal gasification projects and in the eastern gas shale project.
Scope of Work

A. Velocities and Attenuation in Dry and Wet Geothermal Conditions

Compressional and shear wave velocities were measured in water-filled Berea sandstone as a function of pore pressure, with a constant confining pressure of 300 bars. Measurements were made at 145°C and 198°C. At 145°C, compressional velocity increased from vapor saturated (low pore pressure) liquid saturated (high pore pressure) conditions, whereas shear wave velocity decreased. For compressional waves there was a velocity minimum and increased attenuation near the liquid-vapor transition. Results at 198°C show decreases of both compressional and shear velocities and a small velocity minimum for compressional without marked attenuation. At both temperatures, $V_p/V_s$ and Poisson's ratios increased from steam to water saturated.

Results are compatible with mechanical effects of mixing steam and water in pore space near the phase transition and may be applicable to in situ geothermal field evaluation.

B. Microcracking and healing in the Earth's Crust

In a study of the cathodoluminescence (CL) of quartz in granites and pegmatites we discovered that quartz luminesces blue. Many blue luminescing quartz grains have red luminescing structures within them. These red structures are often in linear, elongated domains, which are indistinguishable under the microscope with either ordinary or polarized light.

We interpret domains of red CL quartz as lower temperature filling of microfractures and open subgrain boundaries in deformed higher temperature blue CL grains. The combination of secondary fluid inclusions, formed at depth 8-10 km, and red luminescing quartz domains suggests a continuous process of cracking and healing in the crust. Thus cracking and healing may be much more abundant and common in crustal rocks than previously thought. This conclusion has important bearing on the evolution of quartz and feldspars, in the crust particularly for problems related to pore pressure and transport such as metamorphism, rock physical properties and deep seated geothermal energy potential.
Scope of Work

This investigation concerns mobility of major, minor, and trace elements during contact metamorphism of carbonate rock. Large contrasts in chemical potentials of \( \text{SiO}_2 \), \( \text{Al}_2\text{O}_3 \), and \( \text{CaO} \) across a granitic pluton-limestone contact may induce metasomatism and calc-silicate skarn formation. In addition, rare earth and transition metal elements may act as tracers, and their redistribution during metamorphism may record convective cooling processes.

The late Jurassic Notch Peak Intrusive, a porphyritic quartz monzonite body is intrusive into Cambrian limestones and shaly limestones in western Utah. The Notch Peak intrusive discordantly intersects nearly all depositional environments of a carbonate platform edge and outer shelf of Cambrian age. This is thus an ideal area to study metamorphic changes in carbonate rocks. Outcrop is excellent, the stratigraphy varied and already mapped, and the petrology of part of the unmetamorphosed section has recently been studied in detail. Topographic relief of over 1000 meters permits comparative studies of effects of heat transfer and movements of solutions both parallel to and perpendicular to bedding.

Results of this study may have an application toward radioactive waste disposal and the degree to which radioactive nuclides may be expected to migrate during geologically significant periods of time.
Scope of Work

The primary goal of our research is to determine the fracture state and fracture stress under simulated conditions at depth where thermally activated processes are expected to play a major role. We will determine experimentally the boundary in P-T-e-σ space between elastic-brittle and transient-semibrittle behavior for selected isotropic and anisotropic crystalline rocks deformed in both hydrous and anhydrous environments. We focus on (1) transient creep flow laws and macroscopic fracture criteria which include effects of thermally activated processes; and (2) physical nature of fractures, to the atomic level, in the semibrittle regime and comparisons of the results with naturally deformed rocks.
Components of natural gas are reactive in the deep subsurface and may not survive under all conditions. Stability of natural gas in reservoirs of various lithologies is being studied using a combined theoretical and experimental approach.

A. Theoretical: A computer program was developed to calculate equilibrium in multicomponent (up to 70), multiphase (solid-liquid-gas) systems simulating subsurface conditions to 40,000 ft. Results show significant differences for survivability of methane in reservoirs of different lithologies. Role of sulfur compounds and graphitic residues is examined.

B. Experimental: A gas chromatograph for analyzing gas mixtures containing both organic and inorganic components is installed. Suitable deep wells have been identified and sampling procedures are being developed. Analytical results for gas composition in deep samples will be compared with those predicted by the computer simulations.
Contractor: WOODS HOLE OCEANOGRAPHIC INSTITUTION  
Woods Hole, Massachusetts 02543

Contract: EG-77-S-02-4392

Title: Organic Geochemistry of Outer Continental Margin and Deep Ocean Sediments

Person in Charge: J. M. Hunt

Scope of Work

Approximately 70 cuttings samples of fine-grained shale from two Gulf Coast stratigraphic tests, South Padre Island and Mustang Island, were analyzed by thermal distillation-pyrolysis gas chromatography supplemented with mass spectrometry. The objective was to determine changes in concentration of individual hydrocarbon classes over a depth range from about 3000 to 16,000 feet. In both wells, the threshold of intensive hydrocarbon generation, as determined by thermal distillation, appears to start at around 10,000 feet. Generation peaks at about 14,000 feet. Distribution of n-paraffins in the C_7-C_{14} range with depth shifted from peaking at n-C_7 at 10,200 feet to peaking of n-C_{11} at 15,700 feet. Also, distribution of n-paraffins broadened with depth. Shifting of the peak yield is due to a combination of later generation of higher molecular weight hydrocarbons (C_9-C_{14}) plus migration of lighter hydrocarbons (C_7-C_8) from source rock. Aromatic hydrocarbons, benzene through xylenes (C_6 through C_8) followed the same trend with C_6 peaking around 11,500 feet and C_8 around 13,500 feet. These data indicate that migration and generation are simultaneous and are causing a natural separation of hydrocarbons of different molecular weights. These results are from thermal distillation of free hydrocarbons in the rock matrix. Hydrocarbons complexed to kerogen also will be studied by pyrolysis-GCMS.
Scope of Work

Experiments show that a zone of dilatation forms around an opening mode crack advancing through rock. The extent of the zone of dilatation determines the amount of rock debris produced by the advancing crack and the amount of new surface area present in the rock after passage of the crack. The relation between rock microstructure, crack-induced dilatation and fracture toughness is being examined with stable crack growth experiments in the laboratory. Some experiments will be done in the presence of water so that stress-corrosion effects that may occur in the earth will be detected. The susceptibility of diluted material adjacent to the crack path to solution will be determined. It is intended to relate these characteristics of crack growth in rock to the microstructure--the size and distribution of mineral phases and the distribution of microcracks in the rock--and to compare them with the observed structure of joints in the field. The results should prove useful in evaluating the fracture characteristics of a rock formation from its structure as determined from core or other samples, as well as contributing to understanding of the basic mechanics of opening mode crack growth in rock.
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