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Energy & Environment Division

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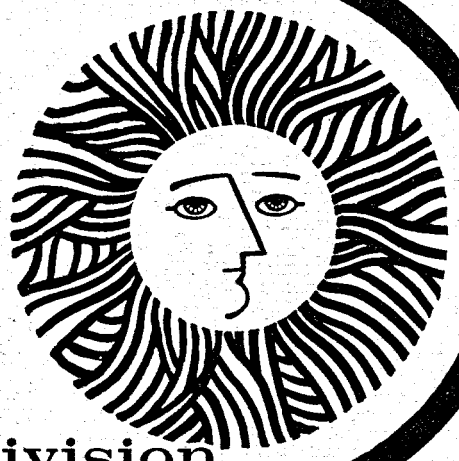
Annual Report 1976



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ANNUAL REPORT

1976

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Energy & Environment Division

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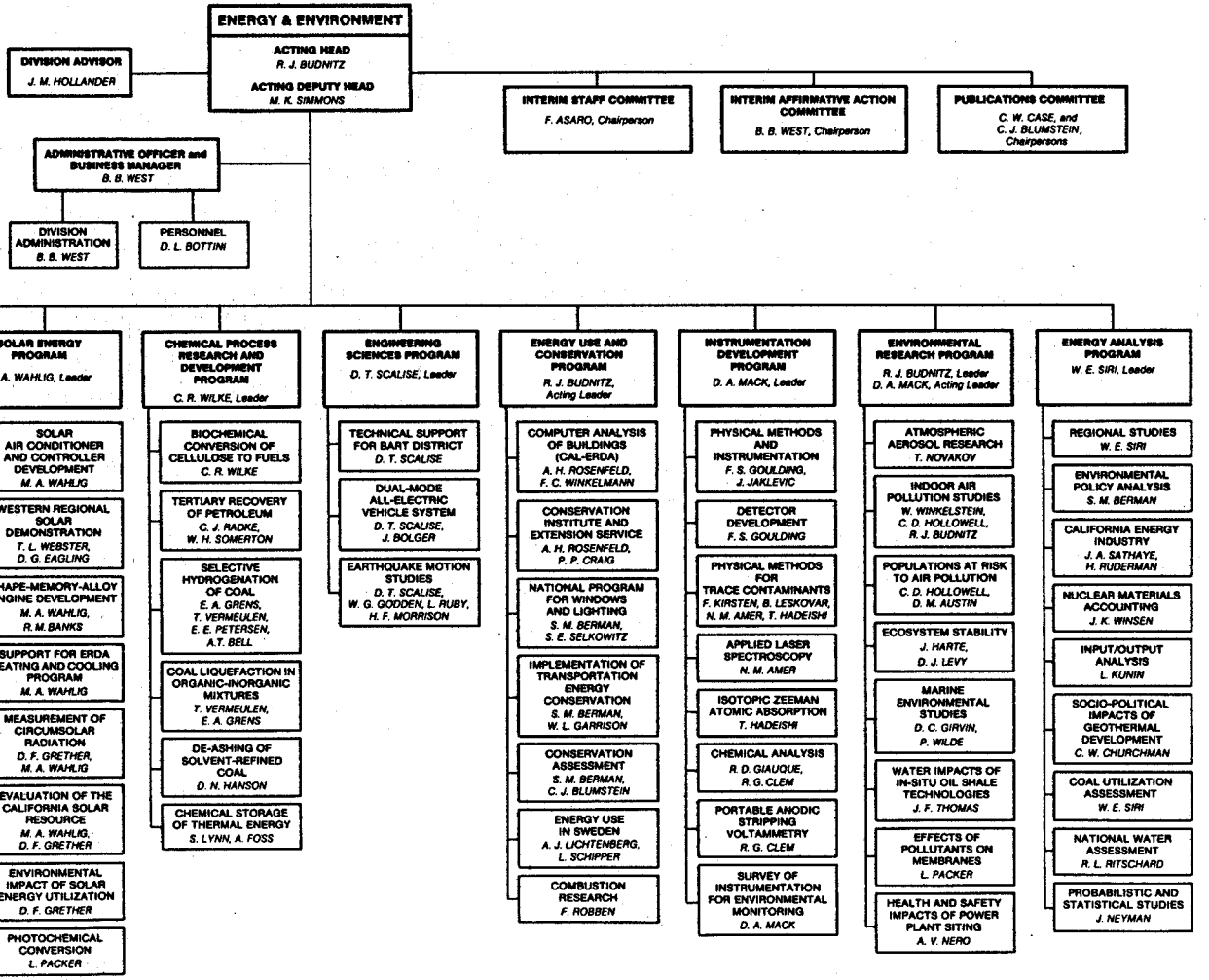

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Geothermal and Geosciences Program

INTRODUCTION

The program of research, development and demonstration in geothermal energy and the geosciences in the Energy & Environment Division continues to expand. New programs have been started and new management responsibilities have been undertaken in the development of this important energy resource and in the growth of fundamental information in the geosciences which will serve a wide range of energy requirements.

There are three major project categories in the geothermal energy program. One is resource assessment, which includes projects on geothermal exploration technology, airborne remote sensing surveys, and the geothermal assessment of lake bottoms. Another major category is the development of field measurement techniques and modeling data analysis methodologies for various geothermal aspects, including land subsidence, variable flow rates in wells, numerical modeling of cyclic storage, interpretation of data from wells at Raft River Valley in Idaho, and the development of a general thermodynamic computer code for simulating power plant cycles. The final category is organization and management. This year LBL assumed management responsibility for the ERDA Geothermal Component Test Facility (GCTF) at East Mesa in the Imperial Valley of California. Also, a management document titled Geothermal Subsidence Research Program Plan is being prepared.

An additional supporting project, the National Geothermal Information Resource (GRID), is charged with assembling data on references for geothermal energy. By the publication of manuals and the operation of a computer data base, this project provides information to all parties interested in geothermal energy.

The several programs in the geosciences form two main categories. One includes scientific studies in brine thermodynamics, earthquake prediction using radon, high precision mass spectrometry, properties of silicate liquids, and rare earth elements in lavas. Another category includes reservoir dynamics, properties of rock-fluid systems, in-situ stress measurements and properties of soils and soft rocks, and stress flow behavior in fractured rock systems.

ERDA GEOTHERMAL COMPONENT TEST FACILITY

J. Angevine

INTRODUCTION

On December 20, 1976, the ERDA Geothermal Component Test Facility (GCTF) began limited operation after 18 months of preparation. GCTF is located on the East Mesa geothermal anomaly of California's Imperial Valley, 20 miles east of El Centro. Originally a project of the U. S. Bureau of Reclamation (USBR), the responsibility for organization and management of the Facility was delegated to the Lawrence Berkeley Laboratory by ERDA during the year.

Conceived by LBL and USBR as the first location open to industry for full scale component tests, construction was started in 1975 by USBR under an interagency agreement carrying funding of $1,040,000 from ERDA. LBL was asked by ERDA's Division of Geothermal Energy to participate as technical advisor to USBR in May 1975. Original plans called for a concrete test pad, manifolds for brine from the existing three geothermal wells, a pipeline from one of the wells, a building for a chemistry laboratory and offices, a machine shop, a paved road and fencing. To provide for the necessary cooling tower, LBL wrote the tower specifications and freed additional funds for tower construction by refurbishing surplus tools which were then installed in the machine shop at no charge to the USBR construction budget.

In April 1976 ERDA assigned responsibility for test operations and management to LBL. While construction proceeded under USBR contract, the management plans were developed at LBL. An LBL supervisor was employed to reside at the Facility and ultimately assume responsibility for the service to each experimenter. Protracted construction contract problems delayed opening the Facility to full operation, but limited work became possible on December 20 when two experiments were permitted to occupy the test area and begin setup work in preparation for testing in January 1977.

As part of the LBL responsibility some promotional activities were carried out during the year to make the availability of the Facility known and to encourage use by industry. A display was provided at the First National Geothermal Conference in Palm Springs and an extensive program of visits to industry was undertaken to discuss the potential for the direct use of geothermal energy.

ACCOMPLISHMENTS DURING CALENDAR YEAR 1976

At the beginning of calendar year 1976, the scope of LBL's involvement with the Geothermal Component Test Facility included only technical advice to the Bureau of Reclamation. LBL personnel conducted several site visits during this period.

In April the ERDA Division of Geothermal Energy requested that LBL accept responsibility for operation of the Facility experimental program. A Test Operations Manager, Jack M. Angevine, was assigned to develop the program and on May 25 the first presentation of the proposed plan was made to ERDA. Following numerous coordination trips to the Bureau of Reclamation Lower Colorado Region offices and several drafts, the plan was released by LBL for ERDA approval in October. The plan was further revised and submitted by ERDA to the Bureau in December where it awaits final approval.

In July LBL hired a Site Supervisor, Ron Phillips, to reside at the Test Facility and to be responsible for all services rendered to experimenters. His duties until mid-December consisted entirely of monitoring the construction activities of the Bureau of Reclamation.

Delays in construction under jurisdiction of the Bureau of Reclamation caused a slip in completion of the contracted portion of the Facility from October until December. Several meetings were called by LBL to assist in expediting completion and on December 20 the Facility was ready to accept two experiments for installation. At the end of December two major items remained to be completed by the Bureau before unlimited operation could be attempted. The injection system had not been tested and only 11 of 24 required flexible joints were available for installation in the brine manifolds. A work-around plan was adopted to provide brine to at least the two early experiments. Disposal of brine in the holding pond was being considered as an injection alternative to allow limited operation.

Early in the year an educational and promotional effort was started to acquaint industry with the Facility and to increase awareness of the potential of geothermal resources. The first major activity was a display and information booth at the First National Geothermal Conference at Palm Springs. A continuing activity through the year was a presentation made at more than 75 personal meetings with industry. Contacts were made and pursued with experimenters already under contract to ERDA and preparing to use the Facility.

The industry presentation was prepared by Jim Davey and made to a broad spectrum of energy consumers with emphasis on those with potential for non-electric uses. More than 100 contacts were made, over 75 of them personal visits. Decision-level managers in the food processing, food machinery, sugar beet, chemical, paper/wood pulp, horticulture and dairy industries were introduced to geothermal energy and to the Test Facility. The entire west coast was covered from Seattle to San Diego during this program. Basic introductory information about geothermal energy including availability and economics was discussed with the participants. An extensive mailing list was compiled, and a brochure was distributed which resulted in articles in five publications by the end of the year.

Twelve experimenters who were either already under contract to ERDA or already involved in geothermal research and development were placed on the Facility schedule. Included in this group are eight industrial firms, one university, and three national laboratories. The technologies under development are in corrosion resistance, mechanical energy conversion, and both conventional and direct contact heat exchange.

In December LBL received direction from ERDA to assume responsibility for the chemistry laboratory at the Facility. Plans for implementing this responsibility were not complete at the end of the year.

ACTIVITIES PLANNED FOR CALENDAR YEAR 1977

Early in the year a contract crew will be provided by ERDA to work under supervision of LBL management on site, the Site Supervisor and a Chemistry Laboratory Supervisor to be hired. Initial activities will consist of establishing operating procedures and physically arranging work space while serving the early experimenters. Some supplies, tools and equipment will be procured to provide the level of support necessary to serve experimenters as planned.

In April a full fledged operation should be possible with all experimental space assigned to an active experiment and the full capacity of the Facility in use. This goal is achievable if the Facility is completed to "turnkey" status by the end of February with the injection system operating reliably and all wells and supporting equipment behaving as planned.

THE INVESTIGATION OF HEAT TRANSFER COEFFICIENTS OF BINARY CYCLE WORKING FLUIDS

R. L. Fulton and B. W. Tliemat*

Recent assessments of the potential of geothermal energy resources have pointed to hydrothermal reservoirs as the most likely source of large amounts of geothermal energy in the next two or three decades. To take full advantage of this source of energy, the binary cycle will have to be used, particularly with brines in the lower part of the temperature range or with brines of higher salinities. In the binary system, the brine is used to heat another, or secondary, fluid used as the

working fluid of a turbo-generator power cycle much as in an ordinary steam power plant. Depending on the brine temperature and other conditions, the secondary fluid may be water, ammonia, refrigerants, light hydrocarbons, other fluids or appropriate mixtures of fluids.

Heat transfer equipment, principally to heat and condense the secondary fluid, accounts for approximately half the capital cost of a binary cycle geothermal power plant. That this cost is significant is shown by the cost estimate for a 10 Mw Experimental Power Generation Facility, prepared jointly by LBL and the Rogers Engineering Company, Inc., of San Francisco. The installed cost of the plant, excluding brine production and injection wells, was expected to be $12 million, of which the heat transfer equipment accounted for $6 million. On the same basis, the heat transfer equipment alone for a 50 Mw plant would cost about $30 million. In such cases, an inexact estimate of the heat transfer coefficients can have serious effects. If the coefficients used in the design are too high, the plant may fail to meet its performance guarantee. If too low, the plant will be overdesigned and wastefully expensive.

Despite the importance of heat transfer in binary cycle plants, there is a real shortage of good heat transfer data for isobutane and other candidate secondary fluids. This is especially true for designs where the secondary fluid is in the supercritical region. Computer studies, LBL's GEOTHM for example, indicate that operation in the supercritical region will be the most efficient. Heat transfer coefficients in this region should be experimentally investigated.

The Binary Fluid Experiment (BFE) has been designed to provide experimental data on heat transfer coefficients of the various candidate secondary fluids. It will establish baseline data on film coefficients for several light hydrocarbons and mixtures of light hydrocarbons, refrigerants and mixtures of refrigerants, and ammonia. Data will be gathered from the BFE for the ranges of heating and condensing temperatures that would be expected for geothermal power plant applications. Reliable baseline data of this type can permit reductions of up to 20 per cent in the cost of heat exchange equipment for a binary cycle power plant. This could represent savings of $50 million on the total capital required for the first five 50 Mw installations.

ERDA is sponsoring several programs to obtain data on brine-side heat transfer coefficients. The brine-side coefficients are important, and are subject to degradiation from corrosion and scaling, but the secondary-fluid side coefficients should not be ignored. Good baseline data for the secondary-fluid side will confirm that any degradiation of overall heat transfer rates in early binary cycle plants will be from brine-side problems.

A fundamental question in present preliminary binary cycle plant designs concerns the inclusion of a secondary-fluid/secondary-fluid heat exchanger (regenerator or economizer). Precise data on heat transfer coefficients for cooling the secondary-fluid vapor will help plant designers settle the question of the regenerator. These data will be gathered early in the experimental program.

The effects of secondary-fluid contaminants is another area in which design data are lacking. Direct contact between heating fluid and cooling fluid, as in proposed direct-contact brine to secondary-fluid heat exchangers, will introduce water and probably noncondensable gasses, such as carbon dioxide and hydrogen sulfide, into the secondary fluid. Some of this water will be dissolved and some will be entrained. It will be necessary to determine the effects of water on the other heat transfer equipment in order to specify the amount of water that can be tolerated economically.

In addition, it is reasonably certain that the secondary fluid will either contaminate or be contained by turbine and pump lubricants. The effects of this contamination on heat transfer should be measured. Information should also be collected on the deterioration of lubricants contaminated by the secondary fluids.

Initial funding for construction of the experimental apparatus was received from ERDA Division of Geothermal Energy in May, 1976. By the end of 1976 the experimental apparatus was approximately 90% complete and checkout of the system had begun.

The BFE is located at the University's Richmond Field Station. The experimental equipment consists of a stainless steel recirculating loop in which the secondary fluid is heated under pressure, expanded to the condensing pressure, condensed, and then repressurized and pumped back to the heater. Because some of the fluids to be investigated are flammable, the experiment is located outdoors and uses pnuematic valves and explosion-proof electrical equipment.

The secondary fluid under investigation is heated inside a single tube by condensing steam on the outside of the tube. Thermocouples accurately located in the tube wall are used to calculate the tube inner surface temperature. The amount of heat transferred is determined by collecting and measuring the quantity of steam condensate formed on the tube. The quantity of secondary fluid being heated is measured with a turbine flow meter, while the secondary fluid bulk temperature is measured with a platinum resistance thermometer.

After passing through an expansion valve to the condensing pressure, the secondary fluid is brought to the condensing temperature in either a direct-contact desuperheater or a tube-in-tube counterflow heat exchanger.

The secondary fluid is then condensed on the outside of a single tube carrying cooling water. Tube wall surface temperature, amount of heat transferred, secondary fluid and cooling water flow rates are all determined with the techniques used in the heater. The condensed secondary fluid is collected in a hot well and then recirculated to the heater by a centrifigal booster pump and a positive-displacement high pressure pump.

Signals from the 83 transducers in the BFE will be recorded on a Kaye Model 8000 datalogger with 129 channel capacity. The datalogger, pnuematic controls and other instrumentation are housed in a trailer located next to the BFE.

The BFE schedule calls for taking initial data on isobutane in the first quarter of 1977. The next secondary fluid to be investigated will probably be the isobutane/isopentane mixture under consideration in the conceptual design of an EPRI-sponsored 50 Mw plant to be located at Heber, California.

FOOTNOTE

*Sea Water Conversion Laboratory, University of California, Berkeley, Richmond, California.

GEOTHERMAL EXPLORATION TECHNOLOGY

N. E. Goldstein, T. V. McEvilly, H. F. Morrison, H. A. Wollenberg

INTRODUCTION

A program for the evaluation of exploration techniques to locate and assess potential geothermal resource areas in north-central Nevada was continued in 1976. During the year field investigations were conducted at specific sites within a large area of elevated crustal heat flow, known as the Battle Mountain high heat-flow area. Geological, geochemical and geophysical investigations were completed around Leach Hot Springs in Grass Valley and Kyle Hot Springs in Buena Vista Valley, Pershing County. Open File Reports[1,2] were issued describing the investigations in Grass and Buena Vista Valleys, respectively.

The parameters studied at each site included heat-flow measurements,[3] geochemistry of trace elements and radioelements of spring waters and spring deposit material, and the following geophysical techniques:

1. Gravity
2. Magnetics
3. Self potential
4. Electric-field-ratio tellurics
5. Magnetotellurics
6. Biopole-Dipole resistivity
7. Dipole-Dipole resistivity
8. Seismological studies
    a. Teleseismic P-wave delay
    b. Microearthquake monitoring
    c. Seismic ground noise
    e. Active seismic refraction and reflection.

The gravity surveys were conducted under the direction of Professor Roswitha Grannell, California State University, Long Beach, and these data were reduced with the assistance of the U. S. Geological Survey, Menlo Park. The active seismic surveys were conducted by a commerical contractor. All other geophysical surveys were conducted by LBL/UCB personnel using, in some cases, special equipment, techniques and analyses developed at LBL and the University of California.

The program is sponsored by the Division of Geothermal Energy, ERDA for the purpose of assisting industry by (1) helping to define the physical properties and characteristics of geothermal systems in the Northern Basin and Range Province, (2) establishing the reliability, efficiency and utility of exploration tools and (3) refining or developing new techniques for exploration.

HIGHLIGHTS AND SIGNIFICANT FINDINGS IN 1976

A. Gravity and Magnetics

Gravity and ground magnetic surveys for structural information were conducted at the sites. At both Grass and Buena Vista valleys the known hot springs areas show subtle gravity highs which are interpreted as due to densification of near-surface valley sediments by precipitating hot spring deposits. A detailed interpretation of the small gravity anomalies was begun to determine the approximate sizes of the hydrothermal deposits.

B. Self Potential

A large negative self potential (SP) anomaly (-300 to -570 mV) was found paralleling the western margin of the East Range, the mountains which form the eastern border of Buena Vista Valley. Because of the unusually large amplitude, width and continuity of the SP effect, it was possible that the anomaly might relate to either thermoelectric or streaming potentials arising from hydrothermal activity. Subsequent detailed geophysical, geological and heat flow holes revealed that the source of the SP effect is probably pyritic and/or graphitic zones in bedrock of the East Range. This finding illustrated the potential problem of misinterpreting SP data, and showed that caution must be exercised in dealing with SP anomalies occurring over valley fill. These may be due to pyritic and graphitic zones at shallow depth in underlying bedrock.

C. Electric-Field-Ratio Tellurics

LBL was the first to apply the little-known method of E-field-ratio tellurics to geothermal exploration. Since our early efforts to use and

describe this technique, the method is now used routinely by the U. S. Geological Survey and industry. Natural telluric fields are measured by means of a tripole electrode array (two co-linear dipoles with one common electrode) that is advanced along a survey line. The electric fields between each pair of electrodes are ratioed to yield the relative amplitude of the E-field in the direction of the survey line. The telluric signal is filtered at two frequencies, 8 and .05 Hz, to provide some measure of depth discrimination.

Over the active Kyle Hot Springs, the E-field-ratio technique gave a sharp, single data-point low at both frequencies, suggesting the presence of an electrically conductive channel feeding the springs. However, over deposits of an inactive spring nearby, the method showed enhanced resistivity, suggesting that this conduit has been sealed to large depth by precipitated hot spring material.

Theoretical analysis and computer modeling is being carried out to assist with data interpretation and a report is being assembled (Beyer, in preparation).

D. Magnetotellurics

The magnetotelluric system uses a SQUID (Superconducting, quantum interference detector) magnetometer for magnetic field sensing. This device was developed by Professor John Clarke, Physics Department, University of California, with funds supplied by the Extramural Program of the U. S. Geological Survey. During 1976, repeat measurements were made at Leach Hot Springs (Grass Valley) to acquire long period data, out to 1000 seconds, for determination of deep crustal structure. Our present emphasis is in data analysis techniques.

E. Resistivity

The resistivity work includes various controlled source methods for obtaining near-surface resistivities; namely, bipole-dipole, dipole-dipole, and an inductive (frequency domain) method.

During 1976 a computer program was completed and applied to the interpretation of dipole-dipole data collected in Grass and Buena Vista Valleys. The program uses the finite difference approach and contains very efficient algorithms which permit fast and efficient operation. The program can accommodate two-dimensional models for dipole-dipole, bipole-dipole, Schlumberger and down-hole electrode arrays. An important feature of the program is that the user can introduce very large models, commensurate with the width of a typical Basin-and-Range valley, 15 to 20 miles. The first part of a two-part report dealing with the method has been prepared.[4]

Frequency domain electromagnetic soundings were conducted in Grass Valley using a combination of equipment originally designed for other purposes. The data gathered were of high quality and were interpreted by means of curve matching. The results compared well with those from other resistivity measurements, demonstrating the usefulness of EM depth sounding. A progress report on the experiment[5] was produced and a final report is in preparation. This experiment marked the first actual field testing of a digital superheterodyne signal averager used to process the conditioned signals.

F. Seismological Studies

Microearthquake studies in Buena Vista Valley were inconclusive because of the lack of activity during the recording period. However, surveys in Grass Valley led to the discovery of three areas of microearthquake swarms south of Leach Hot Springs. First motion analysis indicated a right-lateral movement associated with microearthquakes on the east flank of the Gold Bank hills. The northeast-trend of thezones of microearthquakes suggests the presence of a northeast-trending fault system in the Panther canyon area. The eastern-most zones of microearthquakes match an area of high heat flow near Panther Canyon of the Sonoma Range, which forms the east border of Grass Valley. The possibility of a previously undisclosed hydrothermal system in this area was investigated by means of additional heat flow measurements, and these data will be presented in a joint LBL-U.S. Geological Survey report which is in preparation.

Propagation studies gave some of the most interesting results regarding the size of geothermal systems. Relative times of arrival, amplitude and spectral content of teleseismic and distant man-made seismic events were studied at both Grass Valley and at The Geysers, in California. At Leach Hot Springs in Grass Valley there was direct evidence for a sinter deposit which produced a P-wave advance of 150 milliseconds and an enhancement in frequency content and amplitude of the wave train. At The Geysers clear evidence was found for both P- and S-wave amplitude attenuation at stations within the vapor-dominated field. A separate report on The Geysers experiment is in preparation.[6]

Ground noise experiments were conducted in Grass Valley to investigate the spatial distribution of the ambient background microseisms, in amplitude and frequency, plus parameters such as propagation directions and apparent velocities. Noise level anomalies were found associated with surface hydrological activity at the hot spring and in the center of the valley, presumably associated with the thick low-velocity surficial materials. Hot spring activity produces seismic energy in a frequency band from 3 to 15 Hz; most of the high frequency energy is severely attenuated 1 km from the source. Ground-noise levels reflect thickness of valley sediments and were found to agree with the results of other geophysical methods. A paper on the ground-noise studies is being prepared[7] and work continues on high-resolution wave-number analysis to obtain information on apparent velocities and direction of coherent seismic waves.

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NUMERICAL SIMULATION OF RESERVOIR COMPACTION IN LIQUID DOMINATED GEOTHERMAL SYSTEMS

M. J. Lippmann, T. N. Narasimhan and P. A. Witherspoon

INTRODUCTION

The production of fluids from geothermal systems may result in ground surface displacements due to the lowering of pressures in the reservoir and surrounding rocks. These displacements may not only affect installations directly related to the geothermal field (e.g., well casing, steam transmission lines, power plant) but also nearby roads, buildings, and irrigation canals. Therefore it is important to foresee the magnitude and location of the so-called "subsidence bowl" as soon as adequate data on the geologic structure, stratigraphy, rock properties, and proposed development program become available.

The objectives of this project, started in September 1975, are:

1. Develop computer codes to calculate ground displacements in water saturated porous systems under non-isothermal conditions caused by pore pressure changes;

2. Develop guidelines, based on the geologic characteristics of a system, for locating and managing production and injection wells to minimize pressure reductions and ground deformations.

These programs and guidelines would be applicable to water dominated geothermal systems which at the present time in the U. S. have the largest potential for developing geothermal energy for electrical and non-electrical uses.

ACCOMPLISHMENTS FOR 1976

An improved computer program was developed to calculate the effects of fluid production as well as reinjection on the vertical deformation of water dominated geothermal fields. This mathematical model simulates the transport of heat and water through porous media, including the vertical displacements produced by effective stress changes.

The program named "CCC" (Conduction-Convection and Consolidation) is based on the numerical models SCHAFF[1] for mass and heat transport through saturated porous media, and TRUST[2] for one-dimensional isothermal consolidation. The code can simulate one-, two- or three-dimensional, heterogeneous, isotropic, non-isothermal systems. Deformation parameters may be non-linear and non-elastic; the thermal and hydraulic properties can be temperature and/or pressure dependent.

An integrated finite difference method[3] is used to solve the energy and fluid flow equations. In integral form the flow equation for a slightly compressible fluid (e.g., water) is given by:

$$\frac{\partial}{\partial t}\int_V \frac{\rho}{1+e}\left(e\kappa + \frac{de}{d\sigma'}\right)PdV = \int_S \frac{k\rho}{\mu}(\nabla P - \rho\bar{g})\cdot\bar{n}dS + \int_V QdV \qquad (1)$$

and the energy equation is given by:

$$\frac{\partial}{\partial t}\int_V (\rho c)_M T dV = \int_S K_M \nabla T\cdot\bar{n}dS - \int_S \rho c_F \delta T \bar{v}_d\cdot\bar{n}dS + \int_V qdV \qquad (2)$$

where, t is time, ρ fluid density, e void ratio, κ fluid compressibility, σ' effective stress, P pore pressure, V volume, k intrinsic permeability, μ viscosity, $\bar{g}$ gravitational acceleration, $\bar{n}$ outward unit normal on surface S, Q mass injection rate per unit volume, $(\rho c)_M$ heat capacity per unit volume of the solid-fluid mixture, c_F fluid specific heat capacity at constant volume, δT difference between the mean temperature within the volume element and that on the surface element dS, $\bar{v}_d$ Darcy

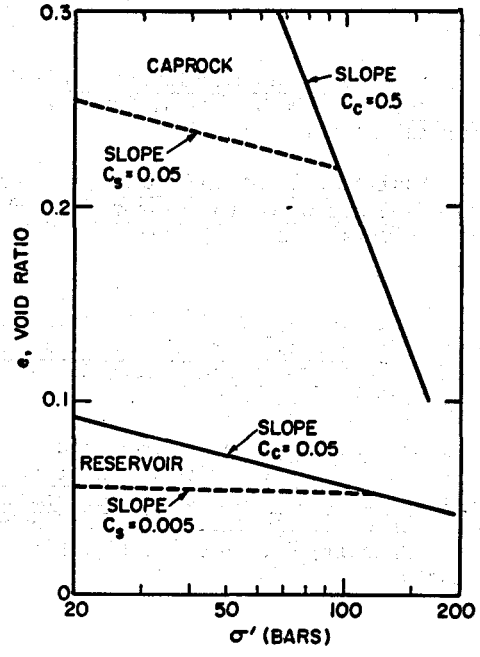

Fig. 1. Plot of void ratio (e) versus effective stress (σ') for hypothetical caprock and reservoir materials. (XBL 7611-7860)

velocity, and q heat injection rate per unit volume.

Concurrent with the mass and energy flow, the vertical deformation of the geothermal system is simulated based on the one-dimensional consolidation theory of Terzaghi. The void ratio at each nodal point is computed by using "e-log σ'" curves (Fig. 1). According to the preconsolidation and effective stresses at the point, the program calculates the void ratio by using either the virgin curve (of slope C_c) or swelling-recompression curves (of slope C_s). The model neglects the hysteresis between swelling and recompression curves. While the pore volume changes with effective stress, the solid volume is defined to remain constant; the thermal expansion of the rock skeleton is not considered. Because of the one-dimensional nature of the consolidation model, the pore volume changes caused by the void ratio changes are directly reflected in a vertical deformation of the individual volumetric nodes.

The deformations computed by this model are restricted to those of the reservoir and neighboring saturated formations which release water from storage to compensate, partly or wholly, for the fluid withdrawn. These vertical displacements may or may not be directly expressed at the ground surface. The external loading of the overburden, caused by the vertical deformation of the deeper geothermal system, may result in displacements at the surface that may be different in magnitude and direction. Future versions of this model will include the computation of vertical and horizontal displacements at the ground surface itself.

The flow and energy equations (1) and (2) are interconnected by:

a. the second order equation of state for the fluid

$$\rho = \rho_0 \left[1 - \beta(T-T_0) - \gamma(T-T_0)^2\right] \qquad (3)$$

where, β and γ are coefficients of thermal expansion, and ρ_0 and T_0 are the reference density and temperature, respectively, for the fluid;

b. the Darcy velocity used in the convection term of the energy equation;

c. the temperature and/or pressure dependence of certain parameters.

Because of these interrelations, equations 1 and 2 are solved alternatively by interlacing their solutions in time; this is shown schematically on Fig. 2. The flow equation solves for P, $\bar{v}_d$ and e assuming that the temperature dependent properties of the fluid and rock remain constant. Then, the energy equation is used to obtain T assuming that $\bar{v}_d$ and pressure dependent properties remain constant. Since the temperature varies much more slowly than the pressure, much smaller time steps have to be taken in the flow cycles than in the energy cycles (Fig. 2) in order to compute pressure variations accurately.

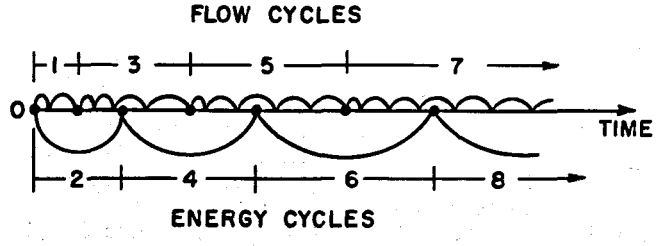

Fig. 2. Interlacing of flow and energy calculations. (XBL 7611-7862)

A number of simplified geothermal systems were studied to determine the effects of reservoir and caprock heterogeneities on the resulting compaction, as well as the effects of different production-injection schemes. The preliminary results obtained were summarized in a paper presented at the Second International Symposium on Land Subsidence.[4] It was shown that:

1. Reservoir heterogeneities may cause the largest compaction to occur away from the producing wells and not at the wells themselves;
2. Even when all produced water is reinjected, some amount of deformation can be expected;
3. When the systems are normally consolidated, it may be necessary to have rates of reinjection that are larger than the production rates in order to minimize the effects of consolidation;

4. Compaction of water dominated geothermal systems with large temperature differences and complex fluid flow patterns will be difficult to simulate using isothermal models.

PLANNED ACTIVITIES IN 1977

1. If adequate data become available the application of program CCC to actual geothermal systems (e.g., Wairakei, New Zealand, or Cerro Prieto, Mexico) will be attempted.
2. Modifications will be made to the program to compute horizontal as well as vertical ground displacements.
3. The effects of geological heterogeneities will be further studied using three-dimensional models with non-uniform caprocks and differently shaped lenticular structures, intercalated in the reservoir.

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RESULTS OF RESERVOIR EVALUATION TESTS, 1976 EAST MESA GEOTHERMAL FIELD, CALIFORNIA

D. G. McEdwards, T. N. Narasimhan and P. A. Witherspoon

INTRODUCTION

To assist the U. S. Bureau of Reclamation in the evaluation of the East Mesa Geothermal Field, located at the southern end of California's Imperial Valley, the LBL Geothermal Group conducted reservoir tests at the field for a four-month period form January 2 to April 19, 1976. The field is used by the Bureau as a design testing facility for desalinization and electrical power generation processes which attempt to mine the energy contained in water at 350°F that exists in the sediments below 4000 feet. The well tests serve to define the permeability and storage characteristics of the deep water-bearing rocks and to elicit information about reservoir structure. This information is imperative for a judicious management of the available geothermal resource. This report presents the findings of the reservoir well tests.

PHYSIOGRAPHY AND GEOLOGY

The East Mesa Field is located 20 miles east of El Centro, California, in the Imperial Valley (Fig. 1) which is part of a large structural feature known as the Salton Trough, a sediment-filled depression forming the landward continuation of the East Pacific Rise and the Gulf of California.[1] The East Pacific Rise is one of several geological sutures in the crust of the earth along which adjoining crustal plates move apart, causing thinning of the crust and upward movement of molten rock. This crustal extension is responsible for the formation of the Salton Trough and the Gulf of California, and provides the heat source for the several geothermal resource areas in the Imperial Valley. As a consequence of this crustal extension many faults occur within the Valley, trending generally in the northwesterly direction. The major active faults close to the field are the San Andreas, located approximately 20 miles from the East Mesa Field on the eastern margin of the Imperial Valley, and the Imperial Fault, located approximately 15 miles to the west of the field. Three local faults have been mapped within the field itself.

The Imperial Valley is a broad depression, approximately 60 miles wide at the geothermal field location. It trends northwest to southeast becoming wider toward the Mexican border. It is about 60 miles long and is bounded on the east by the Chocolate Mountains, which rise to an average elevation of 2000 feet, and on the west by the Fish Creek and Coyote Mountains which attain a local average elevation of 3000 feet. Salton Sea, with an average surface elevation of about-230 feet, occupies the northern part of the valley. A greater part of the valley south of Salton Sea lies below sea level and benefits from the All American and Coachella canal systems of the Colorado River. The East Mesa geothermal field occurs in the unirrigated desert lands located in the southeastern part of the Imperial Valley, about 10 miles to the east of the agricultural town of Holtville.

At East Mesa, the reservoir rocks are essentially flat-lying, poorly consolidated, late Pliocene to late Pleistocene, deltaic sandstones, siltstones and clays believed derived from the Colorado River, and comprise a total thickness of over 10,000 feet on top of crystalline basement rock. A predominantly clay strata sequence approximately 1900 feet thick

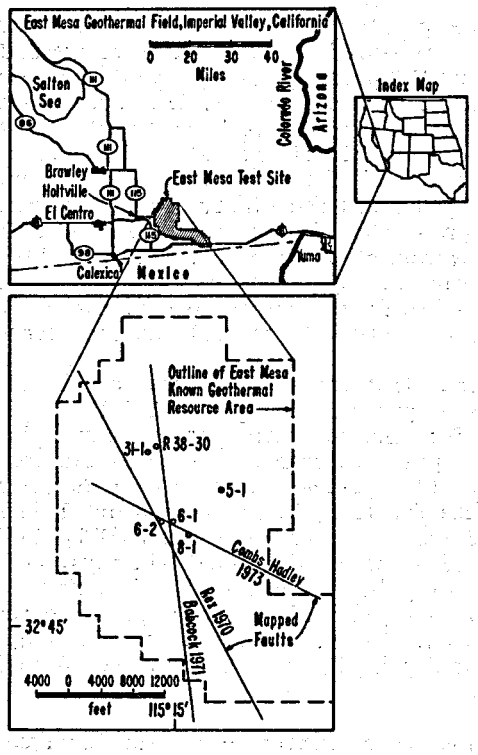
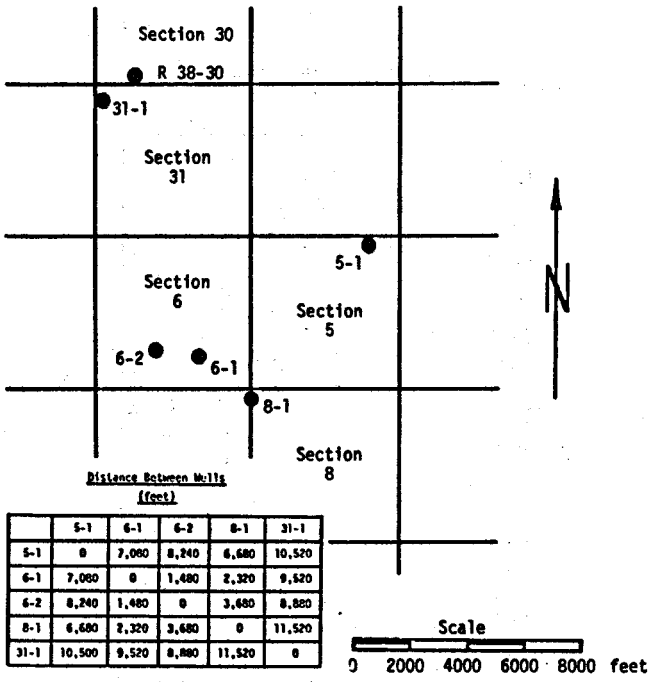


Fig. 1. Location map of the East Mesa Geothermal Field, Imperial Valley, California. (XBL 765-2871)



Distance Between Wells (feet)

	5-1	6-1	6-2	8-1	31-1
5-1	0	7,080	8,240	6,680	10,520
6-1	7,080	0	1,480	2,320	9,520
6-2	8,240	1,480	0	3,680	8,880
8-1	6,680	2,320	3,680	0	11,520
31-1	10,500	9,520	8,880	11,520	0

Fig. 2. Layout of the East Mesa Geothermal Well Field, Imperial Valley, California. (XBL 771-7309)

caps the reservoir and hence no surface evidence of geothermal activity is seen. Within the field, three supposedly vertical intersecting faults have been mapped[1] (Fig. 1). It is thought that one or more of these faults and/or their intersection may act as vertical channels that allow hot water to rise from depth and cooler water to return to depth in a convective cycle. This convective regime is believed to be sustained by heat derived from the tectonic processes associated with the proximate East Pacific Rise. The surface heat flow is about five times that of the earth's average.

THE WELL FIELD

The Bureau of Reclamation has drilled five wells to an average depth of 6000 feet, tapping geothermal fluids under artesian conditions with average well head pressures of about 70 psi. A map of the East Mesa Well Field is shown in Fig. 2 while details of the wells are given in Table 1.

DESCRIPTION OF TESTS

Two interference tests were conducted at East Mesa during 1976. These tests involved removing fluid from one well (the production well) at a constant rate and monitoring the induced pressure changes in a neighboring well (the observation well). Temperature surveys of four wells were also run in conjection with the well test (Fig. 3). Details of the theory of well testing and the method of analysis are presented by Narasimhan and Witherspoon[3] elsewhere. Specific methods used at East Mesa to control and measure fluid flow at the production well and to record pressures in the observation well are discussed below.

Since the geothermal wells at East Mesa are under artesian conditions, well flow could be achieved by simply opening the well head valves. Environmental concerns regarding the disposal of produced hot water limited test production flow rates to about 100 gpm. Flow rate was controlled by means of an orifice plate with a 3/4 inch diameter aperture. In addition to regulating flow, the orifice plate also helped to maintain sufficient back pressures to prevent steam formation within the well. Temperature and pressure information at the well head during production was obtained by means of a bourdon tube and thermocouple arrangement placed upstream of the orifice plate. Once past the orifice, a portion of the fluid flashed to steam and the rate of flow of the remaining liquid portion was measured by passing the liquid through a weir box arrangement with a clock driven water level recorder. Total flow was calculated using the liquid flow rate and the fractional part of total flow converted to steam at the recorded well head temperatures and pressures.

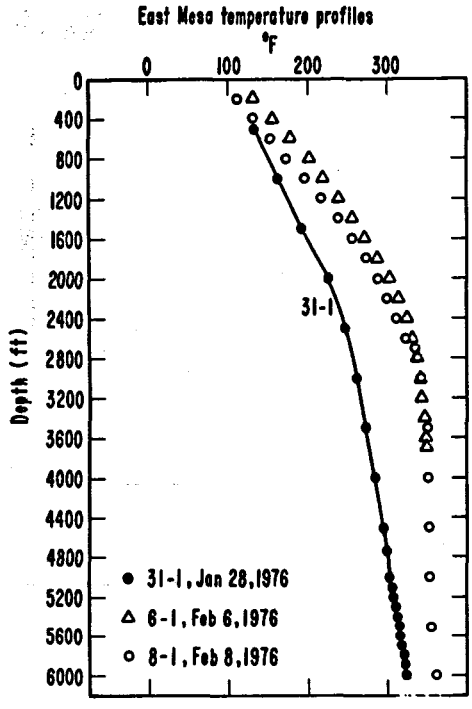


Fig. 3. Temperature Profiles in wells 6-1, 8-1, and 31-1, East Mesa Geothermal Field, Imperial Valley, California. (XBL 765-2872)

The pressure changes in the observation wells were measured using a sensitive downhole quartz crystal pressure gauge capable of resolving pressures to within 0.01 psi. The gauge was placed downhole at an appropriate depth dictated by the temperature profile of the well and the temperature limitations of the tool. Pressure information from the gauge was fed electronically to panels located in a house trailer on the surface. The surface equipment provided both strip chart and printed digital paper tape records in units of psi. Pressure data accurate to 0.01 psi could be monitored at intervals as small as one second.

The first interference test consisted of placing the pressure tool in well 6-1 at a depth of 1100 feet and recording, at ten minute intervals, the pressure changes caused by flowing well 6-2, 1500 feet distant, at a rate of 90 gallons per minute for 11 days. At the end of 11 days, well 6-2 was closed and pressure buildup in 6-1 was recorded for an additional six days. While the pressure drop in well 6-1 was sufficiently large to permit analysis, simultaneous pressure reading taken in well 8-1, 2300 feet away, and at a 1500 foot depth, did not show any such drop in pressure.

The second interference test involved well 31-1 and well R38-30, the latter drilled by a private company (Republic Geothermal) on leased acreage. The pressure tool was placed in R38-30 at 1500 feet and well 31-1, located 1250 distant, was flowed at 130 gpm for 10 days. After 10 days the well was closed and the build-up pressures in R38-30 recorded for an additional 7 days.

Table 1. East Mesa Well Data (after Mathias[2]).

Well	Depth		Bottom Temperature		Producing Interval		Lower Casing o.d.
	feet	meters	°C	°F	feet	meters	inches
6-1	8015	2443	399	204	6201-7982	1890-2433	7
6-2	5958	1816	340	188	4790-5959	1460-1816	7-5/8
5-1	6004	1830	315	157	5007-6004	1526-1830	7-5/8
8-1	6001	1829	354	179	4948-6001	1508-1829	7-5/8
31-1	6175	1882	309	154	5420-6175	1652-1882	7-5/8
R38-30	8890	2710	N/A	N/A	4890-8890	1491-2710	7

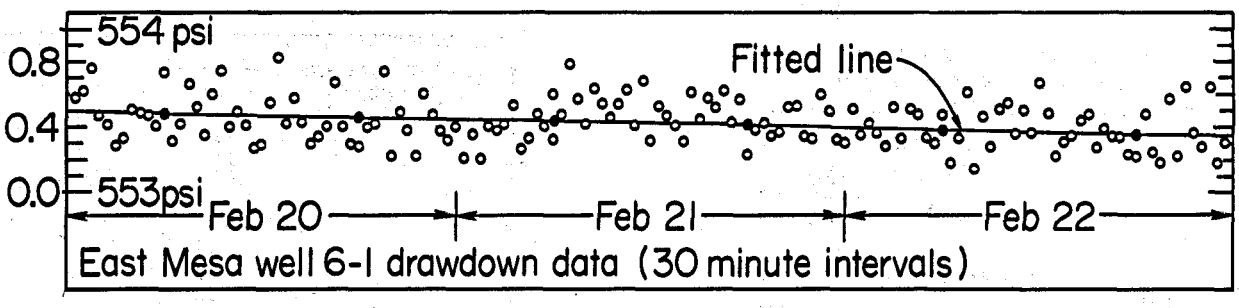


Fig. 4. Water pressure data from well 6-1 showing the noise level in the measurements. (XBL 765-2876)

RESULTS AND INTERPRETATION

A segment of the water pressure data collected from 6-1 is shown in Fig. 4. It can be seen from this figure that the pressure data is subject to considerable background noise. It is not definitely known if this noise is caused by the instrument-cable system or by natural phenomena such as microseismic activity.

The interference test between wells 6-2 and 6-1 indicated that the pressure data from the latter had a noise level of about 0.5 psi about the mean, while the maximum pressure change induced at 6-1 by the production at 6-2 was only about 0.7 psi over 11 days. In order to remove the effects of the noise on the pressure data and to enable meaningful interpretation of the response of the reservoir to the fluid withdrawal at well 6-2, a non-linear regression technique was applied to the data collected from well 6-1. A portion of the mean curve calculated is shown in Fig. 4.

Analysis of the drawdown data from the first interference test indicated that in the region of wells 6-2 and 6-1, the transmissivity and the storativity parameters of the reservoir could be represented by $kH = 11{,}200$ millidarcy feet and $\phi CH = 5.7\times10^{-3}$ feet per psi, where k is permeability, H is reservoir thickness, ϕ is porosity, and C is the combined compressibility of water and rock. The second interference test revealed that the reservoir is probably more permeable in the region of wells 31-1 and R38-30, yielding a kH value of 29,500 millidarcy feet and $\phi CH = 2.1\times10^{-3}$ feet per psi. The differences in the reservoir parameters obtained from the two tests suggest that the geothermal reservoir may be heterogeneous. The calculated parameters indicated by the tests are in substantial agreement with the earlier tests conducted by the Bureau of Reclamation and with the average permeability values calculated from synthesized well log data. In Figs. 5 and 6, the drawdown data from the two interference tests are shown plotted on a log-log paper and fitted, using a curve matching technique[4,5] to the analytical solution (Theis curve).

Examination of the difference between the theoretically expected pressure variation and the actual pressure variation from the two tests as seen from Figs. 5 and 6 lead to two hypotheses concerning the structure of the reservoir. Within distance limits of 200 to 1700 feet from well 601, depending upon direction, there exists a recharge boundary of some nature, such as a zone of greatly increased permeability or a vertical fault plane that acts as a fluid conduit. Again, near R38-30, within 1100 to 2400 feet, depending upon direction, a barrier boundary exists. This barrier boundary may be a fault that is impervious to flow or it may be a zone of greatly decreased permeability. It seems reasonable that the three near-vertical faults crossing the site play the role of such hydrologic boundaries. Further testing is needed to develop a more complete picture of the structural character of the reservoir.

MICROSEISMS

A few hours before the first flow test began, a pressure anomaly of 3 psi above noise level was recorded in well 8-1 (Fig. 7). Concurrent pressure records in well 6-1 did not contain this anomaly. The Bureau of Reclamation maintains a seismic net at the site, and a check of the seismic net records revealed a small seismic event had occurred at about the same time as the pressure anomaly. This suggests a probable microseismic origin for the observed anomaly. That the disturbance was picked up at 8-1 and not 6-1 suggests the presence of an energy absorbing boundary between the two wells. It is interesting to note here that a fault mapped by Combs and Hadley in 1973 runs between the two wells.

These observations give promise to the development of a new reservoir testing technique. A record of passive downhole pressures, recorded at small time increments, and the correlation with concurrent microseismic data, may be amenable to analysis regarding reservoir structure, permeability and other parameters. Little is known about the influence of microseisms on pore pressures because until recently sensitive pressure tools that could measure pore pressures rapidly with high resolution and over extended time periods have not been available for use.

PLANNED ACTIVITIES

The tests so far conducted have yielded valuable preliminary data on the physical parameters and geometry of the geothermal reservoir at

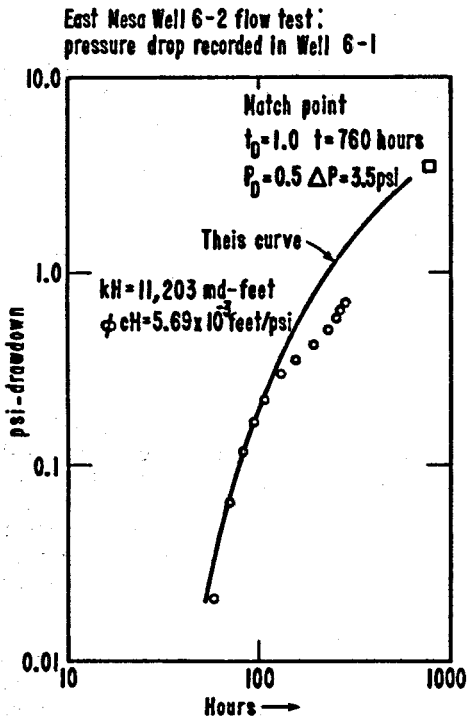


Fig. 5. Interference test 1: log-log plot of drawdown data from well 6-1. (XBL 765-2874)

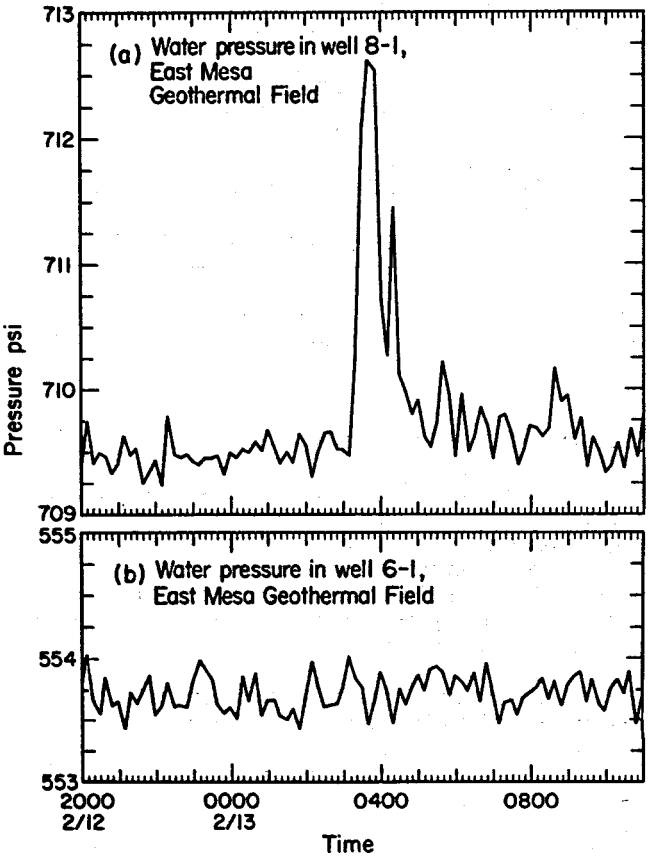


Fig. 7. Water pressure data from wells 8-1 and 6-1, with the former showing an anamalous, 3 psi peak. (XBL 765-2875)

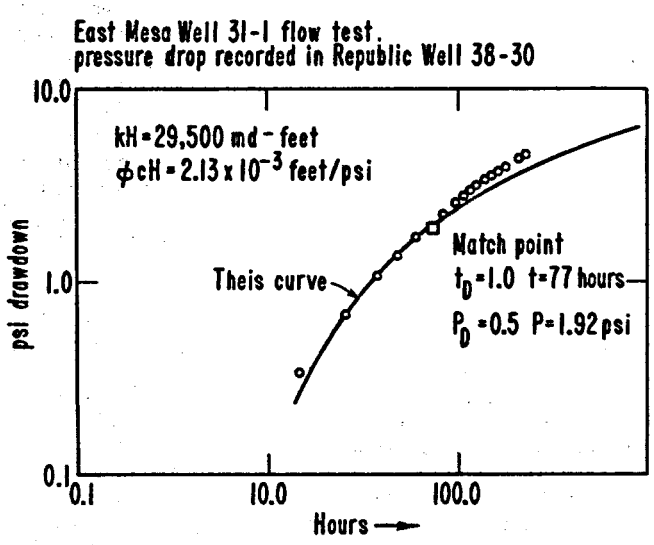


Fig. 6. Interference test 1: log-log plot of drawdown data from well R38-30. (XBL 765-2873)

East Mesa. Further tests are planned for early 1977, and it is hoped they will provide an improved picture of the geothermal resource.

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INTERPRETATION OF PRELIMINARY PRODUCTION-INTERFERENCE RRGE 3, RAFT RIVER VALLEY, IDAHO, JUNE 1976

T. N. Narasimhan and D. G. McEdwards

INTRODUCTION

Following the reservoir testing activities of 1975,[1] a third well, RRGE 3 was drilled and completed in Raft River Valley, Idaho by May, 1976. Subsequently the Idaho National Engineering Laboratory carried out further production-interference tests in June 1976 to obtain more data on reservoir performance. This report is an interpretation of the data collected by the INEL during the aforesaid test. According to the data provided by INEL, the details of the test are as follows:

Producing Well:	RRGE 3
Duration:	193.5 hours, from 1230 hours on June 8 to 1400 hours on June 16, 1976.
Production Rate:	Variable; started at about 152 gpm and ended at about 137 gpm.

The producing well, RRGE 3, was monitored with a Hewlett-Packard downhole pressure gage with the instrument positioned below 5,000 feet, presumably opposite the sand face. RRGE 1 and RRGE 2 were used as observation wells. RRGE 1 was monitored with a Hewlett-Packard downhole pressure gage set at approximately 1,000 feet below ground level. On RRGE 2 well-head pressures were recorded with a surface pressure gage of the same accuracy as the downhole gages.

The average pressure at the location of the instrument within RRGE 3 declined from about 2453 psi at the commencement of production to about 2390 psi at shutdown for a total drawdown of 63 psi. In RRGE 1, the average presures at the location of the instrument declined from about 498.8 psi at the start to about 498.3 psi at the time of shutdown for a total drawdown of about 0.5 psi. The well-head pressures at RRGE 2 fluctuated around an average of about 128.5 psi and no significant trend of pressure decline in the data was discernible during the period of production.

INTERPRETATION

The interpretation presented below relates to drawdown and buildup data collected from RRGE 3 and drawdown data collected from RRGE 1.

Drawdown Data, RRGE 3

The drawdown data from RRGE 3 are considerably affected by fluctuations in the production rate during the first 60 hours. Figure 1 shows the production rate from RRGE 3 as a function of time. Attempts to interpret the data by conventional type curve techniques proved futile since the perturbations introduced by the variable discharge were too strong. A general technique of interpreting the data was developed[2] resulting in a computer program capable of analyzing well test data with arbitrarily variable discharge. Using this new technique, the data from RRGE 3 was analyzed in two different ways. The first analysis pertained to the drawdown data collected during the first 18 hours after the start of production, since early drawdown should be relatively free from boundary and other effects. The second

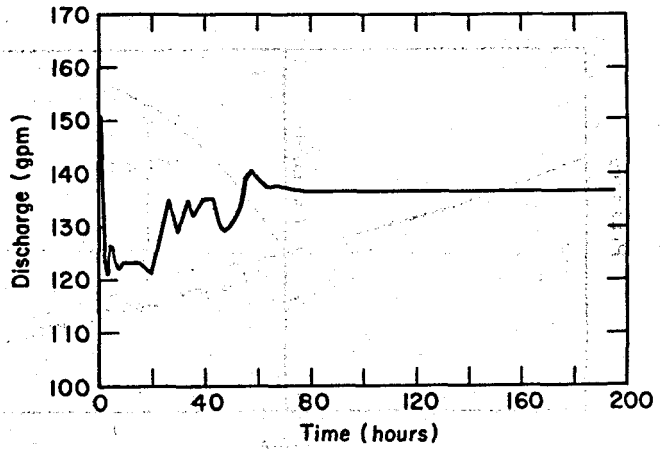

Fig. 1. RRGE 3 Production history. (XBL 773-642)

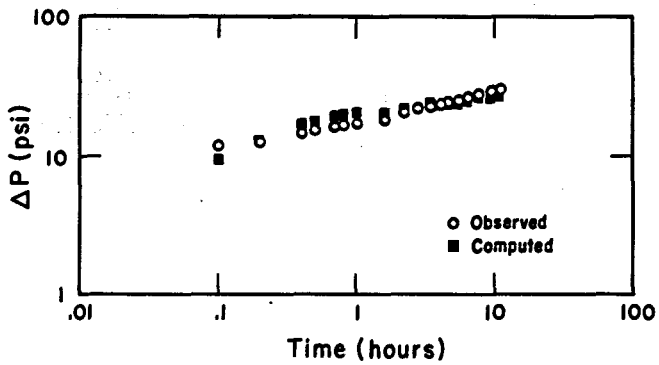

Fig. 2. RRGE 3 Production test-drawdown analysis by variable discharge method. (XBL 773-646)

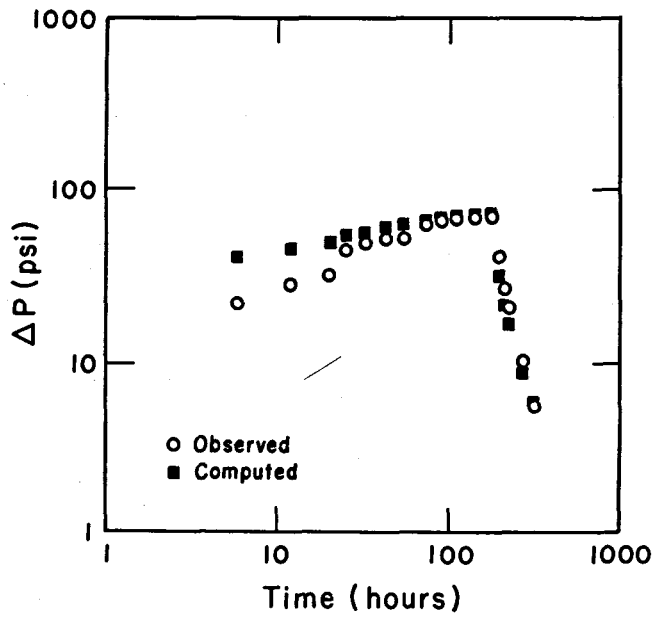

Fig. 3. RRGE 3 Production test-drawdown and buildup analysis by variable discharge method. (XBL 773-647)

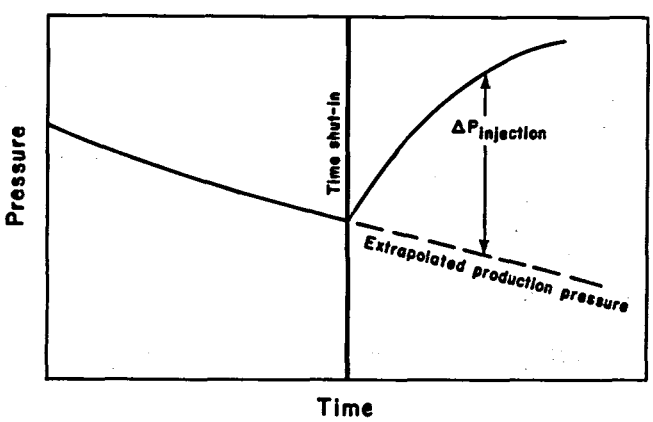

Fig. 4. RRGE 3 Buildup analysis-schematic definition of $\Delta P_{injection}$. (XBL 773-638)

analysis related to all the drawdown data and part of the build-up data, with the assumption that no boundary effects were present.

A log-log match of the observed drawdowns and those computed by the variable discharge model during the first 18 hours of production is presented in Fig. 2. Computations based on this match indicate kH of about 12,000 millidarcy feet in the vicinity of RRGE 3. Since RRGE has 3 legs of differing lengths and orientations, it is not possible to evaluate the effective well radius; hence one cannot reliably compute ϕCH. However assuming a ϕCH of 1×10^{-3}ft/psi, it is estimated that the effective radius of RRGE 3 is about 36 feet.

A log-log match of the entire drawdown data plus part of the build up data with those computed by the mathematical model is presented in Fig. 3. As seen from this figure, the match is very reasonable after about 20 hours of production. Computations based on this match have indicated a kH of about 6400 millidarcy feet. Assuming a ϕCH of 1×10^{-3} ft/psi, the effective well radius is about 29 feet.

Build-up Data, RRGE 3

In order to interpret the build-up data from RRGE 3, the following procedure was used. Shutting down the well was treated as effectively equivalent to superimposing an injection well on the production well commencing at the time of shutting down. The rate of injection was set equal to an average rate obtained by dividing total production during the test by the total duration of production. This average rate worked out to be about 135 gpm.

As shown schematically in Fig. 4, the build-up due to injection, referred to as $\Delta P_{injection}$, is the difference between the observed pressure and the extrapolated production pressure. The conventional technique of curve-matching was employed to analyze the build-up data, $\Delta P_{injection}$, and the results are shown in Fig. 5. Computations indicate a kH value of about 5500 millidarcy feet for the reservoir in the vicinity of RRGE 3. This

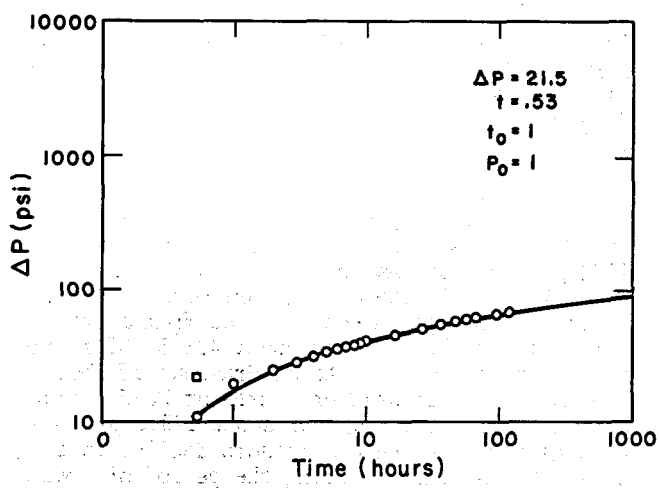

Fig. 5. RRGE 3 Production test-buildup analysis. (XBL 773-644)

analysis yields an effective radius of about 65 feet for RRGE 3.

Drawdown Data, RRGE 1

The pressure data collected from RRGE 1 was masked by significant high frequency noise with the amplitude in excess of about 0.7 psi at times. The cause of the noise is not known exactly, but it is likely that the noise may be related to the instrument-cable system. Nevertheless, on plotting the observed pressures at 10-minute intervals it was possible to discern the cyclic fluctuations caused by earth-tides as well as an overall declining trend caused by the production of RRGE 3.

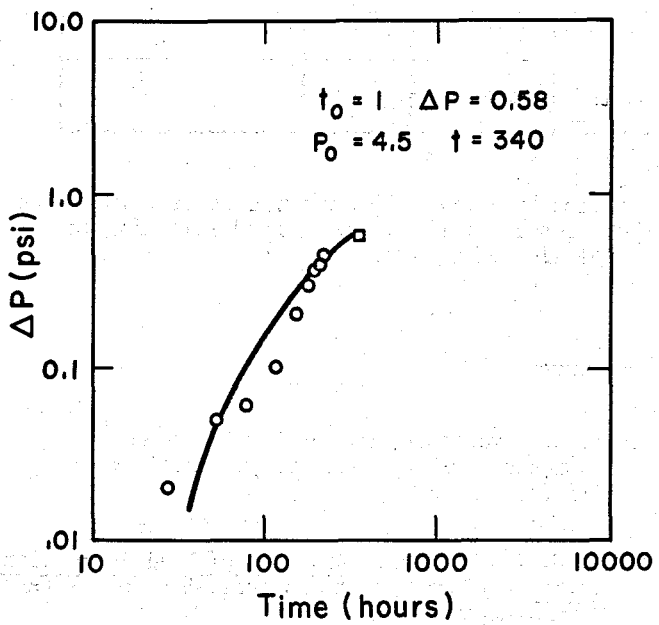

Fig. 6. RRGE 1 Interference test-analysis by Theis method. (XBL 773-643)

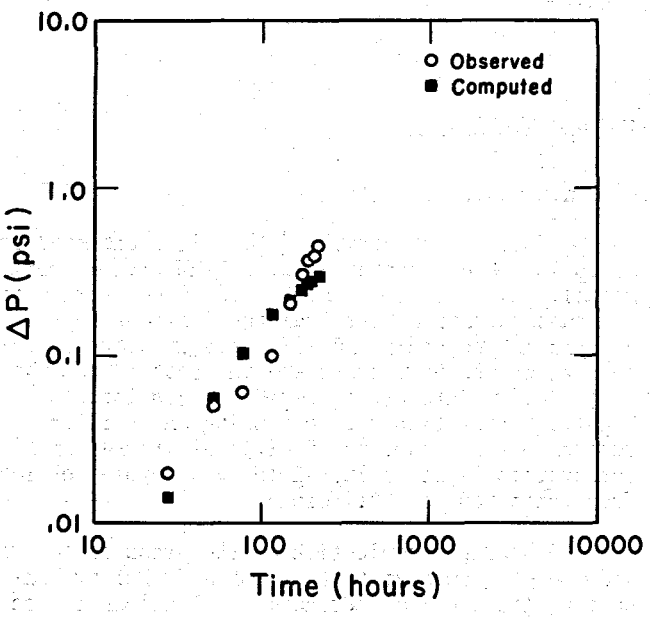

Fig. 7. RRGE 1 Interference test analysis by variable discharge method. (XBL 773-645)

To interpret the data, the first step was to compute the changes in the earth's gravity at the Raft River site during the period of the test. Our previous experience[1] at the Raft River site had indicated that the gravity wave tends to lag behind the pressure wave by about 45 minutes. Using the calculated values of gravity as a guide, the mean-line of pressure variation was first drawn through the observed data by eye judgment. Using this average line and making allowances for the difference in phase between the gravity and pressure data, pressures corresponding to zero gravitational effect were read off from the mean-line referred to above. These pressures were then used for interpretation.

As a first approximation, Fig. 6 shows a log-log match of the observed drawdowns with the Theis type curve. Although the match is not very good, the fit does yield reservoir parameters (kH - 101,000 millidarcy feet and $\phi CH = 1.23 \times 10^{-3}$ ft/psi) which appear reasonable in the light of previous knowledge.[1]

The same data were analyzed with the help of the variable discharge computer technique of Tsang et al.[2] The match obtained with the computer is presented in Fig. 7 and computations indicate a kH of about 222,000 millidarcy feet and a ϕCH of 1.654×10^{-3} ft/psi, which agree remarkably with values of kH = 228,000 millidarcy feet and $\phi CH = 1.19 \times 10^{-3}$ ft/psi, obtained during an earlier interference test between RRGE 2 and RRGE 1.[1] For convenience of comparison, the results of interpretation are summarized in Table 1.

DISCUSSION

Although the variable discharges encountered and the noise present in the data from RRGE 1 tend to undermine the confidence one has in the computed values of kH and ϕCH, the interpretations do enable us to make certain reasonable qualitative judgments on the nature of the Raft River geothermal reservoir.

Both the drawdown and the build-up data from RRGE 3 suggest that the reservoir has very limited permeability near RRGE 3, yielding a kH of about 6,000 millidarcy feet, which is about an order of magnitude less than that computed from the earlier[1] production test at RRGE 3. On the other hand, there is reasonable certainty that the production at RRGE 3 indeed created measurable pressure changes at RRGE 1, leading to a kH of about 100,000 millidarcy feet in the region between RRGE 3 and RRGE 1. This estimate of kH compares favorably with the kH value of about 200,000 millidarcy feet, calculated from the earlier[1] interference test between RRGE 2 and RRGE 1.

An interesting fact is that the surface pressure gage at RRGE 2 apparently failed to pick up the effects of RRGE 3 production. Whether this implies the existence of some discontinuity between RRGE 3 and RRGE 2 is not quite clear. Further long-duration interference tests will be necessary to establish the nature of continuity between RRGE 3 and RRGE 2.

TABLE 1. SUMMARY OF TEST RESULTS

Name of Test	Data Collected from	Type of Data	Type of Analysis	kH md-feet	ϕCH ft/psi	Remarks
Production-Interference Test, June,1976	RRGE 3	Drawdown (0-18 hours)	Variable Discharge	12,000	$1.31/r_w^2$	$r_w \approx 36$ feet; if $\phi CH = 10^{-3}$ ft/psi
		Drawdown and build-up (0-316 hours)	Variable Discharge	6,400	$0.864/r_w^2$	$r_w \approx 29$ feet; if $\phi CH = 10^{-3}$ ft/psi
		Build-up	Theis	5,500	$4.23/r_w^2$	$r_w \approx 65$ feet; if $\phi CH = 10^{-3}$ ft/psi
	RRGE 1	Drawdown	Theis	101,000	1.23×10^{-3}	
		Drawdown	Variable Discharge	222,000	1.65×10^{-3}	
Production Test, RRGE 2, September,1975.	RRGE 2	Drawdown	Theis	47,000	2.91×10^{-2} if r_w=1 ft.	
Interference Test, October,1975	RRGE 1	Drawdown	Theis	228,000	1.19×10^{-3}	

While it is apparent that the reservoir has limited permeability near RRGE 3, the geological conditions that have caused this decrease in permeability are not well understood. The fact that a regional continuity apparently exists between RRGE 3 and RRGE 1, as evidenced by the pressure response observed in the latter, leads to an inference that the decrease in permeability reflects local heterogeneity in the reservoir near RRGE 3.

Overall, the present test confirms that the reservoir extends for over a mile southeast from RRGE 1.

PLANNED ACTIVITIES

A fourth well, RRGE 4, is expected to be drilled by April 1977 for purposes of reinjection. More reservoir tests are planned following the completion of this well.

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CYCLE STUDIES AT LBL USING PROGRAM GEOTHM

W. L. Pope, H. S. Pines, M. A. Green, and J. D. Williams

INTRODUCTION

LBL is developing a general thermodynamic process computer code, GEOTHM.[1,2,3] This code has developed through funding from the U. S. Energy Research and Development Administration, Division of Geothermal Energy (ERDA-DGE); its principal use is for the conceptual design and optimization of geothermal power plants. However, because of its versatility, it can also be used to design and optimize fossil fuel plants, nuclear and solar plants, ocean thermal gradient plants, and hybrid combinations of the above. This report describes the GEOTHM code structure and development and some of the studies this group has conducted with GEOTHM for ERDA and the Electric Power Research Institute (EPRI).

A primary objective of the LBL cycle studies group is the documentation of GEOTHM with a user's manual. This will be accomplished with a series of in-house sponsored User-Training Sessions (beginning in the summer of 1977) for industry representatives who have expressed interest in the use of the code. Interest in GEOTHM is growing. The Bechtel Corporation has been using an earlier version of the code, and Pacific Sierra Research Corporation is accessing GEOTHM via remote terminal from Santa Monica, California.

A secondary objective of the group is to provide ongoing support to ERDA-DGE and EPRI by conducting technical and economic evaluations of contractor proposed geothermal plants and subsystems. This support requires that GEOTHM be capable of

modeling geothermal power cycles of arbitrary configuration for a variety of candidate working fluids (for binary and hybrid cycles) and fluid mixtures, for general environmental properties, site specific resource conditions, and new process component developments.

DESCRIPTION OF THE CODE

Design Flexibility

GEOTHM is being developed along similar lines as other thermodynamic cycle programs, for example, GEOCOST, developed by Batelle Pacific Northwest Laboratory,[4] but emphasis at LBL is toward a more flexible and efficient code with strong thermodynamic or technical characterization of process elements.

GEOTHM is a versatile thermodynamic cycle simulator for a number of reasons:

1. The thermodynamic processes are modularized into fundamental building blocks. These blocks may be arranged in many different ways to simulate virtually any type of flash, binary, total flow[5] or hybrid geothermal system.

2. The calculation of the fluid thermodynamic properties is separated from the thermodynamic process calculation. This factor facilitates the development of new process models and the packaging of a separate fluid properties program.

3. The program is fast. Due to recent improvements in all of GEOTHM's iterative convergence routines, a typical geothermal power plant cycle calculation requires only about 75 milliseconds of computation time on the CDC 7600 computer.

4. In the most recent phase of GEOTHM's development, the thermodynamic cycle generator can be used like a function generator which can be driven by a mathematical optimizer routine which optimizes the design of the cycle with respect to any user-specified criterion. This single step optimization mode reconciles the manyindividual thermodynamic and cost parameters of the system, generating an optimum total system design.

5. GEOTHM's major disadvantage is its size—over 90 subroutines and 8000 Fortran statements. Since the program is so flexible, facility in the use of the input-output routines requires an initial orientation period. A fully documented user's manual is forthcoming.

The thermodynamics process routines of GEOTHM can be used to simulate various types of power plant components. These include turbines, pumps, fans, flash tanks, heat exchangers, cooling towers, condensers, steam boilers, etc. The program will design these components in sufficient detail so that a reasonable cost estimate can be made.

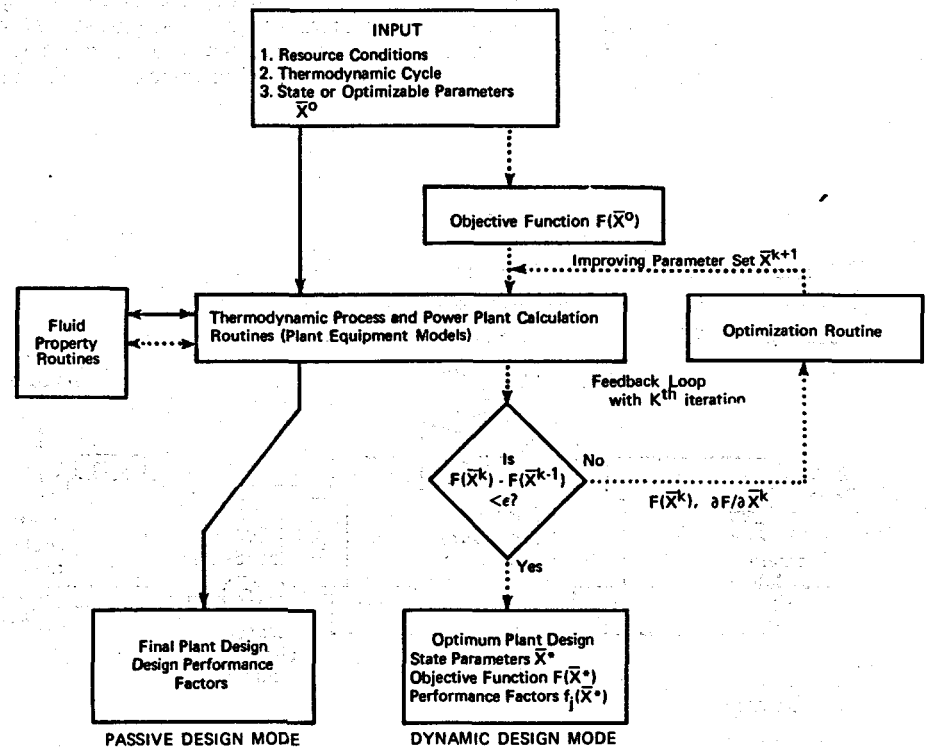

Fig. 1. A schematic flow diagram of GEOTHM operating in passive and dynamic modes (solid flow lines are passive design mode; dotted flow lines are dynamic design mode). (XBL 766-2935)

Since the process routines are modularized, new equipment models can be added. For example, the program currently models four types of counter flow heat exchangers with overall coefficient, U, as input. More recently, subroutines have been written and tested for the detailed design of complex exchangers:[6] general multipass, cross flow shell and tube types with typical commercial shell side leakage characteristics.[7] This design technique will be expanded for condensers and boilers and incorporated into GEOTHM early in 1977.

The greater part of the GEOTHM program is devoted to the calculation of working fluid thermodynamic properties. GEOTHM uses several equations of state[8,9,10] to describe the properties of over 30 pure substances. Most recently we have programmed an NaCl brine properties model developed by Pitzer and Silvester[11] of UC which is valid for temperatures in excess of 300°C and dissolved soild concentrations up to 300,000 ppm.

Thermodynamic Cycle Design: The Passive Mode

GEOTHM designs a geothermal power plant according to the logical scheme depicted in the simplified flow diagram (Fig. 1). The user specifies the following input data: resource and sink conditions, net power production constraint, the configuration of the thermodynamic cycle, and the thermodynamic efficiency and cost factors for the various components in the plant. GEOTHM also requires a set of thermodynamic cycle or 'state' parameters which provide the minimum information necessary in order to calculate the thermodynamics of the entire plant.

As an example, the simple bi-fluid cycle in Fig. 2 is completely specified by the following six state parameters: (1) turbine inlet pressure, (2) turbine inlet temperature, (3) condenser exit temperature (assuming saturated liquid), (4) the pinch point temperature difference across the brine heat exchanger, (5) pinch point temperature difference across the water cooled condenser, and (6) the cooling tower approach to wet bulb temperature.

Given the system state parameters and other required input data, the thermodynamic process and fluid property routines which constitute the heart of program GEOTHM will design the plant to satisfy the net power production constraint. In designing the plant, the program calculates and prints out a set of system design performance factors such as cycle efficiency, resource utilization, fluid mass flows, heat exchange areas, equipment power requirements, and the associated costs of this equipment. Since for fixed efficiency and cost factors, the final plant design is completely determined in GEOTHM by the user-dictated set of system state parameters, the program is defined to be operating in the "passive design mode."

Thermodynamic Cycle Optimization: The Dynamic Design Mode

The logical structure of the passive design mode permits the program to serve as a function generator which is steered by an optimizer routine which optimizes the design of the thermodynamic cycle with respect to that particular function. This is achieved by introducing the optimizer routine as a feedback loop modification of the passive design mode.

The user initiates the optimization process by inputing a first-guess set of system state parameters, now called optimizable parameters. The user must also specify which one of the system's

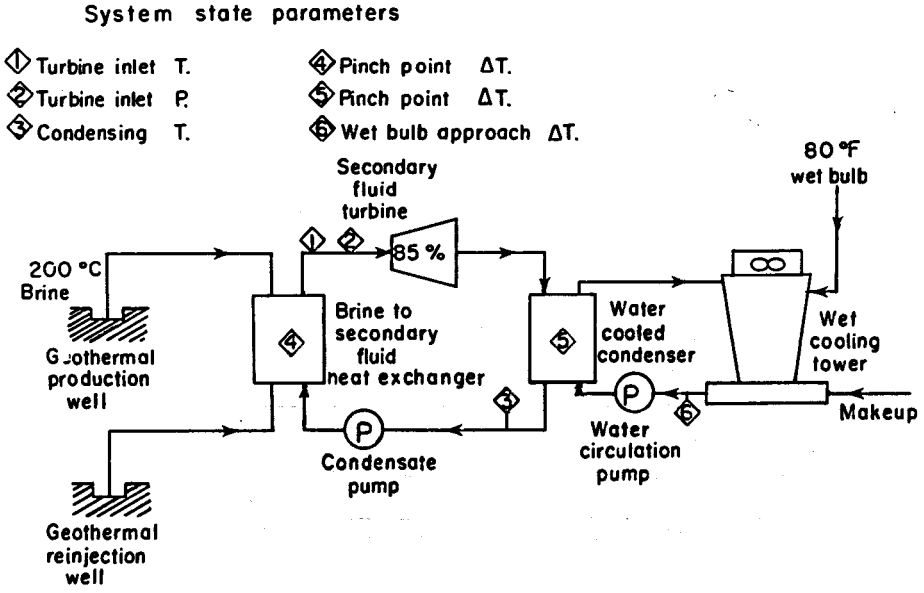

Fig. 2. Simple binary geothermal power plant cycle. (XBL 768-3899).

particular design performance factors is the objective function to be minimized or maximized. The optimizer then steers the program in an iterative fashion and computes an improving sequence in the set of optimizable parameters which rapidly converges upon the optimum system design. When the optimizer routine directs the program to design and optimize the system, GEOTHM is defined to be operating in the "dynamic design mode."

Any of the thermodynamic cycle's design performance factors can be singled out as the objective function to be minimized or maximized by the optimizer. Some example thermodynamic objective functions include maximum cycle efficiency and maximum resource utilization. Example cost objective functions are minimum busbar cost of energy and minimum plant capital cost.

The dynamic design mode is best illustrated in the following manner. For a fixed set of efficiency and cost factors, the design of the simple binary plant in Fig. 2 is completely determined by the previously described set of six optimizable parameters. The set of all possible designs for this plant can be described by a design surface in a 7-dimensional mathematical space corresponding to the six optimizable parameters and the objective function. For purposes of visualizing this surface, four of the six optimizable parameters can be frozen at their optimum design values.

The three dimensional computer generated plot illustrated in Fig. 3 was done the above way and depicts possible turbine inlet conditions for the plant. The x and y axes represent the turbine inlet pressure and turbine inlet temperature respectively, while the z-axis measures the busbar cost of energy for a specific turbine inlet design point on the design surface. Theoretically, there are an infinite number of possible turbine inlet conditions, each corresponding to a different plant design, which define this continuous landscape-like surface. For all such designs, however, there exists a single unique optimum design which minimizes the value of the objective function. This optimum design corresponds to point of minimum elevation on the design surface which on this plot, corresponds to the point of inter-

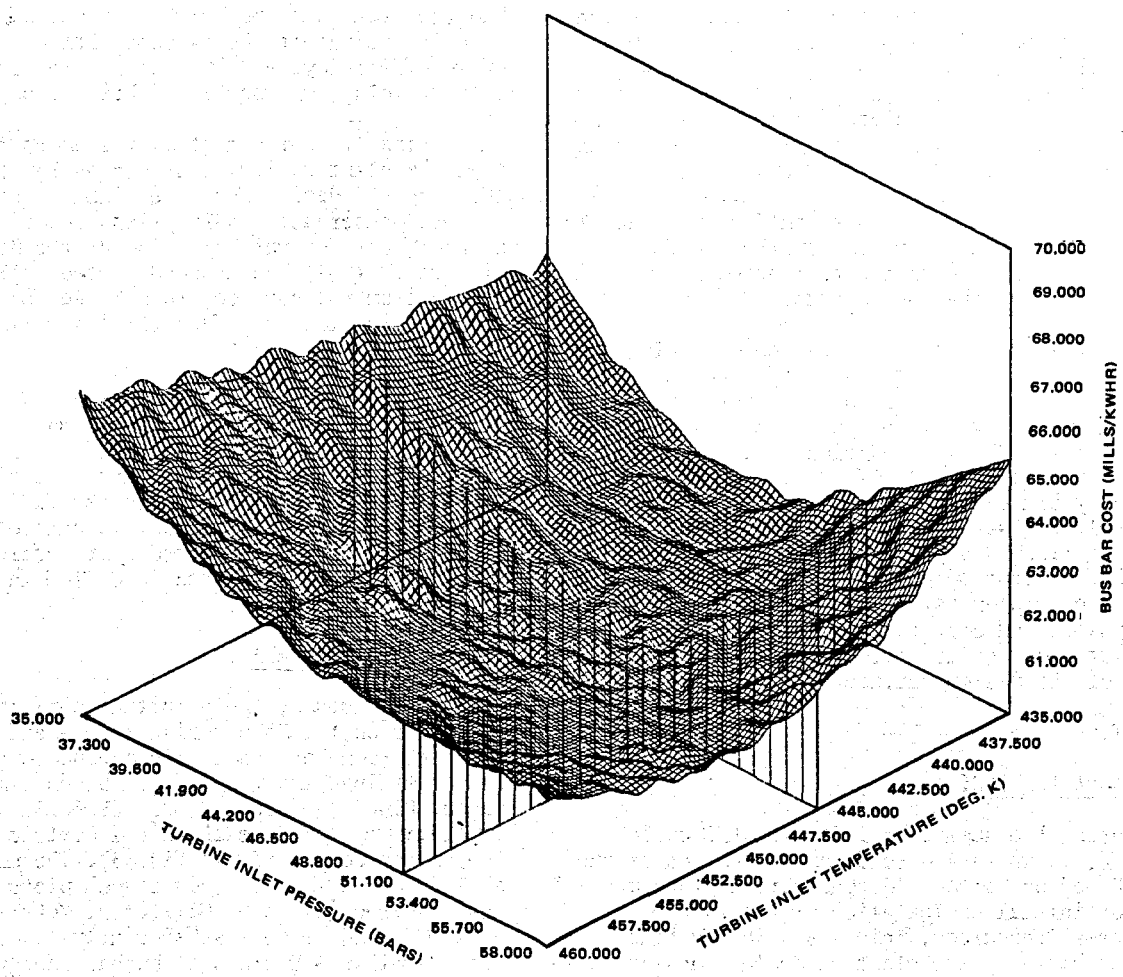

Fig. 3. Energy cost design surface for a 50 MWe binary cycle power plant-isobutane (Ref. 15). (XBB 769-8095)

section of the two reference planes.

Given a first-guess plant design corresponding to a particular point on the design surface, the optimizer calculates the local curvature of the surface in the vicinity of this point. Utilizing this information about local surface curvature, the optimizer generates a sequence of steps along the surface which rapidly converge upon the optimum design point. This process is analogous to a stream with headwaters in the high country whose flow is guided by the combined forces of gravity and local topography to seek out the lake at the bottom of the gravity potential well. Assuming that there is one unique global minimum elevation on this landscape, the water will always flow into the same lake for any given point of origin. In a similar fashion, the optimizer will always converge upon the optimum design for any reasonable initial-guess design. Typically, only about 300 design points or cycle calculations are required for cycle optimization beginning from an arbitrary first-guess design.

The efficiency of this optimizational mode becomes apparent when contrasted with standard multi-parameter optimization methods. These brute-force methods actually construct the entire design surface by computing all possible design permutations in the n-dimensional design space and then comparing the values of their objective functions for the minimum value. To achieve the same resolution as the design surface illustrated here, which was computer generated from a 30 by 30 grid of design points, brute-force would require 30^6 separate cycle calculations. This would require nearly 1.75 years of computation time on the CDC 7600 computer, whereas the same optimization run with GEOTHM takes less than 30 seconds.

Typically, three of the six optimizable parameters – the heat exchanger and condenser pinch-points and the wet bulb approach temperature– are fixed at some practical design value. Only the turbine inlet and exit conditions are varied in order to bring the number of cycle calculations required by brute-force optimization to a manageable level. By sacrificing these degrees of freedom, the optimum design determined by brute-force cannot be the true optimum design for the total system. The complex nature of the interacting thermodynamic and cost relationships which govern a total system design is vividly reflected in the texture of the design surface.

APPLICATIONS

LBL Support for EPRI

During the summer of 1-76, the LBL cycle studies group was asked to do an evaluation of the first "Proof of Concept" demonstration plant proposed for initial exploitation of the vast U. S. hydrothermal resources. This was a 50 MWe binary cycle geothermal power plant conceptual design[12] for the Heber reservoir proposed by the Ben Holt Company to EPRI. This evaluation came at a very opportune time because it allowed us to test the recently developed optimization algorithm on a binary cycle of great practical significance.

LBL adopted the following self-imposed objectives for the review:[13]

1. Verify Holt's design objective (i.e. minimum energy cost? maximum yield?);
2. Investigate plant and energy cost reductions through multi-parameter optimization;
3. Perform sensitivity studies in areas not investigated by Holt.

Initially passive mode calculations were performed to allow us to check the accuracy of our computer model vs. Holt's. The agreement was excellent. The dynamic mode was then used with maximum yield as the objective function using 3 parameter optimization. We found that Holt's baseline binary design clearly had maximum energy yield as a design basis – by our calculations, Holt's design was within 0.3% of maximum achievable yield for his assumed exchanger pinch point delta T's.

Then with our direct and indirect cost factors normalized to Holt's, we found that with 6 parameter optimization, the overall 50 MWe plant cost could be reduced by about 13% ($3.7M). This had the companion benefits of about an 8% reduction in the busbar energy cost without affecting cycle efficiency, and only an 11% reduction of energy yield (Kwhr per lb of brine flow).

Finally, our sensitivity studies indicated that the plant capital cost and energy cost of the proposed design would be significantly affected by more conservative assumptions regarding the exchanger cost per unit area and/or the design well flow rate. (Holt had assumed pumped wells, shafts driven from the surface, to achieve about a 45% increase in flow over free flowing wells at the Heber site.)

Our study of the Holt design was later reviewed by principals within EPRI, and we have been asked to include hydrocarbon mixture routines to GEOTHM's fluid properties package for similar follow-on perturbation studies in the fall of 1977 when Holt's next design study is completed. Starling's hydrocarbon mixture properties routines[14] will be adapted to GEOTHM in the summer of 1977 for this work.

LBL Support for ERDA

Intrigued by these initial optimization successes on the Holt design review and the exceedingly complex trade-offs conducted by GEOTHM in optimizing binary cycles in seven dimensional space, Pines and Green[15] used GEOTHM's output capacity to produce the 3-D isometric plots of the energy cost surface (Fig. 3). The unique capability of GEOTHM to produce such plots at low cost was recognized by Clifton B. McFarland of ERDA-DGE, and we were subsequently asked to generate similar 3-D plots of busbar energy cost as a function of resource temperature and resource utilization efficiency, η_{RU},[16] for various standard geothermal processes.

A brief study of the energy cost, resource

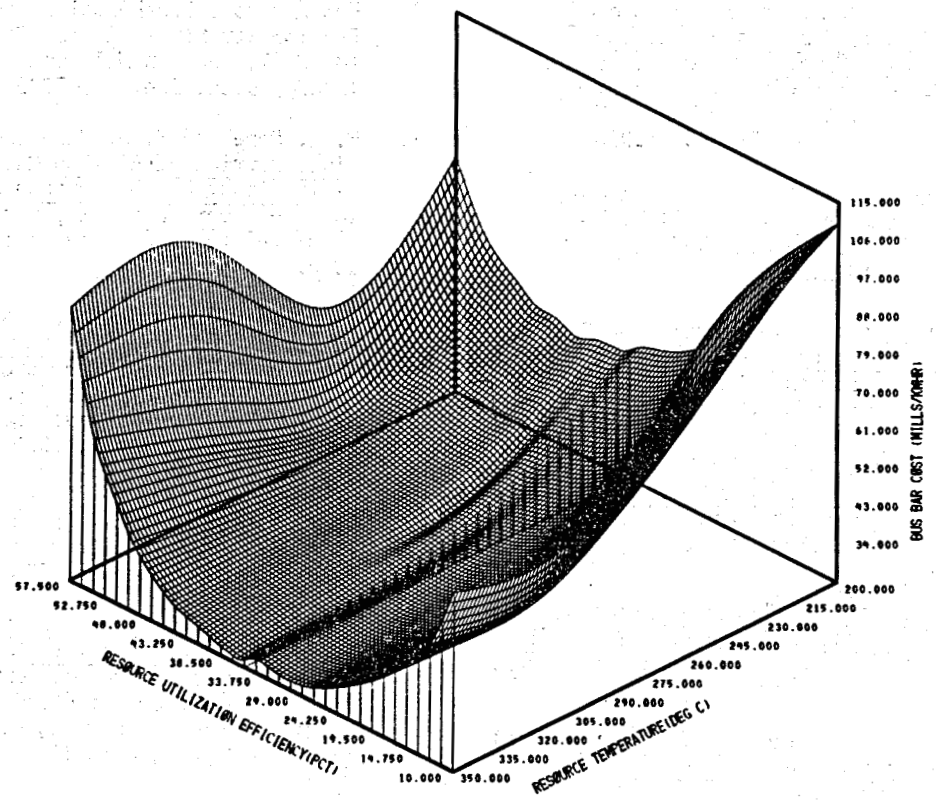

Fig. 4. Energy cost as a function of resource temperature and resource utilization efficiency for a 50 MWe binary cycle-isobutane (Ref.17). (XBB 772-1274)

utilization efficiency, and resource temperature (EC-RUE-RT) surface for simple binary cycle plants was conducted,[17] and the results were presented to the third meeting of the "Centers of the Analysis of Thermal-Mechanical Energy Conversion Concepts" panel headed by Joseph Kestin.

Figure 4 is an EC-RUE-RT surface for a typical 50 MWe, binary cycle power plant with pure isobutane as the working fluid. Plots of this type are quite general and useful for developing cost effective design criteria for all energy cycles. Resource utilization efficiency, η_{RU}, as defined here is a ratio of the resource energy extracted in the process to the maximum available energy, and unlike a Carnot Efficiency, η_{RU} has physical meaning for all thermal processes in which the resources are limited--in other words, all processes.

The LBL cycle studies group has been directed by ERDA-DGE[18] to continue this work with a high priority, and our plans for other fluids and geothermal processes will be detailed to Prof. Kestin's panel when it meets at LBL in January 1977.

LBL Support to ERDA Contractors

H. S. Pines and GEOTHM are currently collaborating with engineers from Pacific Sierra Research Corporation in the conceptual design and optimization of a large geothermal, preheated, coal fired power plant suggested to help meet future energy needs of the city of Burbank, California.

SUMMARY

This paper has demonstrated a number of applications for which program GEOTHM can be used. The application of the program is by no means limited to the cases described, nor is it limited only to geothermal power cycles. It is expected that program GEOTHM can be applied to a host of thermodynamic systems which use a variety of working fluids to generate mechanical power, refrigeration, or transfer thermal energy from one place to another. Program GEOTHM is growing; its development is not complete. This report represents program GEOTHM as a photograph represents a growing child.

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GEOTHERMAL SUBSIDENCE RESEARCH - LEAD PROGRAM MANAGEMENT

T. L. Simkin

INTRODUCTION

The purpose of Lead Program Management is to take a major research issue such as potential geothermal land subsidence, and develop a comprehensive research program to discover means to assess, control and mitigate impacts to an acceptable degree. Such research would support the research needs of the Energy Research and Development Administration.

The individual research projects formulated for this program were prepared so that research may be contracted to selected capable organizations. Thus, the research projects are described in the form of outlined scopes of work within a document which will be publicly available. This document will be produced as an LBL report and will be entitled "Geothermal Subsidence Research Program Plan." The Research Program Plan includes a description of the total integrated geothermal

subsidence research schedule, the major research categories and priorities for individual research projects to be undertaken.

Two teams of professionals were used to develop the program plan. One team basically prepared the plan and the other reviewed and recommended changes. The first team consisted mainly of LBL personnel, and the second team came from independent industry, academic and government organizations.

Need for Research

Development of alternative energy sources is moving ahead in a number of fields including geothermal. Many opportunities are available for development of these resources. However, constraints have been identified that may actually restrict development. Geothermal energy is not without its own set of potential development problems. Removal or injection of geofluids from or into geological formations has been known to induce seismic phenomena and land surface and subsurface deformation under certain conditions. The research program conducted by LBL focuses on the latter issue of land formation deformation, commonly referred to as "subsidence."

Unexpected and uncontrolled land deformation may have major social, environmental and economic consequences. However, varying degrees of subsidence occurring under controlled conditions may be entirely acceptable.

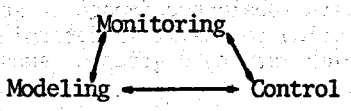
The goal or objective of geothermal subsidence research is to control or mitigate potential geological formation displacements associated with geothermal development within acceptable limits. In this way, acceptable geothermal programs will proceed without delays, and siting flexibility will be increased.

Successful subsidence research will provide:

1. The means for developers to build and operate geothermal facilities within accepted degrees of potential land deformation, and
2. The basis for policy makers to approve and monitor such facilities.

INTEGRATED RESEARCH ACTIVITIES

The framework for successful geothermal energy facility planning and development in the future will consist of the interaction of three major activities:



Integrated regional and site specific surface monitoring combined with advanced instrumentation and techniques to measure subsurface geological formation movement will be used. Based on geological information, models could predict the rate and degree of potential movement from the reservoir up to the land surface. Specific control methods, such as well location and injection processes, would be used.

Based on the anticipated inter-relationships of monitoring, modeling and control programs, the facility development could be approved. Once production of geofluids started, the monitoring results could be continuously compared to the limits anticipated in the model. Changes in the control process would then be directed by the results of such comparisons.

SUMMARY REVIEW OF RESEARCH CATEGORIES AND PROJECTS

Summary descriptions of the major recommended research encompassed by the total geothermal subsidence program are presented below. Detailed descriptions of the individual research programs will be found within the Research Program Plan to be issued by LBL and previously described in the Introduction.

The major research categories are:

1. Development of direct monitoring instrumentation and techniques necessary to assess differential vertical and lateral deformation at substantial depth within the reservoir and overburden;
2. Development of a methodology to monitor vertical and horizontal ground movement in order to distinguish between subsidence directly related to a geothermal facility and subsidence caused by other man-induced phenomena, or natural stresses;
3. Evaluation of the economic effects caused by varying degrees of geothermal land subsidence related to physical systems, such as structures, and environmental factors, such as drainage patterns;
4. Development of indirect field methods for estimating deformation at depth, such as geophysical techniques and instrumentation;
5. Development of case histories and subsidence risk evaluations based on field related studies;
6. Evaluation and ultilization of geothermal subsidence models;
7. Investigation of the physical processes of subsidence;
8. Laboratory testing;
9. Development of reservoir operational policy that will minimize the adverse effects of land subsidence and maximize the production of geothermal energy.

Each category requires one or more research projects depending on the scope of the work required to meet the objectives. Work packages or projects within each category are organized based on recognition of several factors, including:

1. Specialist organizations will be selected to perform complete projects.

2. Projects will be scheduled so that results from one project will be available to other related projects.

Six research projects are anticipated to be initiated in FY 1977. The completion of the total R & D program as outlined below is scheduled for FY 1980.

Research Project Abstract

- Category 1. Development of Direct Monitoring Instrumentation and Techniques Necessary to Assess Differential Vertical and Lateral Deformation at Substantial Depth.

Present methods for measuring or assessing differential compaction at depth in a well are limited. The need is great to improve capabilities for the anticipated depths and hostile environments of geothermal formations.

Research Objective: Develop the capability to measure vertically between two points in a geological formation at substantial depths. Measurements will be made under the hostile conditions of temperature, pressure, salinity and potential for corrosion that exists in geothermal reservoirs. Accuracy desired is 0.05 foot per 100 feet of interval distance. There is a desire to measure lateral movement, but the current emphasis is directed toward vertical deformation.

Project 1. Assess the state-of-the-art and recommend concepts for prototype development.

Present capability for measuring differential compaction or expansion at depth is limited. However, the capabilities of available instruments will be evaluated and means for upgrading these capabilities will be investigated. A survey of instrumentation suppliers and researchers will be conducted to identify opportunities for using advanced instrumentation technology. New measurement concepts will be identified, if possible. A program scope of work will be prepared for each promising concept which will include recommendations for prototype development, field testing, and performance evaluation.

Project 2. Develop prototypes and conduct field testing.

Prototypes will be developed for each of the most promising concepts. Laboratory testing and calibration will be performed. The prototypes will be field tested and their performance will be evaluated.

- Category 2. Development of a Methodology to Monitor Vertical and Horizontal Ground Movement to Distinguish Between Subsidence Directly Related to a Geothermal Facility and Subsidence Caused by Other Man-Induced Phenomena or Natural Stresses.

A geothermal development program needs methodology guidelines appropriate for monitoring horizontal and vertical ground displacements associated with geothermal operations both at the surface and at depth, for the purpose of differentiating between subsidence resulting from a geothermal project and subsidence that may be caused by other activities of man or nature. Recent efforts have been initiated in this area. However, no general guidelines for acquiring and analyzing relevant baseline data are available.

Research Objective: Provide methods and guidelines for planners to use for distinguishing between subsidence directly related to a geothermal project and subsidence caused by natural or other phenomenon. A guideline cannot take the place of a detailed field investigation by a competent geologist. Thus, the emphasis is on developing information to a level suitable for plannners to use as guidance in developing or assessing the appropriate field investigations and monitoring programs. The research project in this category will be accomplished using two projects.

Project 1. Develop a methodology for field investigations and monitoring programs based on available information.

Several representative geologic settings will be identified. The topography, structure and rock competence of these settings will be investigated as they relate to requirements for specifying effective field studies and monitoring programs. Information requirements will be determined for specifying the predevelopment condition of the land surface and for monitoring over the lifetime of the geothermal development. Methods will be identified for acquiring field information of suitable quality and precision for performing interpretive analyses.

Project 2. Revise the methodology in the future based on availability of advanced technology.

(Note: Project 2 is scheduled to begin when Research Category 1 is nearing completion.)

- Category 3. Evaluation of the Economic Effects Caused by Varying Degrees of Geothermal Land Subsidence Related to Physical Systems and Environmental Factors.

Assuming that there are acceptable limits of subsidence, it follows there is need for evaluation criteria. A framework needs to be developed so industry and the public can understand the economic risks associated with geothermal subsidence.

Research Objective: Quantify the costs associated with subsidence damage or subsidence effect mitigation to assist in determining the extent to which varying degrees of subsidence will be accepted.

Project 1. Collect available information.

Areas will be identified that have experienced or are experiencing land deformation. Methods will be developed to acquire information on damage costs and costs associated with mitigating measures. Questionnaires and interviewing techniques may be used, since a preliminary review of the available

literature results in identification of only a few useful sources. The acceptability of subsidence and associated consequences will be investigated.

Project 2. Evaluate the economic implications of subsidence.

Subsidence damage costs and subsidence control costs will be determined for several geothermal development scenarios based on factual information of areas known to potentially undergo geothermal production. The range economic risk will be assessed based on the experience developed in Project 1 above. The critical issues will be identified as they relate to the acceptability of varying degrees of subsidence in various settings.

Alternative means for resolving the issues will be investigated as well as costs associated with alternatives.

- Category 4. Development of Indirect Methods for Estimating Deformation at Depth.

Instrumentation is available, in some cases, to measure some reservoir properties.

However, new instrumentation and/or techniques to measure selected indicators of formation deformation is needed. Geophysical techniques would be considered and included in the "indirect methods" category.

Research Objective: Develop the capability to measure geothermal reservoir parameters indirectly related to the displacement and differential compaction occurring during geothermal production and injection of fluids and develop a methodology for estimating the degree of related deformation in the geologic structure.

Project 1. Evaluate available methods and recommend concepts for prototype instrumentation or technique development.

The available methods will be evaluated for estimating deformation in the geologic structure based on measurement of the rate of change in geothermal reservoir properties such as: density, fracture characteristics, temperature, pressure and fluid composition. New methods will be devised, as required, for making these measurements. Concepts for prototype instrumentation will be recommended for cases where available instrumentation will not meet the performance requirements. A field testing program will be developed and methods devised for correlating data from the field tests with direct measurements taken of displacements in the geologic structure.

Project 2. Develop and test prototypes.

Prototypes will be developed and built, as required. Laboratory tests to verify the precision of the instrumentation will be conducted. Direct and indirect field measurements will be correlated and the adequacy of selected indirect techniques will be assessed.

- Category 5. Development of Case Histories and Subsidence Risk Evaluations Based on Field Related Studies.

This research category includes required research based on the field related study. Included is a research project to selectively evaluate subsidence history based on specific case histories and the development of subsidence risk maps of specifically selected areas likely to undergo geothermal development.

Project 1. Assess and document selected case histories of land deformation attributed to geofluid extraction and injection.

Case histories will be assessed and documented in order to provide the developer and government planner with specific descriptions of actual land deformation as it relates to the extraction and injection procedures of geofluids. Case histories will not be limited to geothermal fields but rather encompass other forms of geofluid management, such as hydrocarbon and groundwater systems.

Project 2. Develop subsidence risk maps for selected potential development areas.

In a manner similar to the concept "seismic risk maps", the degrees of severity of potential subsidence will be mapped based on specifically selected indicators within major areas likely to undergo geothermal development.

- Category 6. Evaluation and Ultilization of Geothermal Subsidence Models.

In planning the development of a particular geothermal reservoir, it is desirable to have the appropriate analytical tools available to estimate potential formation movements so precautionary or mitigating measures can be planned. Several mathematical models have been developed into predictive tools. However, the capability of present models to provide accurate predictive results has not been verified.

Research Objective: Assess the adequacy of available computer models by applying them to field situations and recommend future modeling programs that should be undertaken as part of the geothermal subsidence research.

Scope of Work: Select available subsidence models and assess the adequacy of the predictive capability. Subsidence models available to the Subsidence Research Program will be selected. These models will be those available for use by developers and public planning officials. Models that are proprietary in nature may not be appropriate for widespread use and will be selected only under special circumstances.

A list of performance evaluation parameters will be selected. These parameters will provide a basis for comparing the overall performance of the various models selected for study. Parameters will include; input data requirements, degree of com-

plexity, expense of operation, and accuracy of results. The models will be exercised and the results compared using actual historic data and simulated base data. Procedures will be developed for performing a study of sensitive input parameters for each model. The performance of each model will be evaluated including results of the sensitivity analysis. Recommendation for future modeling research will be prepared, as required.

- Category 7. Investigation of the Physical Processes Subsidence.

Subsidence computer codes and analytical instrumentation are based on theory regarding the physical processes of deformation. Developers and public planning officials will analyze geothermal development alternatives; evaluating the issue of subsidence and, at the same time, striving for maximum reservoir productivity. It is expected that research related to skeletal displacement will be necessary to predict accurately cumulative vertical and lateral movement at the land surface caused by the extraction of geofluids.

- Category 8. Laboratory Testing.

The quantitative compaction or compressive characteristics of material from large depths in geothermal formations are for the most part unknown. If it can be shown that volume changes are negligible due to geofluid extraction, which may well be the case for materials previously consolidated to pressures corresponding to a few thousand meters of overburden, then subsidence accompanying development and operation of such geothermal fields would be caused by other mechanisms. Cataclastic movement of fractured material might then be investigated as the major contributor to deformation.

- Category 9. Development of Reservoir Operational Policy.

Research performed in the previous Categories will provide knowledge and information regarding the physical processes of subsidence, the means to estimate potential ground deformation, and the guidelines for judging the economic effects of varying degrees of subsidence. This knowledge and information needs to be applied directly to current and future goethermal reservoir operations. The research in this category will develop practical reservoir management practices as guidelines for use by planners, developers and operations personnel and will provide the means for applying the results of the total subsidence research program.

Research Objective: Develop guidelines and procedures for use by planners, developers and operators of geothermal projects. The guidelines and procedures will assist in developing and operating a geothermal reservoir in a manner that will tend to minimize the effects of subsidence and maximize the reservoir ultilization.

Research Project 1. Acquire reservoir management information and review current research results. Information will be compiled pertaining to present problems facing operators of geothermal projects. Problems may include: well spacing and location, injection techniques, and monitoring methods. A review of the results of research from the Geothermal Subsidence Research Program will be conducted. The adequacy of current research will be assessed as it relates to reservoir management issues based on operational problems.

Research Project 2. Develop operational guidelines and procedures for planners, developers and operators of geothermal projects. The dynamics of the operations management decision making process will be identified. General principles for reservoir operations decision making will be identified. Opportunities for using management tools, such as computer models and monitoring systems, will be investigated. Guidelines and procedures will be developed for planners, developers and operators to use in maximizing the energy obtained from a geothermal reservoir while minimizing the effects of potential subsidence.

- Recommended Baseline Program for Monitoring Networks to Measure Vertical and Horizontal Ground Movement

The following recommended program has not been included in the previous nine major research categories. However, the need for such baseline data development is great and a detailed program is outlined in the Research Program Plan to be issued as an LBL report.

Standard equipment and techniques are presently available for precise monitoring on the land surface of vertical and horizontal ground movement. Today, at a relatively low-cost, high precision networks can be surveyed to detect both natural and induced movement. Such monitoring networks need to be developed at each producing and prospective geothermal field.

NUMERICAL MODELING OF CYCLIC STORAGE OF HOT WATER IN AQUIFERS

C. F. Tsang, M. J. Lippmann, C. B. Goranson, and P. A. Witherspoon

INTRODUCTION

The concept of hot water storage was suggested in 1971-1973 for the purpose of conserving large amounts of heat now wasted in generating electricity and reducing thermal pollution caused by discharge of this waste heat. In addition, success of this concept appears to be necessary to make large-scale total energy systems feasible. Up until recently only very crude studies have been made of the feasibility and efficiency of such a storage system.

During the middle of this year, we developed a computer model at LBL to numerically simulate cyclic storage of large amounts of heated water in a typical aquifer system. The program CCC, which stands for compaction-conduction-convection, was designed to simulate 3-dimensional transient flow of both fluid and heat in an aquifer.

ACCOMPLISHMENTS DURING THE CURRENT CALENDAR YEAR

The first step in the project was to determine the accuracy of the program, CCC, by simulating cases where analytic or semi-analytic solutions were available. Three different cases were studied; the results are quite satisfactory; and we are confident that the program CCC works properly. We then proceeded to look in detail at a particular aquifer storage system. Cyclic storage periods were determined appropriate for the storage system to be used with electrical generation turbine power plants. The idea was to utilize waste heat from turbine exhaust for heat loads such as for district space heating and air conditioning. Heat could be distributed to users through heat manifolds interconnected with the steam plant, underground storage, and users' dwellings. A cycling period covers the following four parts:

1. 90 days injection into aquifer storage system during summer months when heat loads are small and electrical demand high;
2. 90 days rest during autumn months when heat loads approximately equal electrical loads;
3. 90 days production of stored energy during winter months when heat loads are high;
4. 90 days of rest during spring.

A cycle was termed as one 360 day period with one injection, one production, and two rest periods. The storage system is simulated for five cycles when energy recovery percentage is found to reach a limiting efficiency value as can be seen in Fig. 1. For a case where the well penetrates half way into the aquifer, an efficiency as high as 94% energy recovery was obtained in the fifth cycle. Simulation for the full-aquifer penetration case also showed energy recovery about 90%.

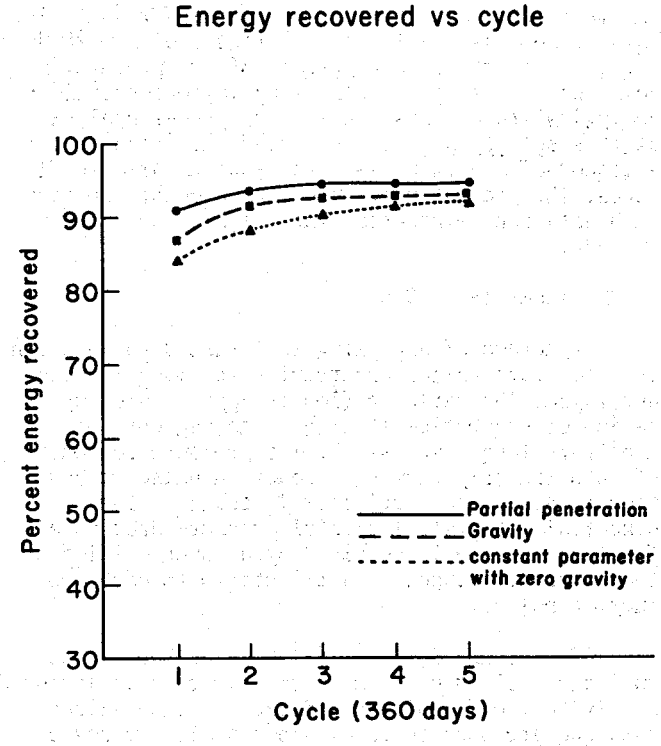


Fig. 1. Energy recovered vs cycle.
(XBL 7612-4523)

This study shows that the possibility for storing large amounts of heated water in an aquifer is quite feasible.

PLANNED ACTIVITIES FOR NEXT YEAR

We are at this time considering a simulation of storage for use in conjunction with a solar energy collection system. We are also planning to perform a parameter study for determining effects of different cycle periods, temperature flow rates, and material properties.

ANALYSIS OF WELL TESTS WITH VARIBLE DISCHARGE

C. F. Tsang, D. G. McEdwards, T. N. Narasimhan, and P. A. Witherspoon

INTRODUCTION

The conventional method of well test analysis necessarily assumes a constant rate of discharge of the producing well. The procedure involves matching a log-log plot of test data (drawdown versus time) to a dimensionless log-log plot that reflects the anticipated analytical behavior of the well test data when the production well is modeled as a continuous line source of constant strength. Well test situations may arise, however, wherein the production rate is not constant. For example, when collecting samples from a geothermal well for chemical analysis, a step-wise increasing or decreasing flow rate of the production well is preferred. Another more immediate example is provided by a set of well

test data recently obtained at the Raft River Geothermal Field in Idaho and sent to LBL for analysis. This set of data reflects the effects of a marked variation in the discharge rate of the production well and is not completely amenable to conventional analytical techniques. It was the proper analysis of this set of data that prompted the research for a method of analyzing well tests with variable flow rates. The present paper presents a method whereby such data can be handled. The research work began in 1976.

ACCOMPLISHMENTS - 1976

A method of analyzing well test data in which the flow rate varies arbitrarily in time has been developed. The variable flow is approximated by a series of sequential straight line segments of arbitrary length and slope. The pressure response of each linearly varying production pulse at any time is derived analytically in terms of the exponential integral. The total pressure drop as a function of time is obtained by a superposition of the reservoir responses attributable to each production pulse.

To account for the influence of boundaries, an image well is used whose contribution is included simply in the formula by addition. The equations obtained are used to calculate drawdown values of a type curve that correspond to a specified flow rate variation and a set of assumed reservoir parameters. With a set of initial guess values of reservoir parameters, a miltiparameter least-squares-fit computer routine is employed to compare well-test drawdown data with predicted type-curve values to search for the best set of reservoir parameters. Thus values for transmissivity, storativity, and the image well distance are determined. Both interference and production tests can be analyzed. In the latter case work is in progress to account for the influence of well bore storage and skin effect, also in a parametric fashion.

The method has been applied to data from seven well tests to evaluate its utility (see Table 1). Three of the analyses involve theoretically generated well test data and four analyses involve field data. The field data were from two well tests conducted at the East Mesa Geothermal Field in southern California and from two well tests conducted at the Raft River Geothermal Field in southern Idaho. The three theoretical cases involve well test data calculated assuming: (1) constant discharge, (2) variable discharge in steps, and (3) exponentially decaying discharge. Three of the four field tests were constant discharge interference tests. In two of these constant discharge tests the presence of a boundary was detected. The last remaining field test involved a discharge rate with a very wide fluctuation.

In all of these cases, a solution was possible and an unambiguous set of reservoir parameters was determined. In the three tests using generated data, the known parameters are reproduced. The analyses of the first three field interference tests yielded reservoir parameters consistent with parameters obtained by the conventional type curve fitting procedures. In the last field case, of strongly varying discharge, which is difficult if not impossible to handle conventionally, the program has successfully yielded reasonable parameters. Figures 1 and 2 show respectively the theoretical case of exponentially decaying discharge rate and the analysis of the Raft River #3 production test, in which the flow rate varied markedly. In the figures, the circles represent observed drawdown

Table. 1. Well tests analyzed by variable flow method.

CASES	Discharge		Barriers		Type Test	
	Constant	Variable	None	Impermeable	Interference	Production
Test Data						
Constant Discharge	●		●		●	
Stepped Discharge		●	●			●
Exponential Decay Discharge		●	●			●
Field Data						
East Mesa Well 6-1	●		●		●	
East Mesa Well 31-1	●			●	●	
Raft River No. 2	●			●	●	
Raft River No. 3		●	●			●

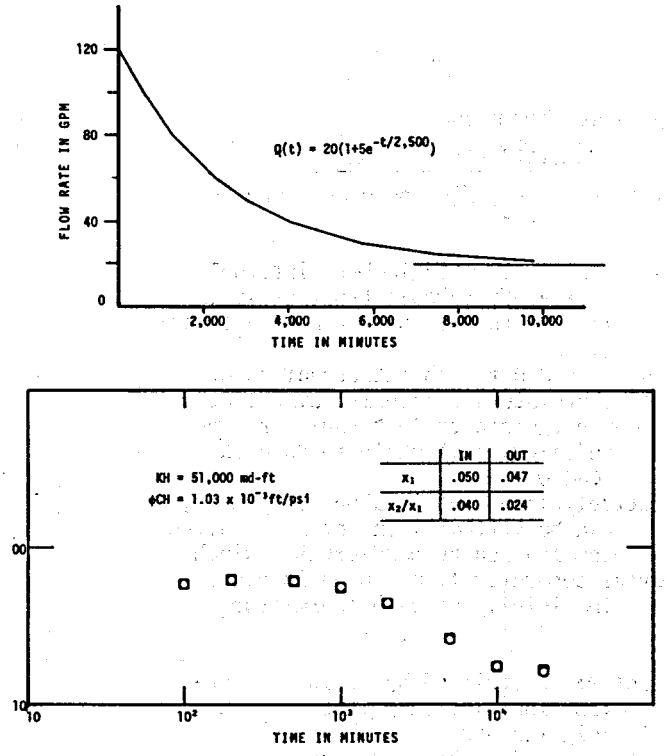


Fig. 1. Exponential decay of discharge. (XBL 773-7923)

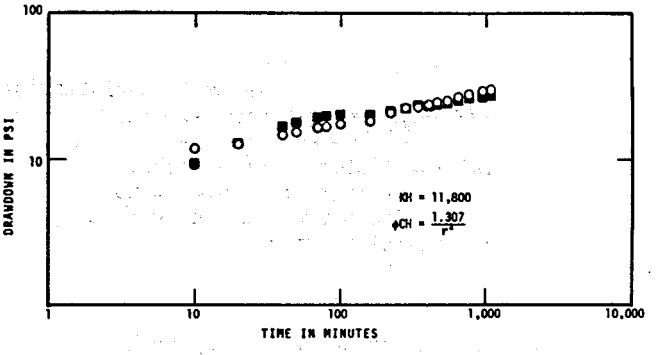


Fig. 2. RRGE 3 Production test. (XBL 773-7924)

data and the squares represent the best-fit drawdown values.

PLANS FOR 1977

Applications of the method will be made in the analysis of field data obtained in the LBL geothermal well testing program. Furthermore, the method will be extended to include the effects of skin and well-bore storage which are important for short time data.

GEOTHERMAL ASSESSMENT OF CALIFORNIA STATE-OWNED SUBMERGED LANDS USING HEAT-FLOW MEASUREMENTS*

P. Wilde,† C. W. Case,† J. Oldson,‡‡ E. Binnal,§ W. Low,§ and F. Parks§

In cooperation with the California State Lands Commission, LBL has completed a study on the exploratory evaluation of the geothermal potential of three state-owned lake bottoms as a first step in the eventual geothermal evaluation of state-owned submerged lands. This project had two goals: (1) a literature search on the techniques and theories for examining the geothermal value of submerged lands[1] and (2) development of an instrument package for preliminary geothermal prospecting which could be operated by State Lands personnel from a small boat on lakes. A modified oceanographic heat-flow probe (Table 1, Figs. 1 and 2)was built by Special Projects and was successfully operated in the field on three California lakes: (a) Salton Sea (54 stations); (b) Clear Lake (89 stations); and (c) Mono Lake (70 stations - see Fig. 3).

The novel feature of the LBL-State Lands probe is that the thermal conductivity as well as the thermal gradient can be measured in place. This is accomplished by taking advantage of the self-heating properties of the measuring thermistors. Calibration work is continuing on the probes in preparation for eventual development of a self-contained package for use in the State's off-shore submerged lands.

Table 1. Characteristics of heat-flow probe.

OCEANOGRAPHIC PROBE	LBL-STATE LANDS PROBE
Two thermistors on rod probe, outrigger type attach to core barrel; may have more	Six thermistors, five on probe, one in the water
All stainless steel	Stainless steel outer jacket, internal fiberglass tube--cut-out of stainless at thermistors, exposing fiberglass
Self-contained recording package, no on-deck read-out	On-deck read-out with interrogation of thermistors controlled by operator
Single strain cable connection between probe unit and surface	Two cables: stain cable to on-deck winch, and electrical cable to on-deck read-out
Heavy, over several hundred pounds, must be raised and lowered with powered winch	Relatively light, up to about 50 pounds, can be lifted by one person, raised and lowered by hand-cranked winch
Thermal conductivity estimated or extrapolated by needle probe measurement of collected bottom sample	Thermal conductivity measured in place in vicinity of each thermistor
Weight essentially fixed by combination of probe and pressure case	Weight may be trimmed by adding or subtracting slotted weights on the weight stand
Probe and pressure case single unit	Probe may be detached and exchanged

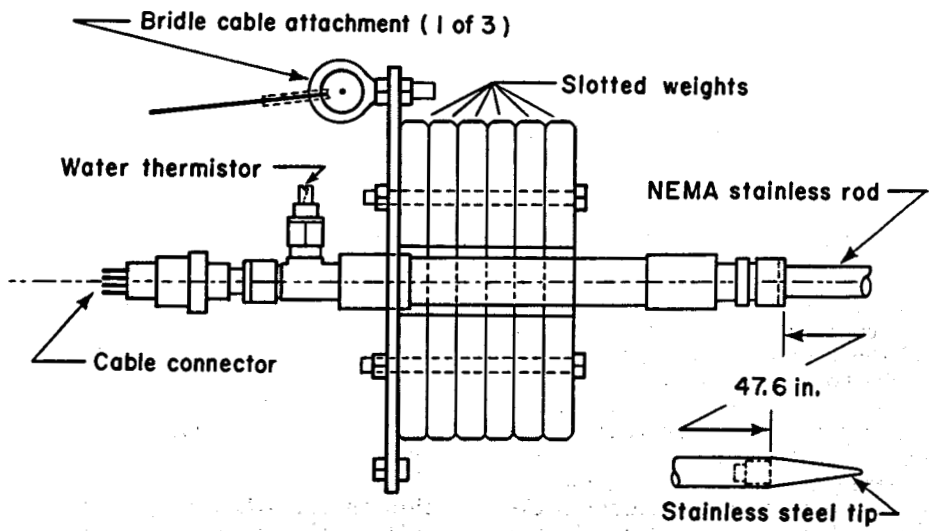


Fig. 1. Heat flow probe. (XBL 773-653)

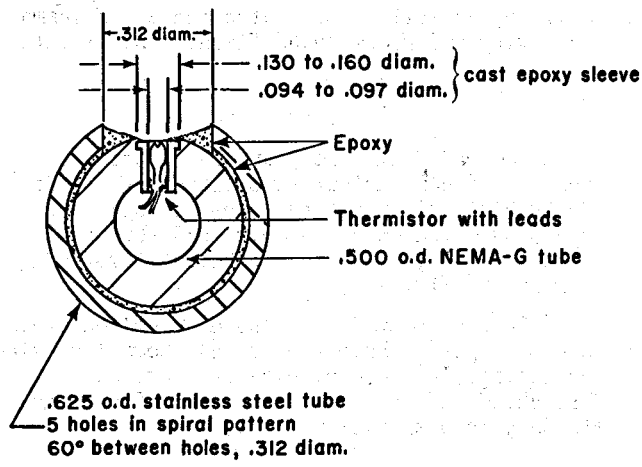


Fig. 2. Thermistor implantment details. (XBL 773-651)

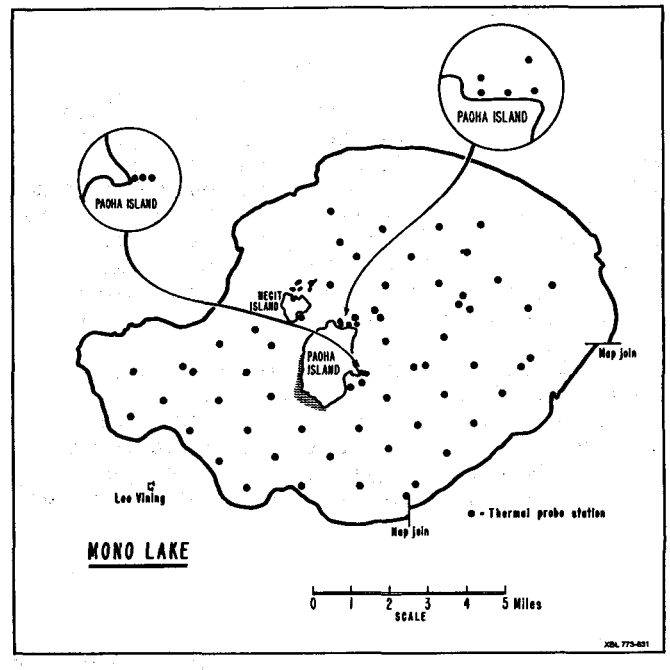


Fig. 3. Mono Lake stations. (XBL 773-631)

FOOTNOTES AND REFERENCE

*Project funded by the Federal Energy Administration/California State Lands Commission through agreement LC 6028.

†Energy & Environment Division.

‡‡California State Lands Commission, present address: Engineering Geoscience, University of California, Berkeley.

§Special Projects.

1. C. W. Case, and P. Wilde, Methods for Geothermal Reservoir Detection Emphasizing Submerged Environments: Lawrence Berkeley Lab. Rept. 4495 (1976).

WORK WITH EG & G, INC.

H. Wollenberg

REMOTE SENSING

Two regions, Rocky Flats, Colorado and Imperial Valley, California, were covered by airborne remote sensing surveys, incorporating multi-spectral photography and thermal infrared sensors. Geologic guidance was furnished by LBL in planning the flights, obtaining "ground truth" during surveys, and evaluating the data. At Rocky Flats, an ERDA facility near Boulder, Colorado, geologic and hydrologic features were discerned which may influence movement of surface and ground waters on to the site and plant fluids from the site. Results of the Rocky Flats surveys and recommended further investigations were described in a report by Lackey, Jones, and Wollenberg[1] which was included in the environmental impact statement for that site.

The surveys in the Imperial Valley, described in detail in a report in preparation by Lackey, Jones, and Wollenberg,[2] were in support of the ERDA (DBER) program of investigation of environmental effects of geothermal energy production. The purpose of the Imperial Valley flights was to obtain a set of baseline data prior to appreciable production of geothermal fluids. Multi-spectral photographs and thermal infrared data disclosed drainage patterns in the Salton Sea geothermal area which pre-date the filling of the Salton Sea as well as the present-day agricultural overprint in the extensively farmed region. These drainage patterns have a strong northwesterly "grain" which may be influenced by faulting. Sharp linear features were also observed on photographs, most likely associated with surface breakage from the 1975

Brawley earthquakes.

GEODOSE AND REACTOR SITE SURVEYS

During FY1976 the Geodose data bank, which is the basis for characterization of rock types by their radioelement contents, gamma-ray exposure rates, and radiogenic heat production, was expanded to include sedimentary and metamorphic rocks. The total number of entries now in the bank are: uranium, 1967; thorium, 1964; and potassium, 1442; permitting calculation of gamma-ray exposure rates and radiogenic heat production for 1417 samples.

The geologic settings of reactor site areas, in support of airborne gamma radiometric surveys by EG&G, were evaluated for eight regions. They included: the Arnold Reactor site region, Iowa; Big Rock Point, Michigan; Bridgman, Michigan; Baxley, Georgia; La Crosse, Wisconsin; Scriba, New York; St. Lucie, Florida; and Trojan, Oregon. Reports covering these areas included brief descriptions of their geology, soils, vegetation and climate, as well as estimated ranges of gamma radioactivity and recommended flight line orientations.

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2. J. G. Lackey, E. B. Jones, and H. A. Wollenberg. Status report, photographic and thermal sensing of geologic and hydrologic features, Salton Trough, California, EG&G Inc. Technical Memorandum, in preparation (1977).

GEOTHERMAL RESERVOIR DYNAMICS

P. A. Witherspoon, C. F. Tsang, T. N. Narasimhan, M. L. Lippmann, and G. E. Assens

INTRODUCTION

The purpose of this long-range project is to provide theoretical and interpretive support to the investigation of geothermal systems for the development of geothermal energy. It is generally addressed to the following objectives:

(1) Understanding the physics and chemistry of mass and energy transport in geothermal systems;

(2) Estimation of the useful life of a geothermal reservoir;

(3) Determination of the optimal rate of energy removal;

(4) Determination of the optimal distribution of production and reinjection points within the reservoir boundaries;

(5) Evaluating the effect of geothermal exploitation on environment; specifically, the subsidence of land surface due to fluid withdrawal.

These objectives are being accomplished through the development of mathematical techniques and computer codes, incorporating thermodynamic, hydrodynamic, and other physical and chemical principles to simulate the behavior of geothermal reservoirs (a) under natural conditions and (b) during exploitation. The convective and conductive nature of these systems and the effect of heat energy on temperature distribution within any producing reservoir are also studied. These studies will also eventually be able to identify the important field parameters which govern reservoir behaviors and determine how accurately they would need to be evaluated. Particular emphasis is being laid on hydrothermal systems which are most likely to provide the capacity of the ERDA mission goal of 6000 MWe by 1985.

This project is directly related to the development of geothermal resources as an economically feasible energy source. It is intimately coordinated with the overall LBL geothermal program. The study of effects of reinjection, subsidence, and other aspects within this project is of such a universal nature that immediate application can be found in many geothermal projects such as Raft River, Cerro Prieto, and East Mesa geothermal fields. The mathematical models currently developed with special emphasis on hydrothermal systems can be easily extended to consider hot dry rocks and geopressure reservoirs.

ACCOMPLISHMENTS DURING 1976

FY1976 represents a year of energetic expansion of the project. The most significant accomplishment is the development of a land subsidence computer program which will be able to simulate the subsidence of land surface in the case of a liquid-dominated geothermal system. Such an investigation will help to estimate the environmental impact of a geothermal project. Another powerful computer code was developed to study geothermal reservoirs where the vapor and liquid phases of the fluid are equally important. The co-existence of liquid and vapor may be very important in a number of producing geothermal fields such as at The Geysers in northern California. The problem of reinjection has also been studied, and it appears that for many cases, under reasonable conditions, reinjection can be safely done without affecting the producing well

for possibly 30 years or more. A new concept of screening the producing well is also suggested that may increase this number by 50 to 100%. An economic feasibility study is being made on the implementation of the screening concept. On the more basic level, a new numerical technique, called the Explicit-Implicit Finite Element Method, has been developed which appears to be superior to current techniques. This may prove to be very significant in the next generation of calculations. More detailed descriptions of these accomplishments are given below.

Numerical Modeling of Geothermal Reservoirs

Mathematical models are being developed to study the behavior of a geothermal reservoir given its physical and geological properties. We have extended our one-phase fluid and heat flow program for multi-dimensional geothermal systems to include presence of sources and sinks. This will enable us to handle either liquid-dominated or vapor-dominated geothermal systems both before and during exploitation. However, many geothermal systems are not one-phase systems. We have adapted the program of T. J. Lasseter which considers two-phase fluids. This powerful program is now being carefully tested. A glossary of names used in its programming was compiled. Several errors were corrected and that part of the program which reads in properties of the fluid and of the porous matrix and transforms them into a table has been completely reconstructed. Initial application to the study of a vapor-dominated system has been made. Slight local heating up near the production well was observed, which may be due to numerical inaccuracies. We are currently studying this problem in detail.

Land Subsidence

Geothermal fluid withdrawal can lead to reservoir consolidation and land subsidence. In some cases, the effects of subsidence can be quite significant. For example, parts of the Wairakei Geothermal Field in New Zealand subsided 12 feet in as little as 12 years. This poses important environmental problems. Physically, this is because of the reduction in fluid pressure accompanying fluid extraction, and the consequent increase in the effective overburden pressure.

A computer program was developed to simulate the effects of production as well as reinjection on the deformation of geothermal reservoirs. The program combines the numerical method of Sorey[1] for mass and energy transport with another method by Narasimhan[2] for one-dimensional (vertical) consolidation. The model is multi-dimensional and solves for reservoir deformation in liquid-dominated, heterogeneous, isotropic, non-isothermal systems. Deformation parameters may be non-linear and non-elastic, while the thermal and hydraulic properties can be temperature and/or pressure dependent.

An integrated finite difference technique[3] is used to solve the flow and energy operations, which are interlaced in time. Pore-pressures and temperatures are obtained, and the pressure changes are used to determine the volumetric and vertical deformations.

Reinjection

Land subsidence and subsequent environmental problems can be minimized through injection of the heat-depleted water in the geothermal reservoir. However, reinjection creates a zone of relatively cold water around each injection well that grows with time and eventually will reach the production wells. After breakthrough occurs, the temperature of the produced water drops and drastically reduces the efficiency of the whole operation. It is thus important to design the system of production and injection wells to prevent injected water breakthrough before a specified time, and to maintain the temperature variations within reasonable limits at the production wells after breakthrough. We have successfully adapted a simple two-dimensional, steady-state model that was developed by A. C. Gringarten and J. P. Sauty of Bureau de Recherches Geologiques et Minieres at Orleans, France. Various tests have been made on the program and we are satisfied that it is working properly. This program is able to handle any arrangement of injection and production wells including the effects of natural regional flow.

Screening of Production Wells from Effects of Reinjection

In connection with the reinjection problem, we have developed a new concept of protecting the producing well from reinjection effects by means of one or more screening wells appropriately positioned in between. The basic idea is that by producing water from the screening wells, one can intercept the cold water and put it back into the injection wells. The physics of the idea has been worked out, and it is found that the time it takes for the cold, reinjected water to break through at the production well may be increased by as much as a factor of two. After breakthrough, the rate of temperature drop at the production well will be less when screening wells are used. The optimum positions and pumping rates of screening wells can be calculated for any distribution of production and injection wells. However, we have not yet made an economic feasibility study including the cost of drilling the extra screening wells.

A New Numerical Method for the Solution of the Diffusion Method

Among existing techniques, the Finite Element Method (FEM) and the Integrated Finite Difference Method (IFDM) are two powerful integral formulations used to solve the diffusion equation numerically. Although these two methods have conceptual similarities, each method has some special features which give it distinct advantages in handling certain classes of problems. We have made an analysis of their conceptual basis. This has led to a hybrid approach combining the special advantages of both the techniques. We call this new technique the Explicit-Implicit Finite Element Method. Based on this, a powerful computer program called FLUMP has been developed to solve diffusion-type problems. As part of the theoretical basis of this work, the stability and convergence of the numerical equation and the convergence of the interactive scheme have been proved. The validity of the program has been verified by solving a number

of problems with known solutions. The program presently considers only two-dimensional or axially symmetric flow regions, but it can be extended to general three-dimensional problems using block isoparametric elements. This new technique and program should be of interest in fields of heat conduction, ground water flow, and chemical engineering.

PLANNED ACTIVITIES FOR 1977

(1) Further improvements will be made on the computer program handling two-phase fluid and thermal flow. Simulation of both vapor-dominated and liquid-dominated systems will be attempted.

(2) Our land subsidence program will be checked against available analytical and experimental results. Attempts will be made on actual field problems.

(3) An economic feasibility study will be made on the reinjection problem in collaboration with C. R. Scherer and his group at UCLA.

(4) The concept of the screening well will be applied to a study of optimal methods for a given distribution of geothermal production and injection wells.

(5) Due to the limitation of manpower and funding, the further development of the new explicit and implicit finite element method will be temporarily suspended. However, exploratory study of the possibility of extending the method to convective transport will be made.

(6) During the second half of FY77, a new subproject will be started to study the double diffusion of heat and salt in porous media to gain an insight into the instabilities that occur when a fluid at a certain temperature and salinity is injected into a reservoir with a different temperature and salinity. Such a study is related to the reinjection problem and is also important in the space-heating problem of hot and cold water storage in underground reservoirs for reuse after a few months.

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PROPERTIES AND BEHAVIOR OF ROCK-FLUID SYSTEMS AT HIGH TEMPERATURES AND PRESSURES

W. H. Somerton

BACKGROUND

The objectives of this project are to develop methods of and equipment for measuring the properties and behavior of rock-fluid systems at environmental conditions of pressure, temperature and fluid saturation which may be encountered in geothermal power development and thermal recovery methods applied in the extraction of fossil fuels. These data are needed in the interpretation of well logs in relation to zonal evaluation, in the study of fluid and heat flow in relation to subsurface reservoir management, and in prediction of well bore stability and possible surface effects associated with fluid withdrawal from the reservoir. Another objective of the project is to develop models and correlations which will permit the prediction of thermal, fluid flow, electrical, and mechanical behavior of rocks under a wide range of environmental conditions.

Methods of measuring the desired properties and equipment capable of making such measurements to temperatures as high as 200°C and pressures of 1000 bars were developed through earlier projects. Support for this project from the Lawrence Berkeley Laboratory began in FY1974. Preliminary design work has been completed on a new test facility capable of measuring all of the desired properties concurrently on the same test specimen to temperatures as high as 500°C and pressures to 1250 bars. Construction work on this new facility awaits receipt of funding.

New laboratory space has been provided for high temperature rock properties research. The existing test facilities have been moved into this space and are being used to continue testing of methods and to generate additional data on a widening variety of rock-fluid systems.

ACCOMPLISHMENTS DURING 1976

Plans for this period are outlined as follows:

(1) Continue to seek funding for the new test facility;

(2) Modify the sonic equipment to increase signal strength and perfect the stacked

crystal method for concurrent measurements of P and S wave velocities;

(3) Continue the development of concurrent measurements of permeability and formation resistivity factors using laboratory sandstones and cores from geothermal areas if available;

(4) Complete development of the multi-fluid thermal conductivity model and complete the liquid-solid contact resistance study. Continue development of the thermal conductivity probe. Continue study of convective heat transfer in porous media.

Accomplishments in the Above Areas were as follows:

(1) Funding of new test facility: Contacts have been made with several major oil company research centers regarding the possibility of grants-in-aid to help support construction of the facility. Encouraging responses have been received from three companies and more are expected.

(2) Sonic velocity measurements: Test equipment has been modified and tests on three laboratory sandstones are nearing completion. Both P and S wave velocities are being measured over a pressure range of 100 - 650 bars, temperatures from 25° to 175°C and brine saturations from 0% to 100%. The results agree with earlier single crystal test data over the same ranges of variables.

(3) Permeability and formulation resistivity tests: The high temperature permeability equipment has been improved to the point that satisfactory results are now being obtained. A dynamic method has been developed in which permeabilities are measured during sample heating which is done at a constant rate of about 1.5°C/minute. When the top temperature is reached (about 190°C), tests are continued at isothermal conditions. Other variables, such as salinity of the injected water, can be investigated at this constant temperature condition. Results of one successful test have been published.[1] Reduction in permeability to distilled water with increase in temperature was about 40%. Further reductions occurred as KCl was added to the flowing water reaching about 70% at the limit. Formation resistivity factors were measured after the addition of KCl showing an increase in the order of 33% from previously measured room temperature values.

No progress was made on other properties in this group, thermal expansion and compressibilities, because of the large amount of effort and time required to obtain satisfactory permeability and electrical resistivity factor results.

(4) Thermal properties tests: The thermal conductivity sphere-pack model was completed and tested against experimental results. Good agreement was obtained in most cases. Knowledge of the quartz content of the sand or sandstone was necessary for good agreement since quartz dominates in determining the rock solids conductivity. The model predicts thermal conductivity of multi-fluid saturated media of known porosity.

The work on liquid-solid thermal contact resistance was completed. It was found that contact resistance, if it did exist, was very small for wetting phase fluids. For non-wetting fluids, a measurable contact resistance value was obtained, but even it was found to have a negligible effect when included in the sphere-pack model. These matters are discussed in greater detail in a recently completed Ph.D. dissertation[2] and in a paper in preparation.[3]

Existing steady-state thermal conductivity equipment has been modified so that studies of convective heat transfer effects can also be made. This apparatus makes possible the study of natural and forced convection in fully liquid saturated systems and the VCC (vaporization-condensation-capillary) effects in liquid-vapor saturated systems. Natural convection is studied by reversing the direction of heat flow from vertically downwards to vertically upwards. Forced convection is studied by monitoring inlet and outlet temperatures of the flowing fluid as well as utilizing the top and bottom heat meters and guard heating. Preliminary results have been obtained which seem reasonable and compare favorably with literature values.

Little progress was made on the thermal conductivity probe method which is to be used in the new test facility. Bench-top tests showed the method to be practical and worthwhile developing for the new apparatus.

The most significant accomplishments are summarized as follows. P and S wave velocity studies with the two-crystal method confirm earlier results which showed a significant reduction of both velocities with increase in temperature. From these data, the effect of temperature on the "intrinsic strength" (G_b/C_b), and thus borehole stability, can be evaluated. The effects of variable fluid saturation on P and S wave velocities confirm that the ratio V_s/V_p should be a good indicator of liquid-gas contacts. Correlation of measured velocity values with changes in porosity under different pressures and temperatures cannot be made until the new test facility is available.

Successful tests were completed showing the effects of temperature, pressure, and salinity on permeability and formation resistivity factors. Large reduction in permeability and increase in formation resistivity factor with increased temperature have confirmed earlier results. Change in salinity of the flowing fluid has been shown to cause additional non-reversible reductions in permeability, but little effect on formation resistivity factor. A systematic study of these variables can now be made within the limits of the existing equipment.

The thermal conductivity model has proven to be very useful for the prediction of thermal behavior of multi-fluid saturated porous media. Knowledge of the quartz content of the rock, its porosity and condition of fluid saturation makes it possible to estimate thermal conductivity with good accuracy. Further testing against all of our accumulated thermal conductivity will make further

refinements possible.

PLANNED ACTIVITIES FOR 1977

Measurements of P and S wave velocities will be continued on additional rock types within the range of variables possible with the present equipment. Analysis and interpretation of findings will be presented in an MS thesis soon to be completed. Efforts will be made to correlate these findings with changes in porosity under the same environmental conditions.

Measurements of permeability and formation resistivity factors will be run on porous rocks ranging from pure quartz sandstones to limestones to establish the effects of increased temperature. Ionic concentrations of mono- and bivalent salt solutions will be varied systematically in an effort to explain the observed phenomenon. Streaming potentials may be measured if this would be useful for the analysis.

The thermal conductivity model will be tested against our large accumulation of thermal data. Suitable modifications and simplifications will be made so that the resulting equations may be used for reliable predictions of thermal conductivity of a variety of rock types under a wide range of environmental conditions. Work will continue on convective heat transfer, relating the magnitude of this effect to measurable properties of the system.

If time permits, additional work will be done on the development of the needle probe method for measuring thermal conductivity and on further development of methods for measuring thermal expansion and rock compressibilities appropriate to the new rock-properties test facility.

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THERMODYNAMICS OF HIGH TEMPERATURE BRINES

K. S. Pitzer,* L. F. Silvester† and P. Z. Rogers*

INTRODUCTION

An understanding of brines is essential for the technical utilization of many geothermal resources. Consequently, in 1975 a study was begun of the solution thermodynamics of brine systems, both simple and complex, weak and strong, covering a wide temperature and pressure range, and combining both modeling and experimental work.

The initial work involved analysis of existing thermodynamic data on simple electrolyte systems using equations developed by Pitzer and co-workers.[1-4] The goal of the modeling was to provide a compact set of equations capable of reproducing at various temperatures and pressures the existing data within experimental error up to practical concentrations (~6M) in terms of parameters having physical significance. The modeling equations for NaCl(aq) solutions were integrated into GEOTHM, an LBL computer program for modeling geothermal power plants.[5]

The program to measure heat capacities arose because of inadequate literature data on electrolyte systems. The experimental program has two goals; (1) to supply data on simple and complex electrolyte systems previously unreported, plus extending existing data to higher temperatures and pressures both along and away from the liquid-vapor saturation curve; and (2) to provide a data base for checking and refining various models.

Though the modeling and experimental work relate directly to electrolyte systems common to geothermal brines, the results are applicable to such areas as biological fluids, battery electrolytes in aqueous and nonaqueous solvents, plating baths, waste effluents, materials corrosion from electrolyte systems, and marine chemistry.

PROGRAM IN FY 1976 AND TRANSITION QUARTER

Planned activities of fiscal year 1976 covered three areas of modeling: strong electrolytes, moderately soluble electrolytes, and moderately weak electrolytes – plus the design and start of construction of a flow calorimeter-densitometer.

A flow design was chosen over the conventional Dewar calorimeter since in a flow system (1) no vapor space exists which eliminates the need for solvent loss corrections, (2) high pressures may be easily confined to capillary tubing and readily varied, and (3) solutions may be continuously changed while maintaining high temperatures and pressures.

Work completed on the high temperature-pressure-flow calorimeter-densitometer included tests on the flow and pressure systems to 700 bars, tests on the temperature bath to 300°C, and the initiation of design and construction of the calorimeter's electronic monitoring instrumentation.

Modeling of strong electrolytes centered on the thermal and volumetric properties of NaCl(aq) solutions. The osmotic-activity coefficient data, enthalpy data, and heat capacity data on vapor saturated NaCl(aq) solutions taken from various sources were fitted to a thirteen parameter equation. The equation reproduced the osmotic data to ± 0.005 for compositions of 0-6M from 0-300°C, enthalpy data to ± 5-10 cal/mole for compositions of 0-5M from 28-100°C, and heat capacity data to ± 0.5 cal/mole-°K for compositions 0-2M from 25-200°C. Details of the model, data analysis, tabulated and graphical displays of the Gibbs energy, enthalpy, heat capacity, partial molal and excess thermodynamic quantities for compositions of 0-6M from 0-300°C are given elsewhere.[6]

Volumetric data on vapor saturated NaCl(aq) solutions, supplied by the LBL GRID program, was evaluated from 0 to 200°C. A model, incorporating the Born charging equation, capable of reproducing the experimental values of $\bar{c}p^{\circ}_2$ and $\bar{v}^{\circ}_2$ from 0-200°C was developed.

Modeling work on moderately soluble electrolytes involved evaluation of literature data on calcium sulfate systems for both pure solutions and mixtures. The aim was to study the temperature dependence of the modeling parameters for 2-2 electrolytes. From the 25°C data, a calcium sulfate dihydrate K_{sp} (2.53×10^{-5}, molal scale) consistent with data on pure and mixed solutions was determined. At other temperatures, only mixture data was available which proved inadequate for fixing the modeling parameters.

The modeling work on moderately weak electrolytes resulted in equations originally developed for strong electrolytes being extended to solutions involving dissociation equilibria. Various sulphuric acid and phosphoric acid systems were analyzed. An improved analysis avoided the ambiguities formerly inherent in determining dissociation constants of weak acids in the pK range 1-3; the analysis gave a pK of 2.146 (molal scale, 25°C) for phosphoric acid. The model gave excellent agreement with experimental data on pure phosphoric acid solutions to 6M, and for phosphate buffer solutions. The work on phosphoric acid was completed and published.[7]

Modeling of sulphuric acid solutions covered thermal and activity data from 0 to 55°C. Superb agreement with solution data at each experimental temperature was obtained using an analysis which explicitly includes appropriate parameters for H^+ interaction with HSO_4^- (the dominant anion at high concentration) as well as for dissociation of HSO_4^- to H^+ and SO_4^{-2}. The completion of the sulphuric acid work is scheduled for fiscal year 1977.

PLANS FOR CALENDAR YEAR 1977

The scope of activities for calendar year 1977 for the experimental program includes final calorimeter-densitometer assembly, materials testing under experimental conditions, and obtaining data for simple and complex electrolyte systems.

Of particular interest will be obtaining data on those systems normally labeled strong electrolytes at room temperature but which show evidence of association at higher temperatures. The aim is to find under what conditions, if any, the solution thermodynamic properties may, or may not, be adequately treated without resorting to association equilibria. In addition, acquiring data on mixed electrolyte systems, which are virtually nonexistent away from room temperature, will be of prime importance in unraveling what factors influence mixture properties.

The modeling work will be closely integrated with the experimental program, both from the point of data analysis, and in suggesting systems and conditions for further study. Modeling will continue on strong and weak electrolyte systems using the available literature data, particularly the sulphuric acid, biosulfate systems, and the combining of the thermal and volumetric data for NaCl(aq) solutions into a single equation of state. Finally, the NaCl(aq) model will be transformed to a constant volume standard state system which allows predictions off the vapor-saturated liquid line. This is very important as a basis for applications of geothermal or geochemical interest.

FOOTNOTES AND REFERENCES

*K. S. Pitzer, Principal Investigator, and P. Z. Rogers, graduate student, are associated with the Materials and Molecular Research Division as well as the Energy & Environment Division.

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IN-SITU STRESS MEASUREMENTS: SEISMIC WAVE VELOCITY

T. V. McEvilly and C-Y. Wang

INTRODUCTION

A field technique for monitoring in-situ stress variations within the earth's crust is being evaluated along with laboratory investigations of measurable physical property changes of crustal rocks under conditions of temperature and stress, appropriate to in-situ conditions. The field study utilizes a mechanical source (VIBROSEIS[1]) of coherent programmable seismic waves and a special recording system. Two vehicles with operators can conduct repeated measurements of travel times of seismic waves reflected from discontinuities to depths of over 20 km in the earth. Stress variations should be evident in variations of times resulting from stress-induced velocity changes. In the laboratory, changes in physical properties of rocks typical of those being sampled in the field are measured for a variety of stress fields and pore water conditions appropriate to tectonic conditions within the earth. Seismic wave velocity, electrical resistivity, and crack formation are monitored with transducers and radiography/electrostatic imaging. Some aspects of the research have been supported in part by the USGS earthquake studies program. Work in FY75 was directed to initial design and fabrication of equipment. A well-developed and simple method of precise monitoring of in-situ stress variation within the upper tens of kilometers of the earth would be a major accomplishment in environmental monitoring. Applications to questions of geological hazards and the safety of structures, effects of reservoir depletion in geothermal or petroleum exploitation, and the prediction of earthquakes are some environmental areas where in-situ stress change monitoring would be of value.

ACCOMPLISHMENTS DURING 1976

It was found mid-year that the special purpose field velocity-monitoring equipment was, in fact, capable of making repeated measurements of velocities within the crust to depths of some 25 km with an uncertainty of 1-2 ms (approximately 0.02% precision). It was seen that, over periods of weeks, no changes in velocity were observable on either short-term (tidal periods of 12 hrs) or secular time scales at a monitoring site near the active San Andreas fault in central California. An order-of-magnitude improvement in monitoring precision was found possible through equipment modifications made in the summer of 1976. Field trials conducted in the fall confirmed that we now have the capability of measuring variations in seismic wave travel-times through the earth's crust with a repeatable absolute accuracy of 0.1 - 0.2 ms for a total pathtime of about 8 sec, i.e., a resolution of changes as small as about 0.002% in average velocity. This advances the state of the art by two orders of magnitude and provides a relatively simple field system of velocity change monitoring. Such a development will now permit searching for systematic variations in an area of known stress variations associated with earthquakes in central California.

Investigation of the physical process in rocks undergoing mechanical instability has been carried out in two directions. In one direction we have investigated (with Professor Richard Goodman) the change of electrical resistivity and pore-water pressure in granite undergoing stick-slip sliding. Clear variations of these parameters have been found to associate with stick-slip instability; the sense of variation has been found to depend upon the constraints on the flow of water, namely whether water is free to move in and out of the rock specimen.[2] It showed that in the "drained" condition (i.e., water is free to move in and out of the specimen), resistivity decreases by a few percent with increasing shear stress on the specimen; the minimum coincided with a sudden release of shear stress, accompanied by an immediate return of resistivity. This sequence of changes bears some similarity to those observed in the field associated with some earthquakes. Pore-water pressure, on the other hand, increases with increasing shear stress, with immediate decreases occurring simultaneously with sudden stress releases. In the undrained condition (i.e., water is not free to move in and out of the specimen) the senses of variation of both resistivity and pore-water pressure reverse direction. Based upon these observations, models have been constructed for the physical process occurring in rock during the stick-slip instability.

Another direction of investigation has been developing a new method for "directly" examining the generation and growth of cracks in stressed rocks.[3] This method combines radiography and electrostatic imaging to define the internal fractures and has been successfully applied to some fine-grained rocks.

PLANNED ACTIVITIES FOR 1977

Upon repair of the VIBROSEIS (damaged in an accident in October 1976), we will continue monitoring velocities adjacent to the San Andreas fault in San Benito County, California, where seismic activity and fault creep are ongoing and, consequently, stress changes are expected in the crust.

The modeling of physical processes during stick-slip instability will be continued and its relevance to processes occurring at earthquake sources will be sought. The mechanical properties of the gouge material invariably found in natural faults will be investigated and its effect on fault movement studied.

We plan to take radiographic images of a stressed sample at several different angles and, using these multiple images, to construct a 3-D picture of the internal crack, thus surmounting the present 2-D limitation in our radiographic study of internal cracks.

We plan to pick up the elastic wave radiation patterns from the cracks, using piezoelectric transducers mounted at various positions on the

specimen. In conjunction with a radiographic image of the internal crack, the radiation pattern will enhance our understanding of the rupture process of rocks.

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NATIONAL GEOTHERMAL INFORMATION RESOURCE (GRID)

S. L. Phillips

INTRODUCTION

The National Geothermal Information Resource (GRID) of the Lawrence Berkeley Laboratory is sponsored by the U.S. Energy Research and Development Administration to develop a comprehensive compilation of worldwide literature and data designed to assist in the research and development of geothermal energy for both electrical and non-electrical uses. Included in this compilation is site-dependent and site-independent material related to geothermal exploration, reservoir engineering, energy utilization, physical chemistry; as well as to environmental, legal, and economic aspects of geothermal energy. The GRID information resource maintains computerized data bases which provide the basis for in-depth literature reviews and critical evaluations of the status of data by GRID's technical staff. In addition, computer-produced bibliographies and data tabulations are generated from the data bases.

The GRID program was initiated in Fiscal Year 1974 with funding provided from the Division of Physical Research. Currently GRID is supported by the Division of Physical Research, the Office of Technical Information, the Division of Biomedical and Environmental Research, and the Division of Geothermal Energy. In addition to ERDA funding, GRID is funded by the Electric Power Research Institute for a study of brine treatment.

In 1975, emphasis was placed mainly on the following aspects of computer data handling:

(1) Applying Berkeley Data Base Management Systems (BKY-BDMS) to GRID for information storage and retrieval;

(2) Compiling and storing data files on computer tapes;

(3) Developing methods for information and numerical data extraction from the literature;

(4) Developing input formats;

(5) Establishing exchange programs with existing computer data centers.

ACCOMPLISHMENTS DURING 1976[1-14]

A bibliography has been completed dealing with the basic properties of aqueous NaCl, KCl, and $CaCl_2$ solutions. Numerical data covering viscosity of sodium chloride solutions at elevated temperatures and pressures have been extracted from reports contained in the bibliographic file. The viscosity data have been tabulated and work has begun to develop equations which will closely fit the existing data.

A brine chemistry data file was established jointly with the LBL Geochemical Engineering Program. Computer formats and programs were developed for handling the data. This file contains numerical data on the chemical composition of brines produced from selected U.S. geothermal wells. Coverage will be extended to include the Cerro Prieto geothermal field in Mexico.

A file on ground subsidence was established to include ground subsidence resulting from mining operations and petroleum production, as well as subsidence associated with geothermal reservoirs. A report reviewing data on subsidence in relation to geothermal energy production has been issued.[1]

A bibliography on the environmental effects of hydrogen sulfide is nearing completion. Information included in this file covers; environmental effects on plants and animals, monitoring methods and instrumentation, H_2S recovery processes, and abatement procedures.

Papers dealing with exploration of the East Mesa KGRA (Known Geothermal Resource Area) have been collected and a bibliography nearly completed. The East Mesa bibliography is a sample file for the larger worldwide exploration file.

The files on physical chemistry of sodium chloride, brine chemistry, ground subsidence, environmental effects of hydrogen sulfide, and the exploration file on the East Mesa KGRA were made available for computer search and retrieval at the request of interested users.

A study of brine treatment, funded by the Electric Power Research Institute, was conducted

as part of the GRID program. Brine treatment deals with the chemical and physical methods that are being used, or might be used for handling geothermal fluids to control the formation of scale by silica, calcite, or sulfides and to minimize the effects of corrosion in pre-utilization, utilization, and post-utilization stages of geothermal power production. A draft report was prepared.

GRID data were exchanged with the U.S. Geological Survey data base in Reston, Virginia, and with the Geothermal Research Institute data base in Pisa, Italy.

PLANNED ACTIVITIES FOR 1977

Compilations on silica solubility, magma, and non-electrical uses of geothermal energy will be made. Existing compilations will be kept current and coverage expanded as needed.

Reviews will be written covering important aspects of geothermal energy exploration and utilization; environmental effects of hydrogen sulfide, exploration at East Mesa KGRA, and others.

Data evaluation activities (e.g., viscosity of NaCl, silica solubility) will continue; a review of the findings of various exploration methods at the East Mesa site is in progress; and work is continuing on the bibliography of worldwide geothermal exploration.

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RADON AS AN EARTHQUAKE PREDICTOR

A. R. Smith, H. A. Wollenberg, D. F. Mosier

PROJECT DESCRIPTION

Russian and Chinese experience suggests that fluctuation of radon-222 in groundwater can be used as an earthquake predictor. The objective of the LBL program is to evaluate this mechanism, and to develop techniques and instrumentation to accurately measure small fluctuations in ^{222}Rn in groundwater.

ACCOMPLISHMENTS IN 1976

(1) Evaluation programs included sampling of well waters in the Oroville area, which is experiencing aftershock activity following the 1 August 1975 earthquake of magnitude ~ 6. Subsequent γ-spectrometric analyses indicate some correlation between aftershocks and ^{222}Rn fluctuations in water from ~ 200 feet-deep bedrock wells. The statistical significance of these apparent concordances is being tested, taking into consideration the spatial as well as temporal distribution of the aftershocks. Discussions have been held with geologists and physicists at Chico State University to formulate a program wherein the bulk of the field work, and later the analytical work, will be conducted by that University, possibly under an NSF grant. In the meantime, active efforts are being made to obtain some interim funding from the Butte County

Board of Supervisors.

(2) Instrumentation to continuously monitor ^{222}Rn, based on components available at LBL, was initially tested on site in Berkeley, then installed with the cooperation of the USGS at a well in San Juan Bautista on the San Andreas fault. This location is within the area of stations where the USGS is evaluating other geophysical parameters as earthquake predictors. The continuous monitoring system has been operating steadily for nearly 3 months. No significant local earthquakes have occurred during that period. Gamma-ray count-rate data showed a marked periodicity which may be related to earth tides.

(3) To evaluate the effects of ground shaking on ^{222}Rn on soil-gas and deep aquifers, well samples were collected and alpha-track detectors emplaced at the Nevada Test Site, in conjunction with schedules of underground nuclear explosions. This project was done in cooperation with Lawrence Livermore Laboratory and USGS personnel. Results of the well sampling indicate no clear response of ^{222}Rn in deep aquifers to ground shaking from underground tests. Of several tests monitored, only one (the closest to the detector array) had any appreciable effect on fluctuations in soil-gas ^{222}Rn contents.[1]

(4) A compact prototype well-water monitoring system, based on an NaI(Tℓ) scintillation detector and γ-ray spectrometer, was designed and assembled. The system will be field tested in FY77.

The concept of a γ-ray monitoring system was described, and early results of the Oroville sampling project were reported by Smith et al.,[2] and were described at the Fall 1976 Annual Meeting of the American Geophysical Union.

PLANNED ACTIVITIES FOR 1977

(1) On-going continuous monitoring at San Juan Bautista, with site support from USGS;

(2) Operation of prototype γ-monitoring system;

(3) Formulation of proposal to NSF with Chico State to conduct area water sampling and radiometric analyses in the Oroville region;

(4) Preparation of a report summarizing the Oroville and San Juan Bautista projects, including statistical analysis of Oroville data.

If funding levels permit, two research studies may be started:

(1) Development and proof of concept of a system to monitor fluctuations in the ^{222}Rn content of natural gas from deep reservoirs, at the wellhead;

(2) Evaluation of the concept of tracing the history of fluctuations of ^{222}Rn in seismic areas by analyzing contents of radon-daughter elements in tree rings.

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IN-SITU PROPERTIES OF SOILS AND SOFT ROCKS

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INTRODUCTION

Recent studies and surveys have identified the need for reliable and improved techniques for in-situ determination of the engineering characteristics and properties of soils and soft rocks as one of the most important geotechnical problems at the present time. Accurate characterization of below ground conditions is essential for success and economy in underground construction and the utilization of underground space. Data on subsurface conditions are imperative for the analysis of problems such as subsidence and ground water pollution that may result from the extraction (and possible reinjection) of underground fluids.

Until recently the primary means for gathering soil and rock data was through sampling and testing of so-called "undisturbed" samples. Limitations to this approach, arising from such problems as sample disturbance, the difficulty of preserving or re-establishing in the laboratory the in-situ environmental conditions, and changes in sample properties owing to unloading and exposure have been recognized for some time. The severity of these limitations has become particularly evident as the volume of offshore and underground construction has increased, hence the emphasis on in-situ testing.

Accordingly, the primary objective of this research is to identify, develop, and implement new

and promising approaches for the determination of soil and rock properties in-situ. A second related objective is to develop methods and practical laboratory and field procedures to establish the durability and susceptibility of property changes of soft rocks after unloading and/or exposure to environmental changes.

The project was started during Spring 1976, and work has been focused on the first objective, although some separately funded research bearing on the second objective has been in progress concurrently.

ACCOMPLISHMENTS DURING 1976

Although our ultimate goal is the development of new, innovative, and improved techniques for characterization of subsurface profiles and properties, emphasis thus far has been on the in-depth review and evaluation of existing methods. For any field problem it is necessary to know the soil or rock types, the location of the boundaries between them, and the location of the groundwater table. In addition analyses of the fluid flow, stability, and stresses and deformation in the ground require knowledge of permeability (hydraulic conductivity), strength, in-situ stresses, and volume change characteristics.

In-situ test methods presently used for determination of these properties have been studied. They include:

(1) permeability tests by pump-in, pump-out, and piezometer methods, including both steady state and transient conditions

(2) the Standard Penetration Test

(3) cone penetration tests of various types, including both static and dynamic methods

(4) the Vane shear test

(5) the borehole direct shear test

(6) pressuremeter methods

(7) methods for determination of in-situ stress

(8) load bearing tests

(9) screw plate tests

(10) down-hole and cross-hole seismic methods

(11) hydraulic fracturing methods

As a result of these studies a report has been drafted which presents a description of the methods, an assessment of the suitability of each for determination of different geotechnical parameters, and their potential for further development. Extensive references are also listed. When completed, this report should serve as a definitive starting point for anyone interested in the subject.

Preliminary study has also been made of several less direct approaches to the deduction of properties in-situ; methods which if further developed might prove very useful in practice. Generally these involve applications of geophysical methods to the determination of the geotechnical properties of soils and soft rocks. They include:

(1) nuclear methods – surface and subsurface

(2) remote sensing approaches

(3) electrical resistivity

(4) dielectric measurements

(5) gravimetric methods

(6) magnetic methods

(7) thermometric methods.

A preliminary experiment has also been done to explore the possibility that soil type identification (e.g., sand, clay) can be made on the basis of acoustic response during steady penetration by a cone penetrometer. The results indicate that it can.

PLANNED ACTIVITIES FOR 1977

Activities planned for the forthcoming year are:

(1) Completion and publication of the previously described state-of-the-art report on in-situ measurement of soil properties;

(2) Further study and evaluation of the suitability and potential for remote and geophysical measurements to provide data, from which quantitative measures of the mechanical properties of soils and soft rocks may be deduced;

(3) Further study of the usefulness of acoustical measurements during cone penetration tests as a basis for determining soil type.

FOOTNOTES

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STRESS FLOW BEHAVIOR OF FRACTURED ROCK SYSTEMS

R. L. Taylor, P. A. Witherspoon, and H. M. Hilber

INTRODUCTION AND ACCOMPLISHMENTS DURING 1976

We directed our attention to physical systems which can be approximately described by the partial differential equations of elastodynamics. Examples of such systems are frequently encountered in structural and geotechnical engineering. Consider, for example, a system of deformable fractured rock. In order to study the behavior of this system, an Initial Boundary Value Problem has to be solved. This is done most conveniently and economically by employing numerical techniques, such as the Finite Element method, which can be implemented into computer programs. Here we assume that the spatial domain of the considered physical system is discretized by the Finite Element method. Consequently the Initial Boundary Value Problem is replaced by an approximating Initial Value Problem, consisting of a set of second order differential equations (equations of motion) plus some initial conditions. Solutions to the equations of motion are most conveniently obtained by computational techniques. In this work we consider methods which are specifically designed for solving systems of second order differential equations by employing a discretization of the time domain and generating approximate solutions in a step-by-step fashion.

Equations describing the dynamic behavior of the physical systems considered here, are, in general, characterized by the fact that their frequency spectrum is spread out over a relatively large domain of the positive real axis. In our study only linear problems have been considered. Hence, each frequency is associated with a mode of vibration, and the solution of the equations of motion can be viewed as the superposition of all individual modal response histories.

In many applications only low mode response is of interest. For these cases the use of implicit unconditionally stable algorithms is generally preferred over conditionally stable algorithms.

Conditionally stable algorithms require that the size of the time step employed be inversely proportional to the highest frequency of the discrete system. In practice this is a severe limitation as accuracy in the lower modes can be attained with time steps which are very large compared with the period of the highest mode.

For unconditionally stable algorithms a time step may be selected independent of stability considerations and thus can result in a substantial savings of computational effort.

In addition to being unconditionally stable, when only low mode response is of interest, it is often advantageous for an algorithm to possess some form of numerical dissipation to damp-out any spurious participation of the higher modes. Examples of algorithms commonly used which possess these properties are Houbolt's method,[1] the Wilson θ-method,[2] and the Newmark family of methods restricted to parameter values of $\gamma > 1/2$ and $\beta \geq (\gamma + 1/2)^2/4$.[3]

The Newmark family of methods allows the amount of dissipation to be continuously controlled by a parameter other than time step. For example, set $\beta = (\gamma + 1/2)^2/4$ and $\gamma > 1/2$; then the amount of dissipation, for a fixed time step, is increased by increasing γ. On the other hand, the dissipative properties of this family of algorithms is considered to be inferior to both the Houbolt and the Wilson methods, since the lower modes are affected too strongly. (It seems all of these algorithms adequately damp the highest modes; see Bathe and Wilson.[2])

In the Wilson method, θ must be selected greater than or equal to 1.37 to maintain unconditional stability. It is recommended[2] that $\theta = 1.4$ be employed as further increasing θ reduces accuracy and further increases dissipation; but even for $\theta = 1.4$ the method is more highly dissipative. For example, it is suggested[2] that to integrate a mode accurately, 100 time steps be taken per period, whereas the generally employed rule-of-thumb is ten steps per period for nondissipative algorithms. From this we conclude that the Wilson method is generally too dissipative in the lower modes, requiring a time step be taken that is smaller than that needed for accuracy.

Houbolt's method is even more dissipative than Wilson's and does not permit parametric control over the amount of dissipation present. Thus despite its shortcomings, the Wilson method is considered by many to be the best available unconditionally stable one-step algorithm when numerical dissipation is desired.

Since it seemed that the commonly used unconditionally stable, dissipative algorithms of structural dynamics all possessed some drawbacks, a research effort was undertaken to see if an improved one-step method could be constructed. The requirements of the desired algorithm were delineated as follows:

(1) It should be unconditionally stable when applied to linear problems ;

(2) It should possess numerical dissipation which can be controlled by a parameter other than the time step. In particular, no numerical dissipation should be possible;

(3) The numerical dissipation should not affect the lower modes too strongly.

We have been able to develop an algorithm which achieves the above requirements and its properties are described in Ref. 4.

We defined and analyzed a three-parameter family of algorithms which contains the Newmark family. A new form of dissipation, called α-dissi-

pation, was introduced by way of these algorithms. The new one-parameter family of methods which is advocated here is a subclass contained in the three-parameter family.

The unfavorable algorithmic dissipation possessed by the Newmark family was demonstrated. Furthermore, we showed that α-dissipation is similar to linear viscous damping and, in itself, is ineffective in the higher modes. The dissipation of our new algorithms, which consists of a combination of a positive Newmark γ-dissipation and negative α-dissipation, was shown to have improved characteristics. Results of a stability analysis of the new family are presented and its algorithmic damping ratio and relative period error are shown to compare favorably with those of the Wilson and Houbolt methods.

CONCLUSIONS

A new family of unconditionally stable one-step algorithms for structural dynamics has been developed which possesses improved algorithmic damping properties that can be continuously controlled. In particular, no damping is possible. It was shown that there are members of the new family which are more accurate in the lower modes than the Wilson method, yet are more strongly dissipative in the higher modes. The new methods involve commensurate storage when compared with the Newmark and Wilson methods and are no more difficult to implement.

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COAL PARTICULATE PROCESSING

D. W. Fuerstenau*

Processing of fine coal particulates is expected to play an increasingly important role in the nation's wealth and economic survival. At present, coal finds cannot be satisfactorily recovered by the conventional methods of extraction. Therefore, the aim of this research project has been to explore new technologies for their efficient and economic recovery.

BACKGROUND

Coal is one of the oldest sources of energy, and it will be the major domestic energy source in the United States for the next several years. Therefore, we must develop means not only to use efficiently the higher grade deposits, but also to utilize the vast tonnages of the lower grade, high sulphur coal deposits (especially in the Eastern United States). One of the major problems in the utilization of coal is the undesirable emission of sulphur dioxide gas into the atmosphere on burning (e.g., in power plants or coking processes), which must be minimized. Such emission is due to the notorious presence of pyrite (FeS_2) in association with coal and shale minerals in natural deposits. Although sulphur is also present in coal in the form of organic compounds, only pyritic sulphur can be removed by mineral processing methods, such as froth flotation and leaching.

OBJECTIVE

The objective of this research project has been to explore new methods for improving the selective removal of pyrite from coal by froth flotation. One such method is based on selectively inducing a hydrophilic character to coal particles through the adsorption of hydrophilic polymers. In order to effectively remove pyrite from coal by physico-chemical methods, a thorough investigation of the characterization of surface-chemical, electrochemical properties and solubility of pyrite in aqueous environments must be made.

ACCOMPLISHMENTS DURING 1976

It has long been known that coal possesses an inherent floatability (hydrophobicity), which varies with the rank of coal – maximum hydrophobicity being for medium- and low-volatile bituminous and semi-anthracite coals. It was thought that the hydrophobicity of coal could be reduced by the adsorption of hydrophilic polymers such as polyacrylamides, starch, etc. Polyacrylamides, which are widely used in many industries and easily available, were experimented with first. "Pure" natural samples of anthracite were used in all the experiments. In order to find the optimum amount, type and conditions under which polymers can render coal particles

hydrophilic, adsorption isotherms of these polymers were determined. Using a nephelometric method for measuring very small amounts of commercial polymers of high molecular weight (> 10^6), the calibration curves for Magnifloc 905N, Separan NP10, Methocel F4M and Purifloc N-17 have been established. The adsorption isotherms of these polymers on minus 37-micron anthracite particles at pH 7.6 in the range 1 - 100 mg/l, showed that approximately 90% of polymers were adsorbed on coal. The high molecular weight Magnifloc (10^7) was adsorbed slightly more than Separan (10^6).

Flotation of Coal

The modified Hallimond tube flotation experiments were carried out to determine the effect of polymer adsorption on the flotation of pyrite and fine anthracite particles. Though our preliminary results are not really conclusive, it was confirmed that polymers do reduce the flotation recovery. The flotation of coal was also decreased as the suspension pH was changed away from 6.7, in both the acidic and basic direction. Surprisingly, the flotation recovery of both pyrite and coal behave very similarly with regards to pH, even in the absence or presence of polymers. However, it was expected that xanthate collector (which is used to induce hydrophobicity on pyrite) would still adsorb selectively on pyrite, thus resulting in the flotation and separation of pyrite from the polymer-coated hydrophilic coal particles. A number of polymers, such as polyacrylic acid, polyethylenimine, Methocel and combinations thereof, besides polyacrylamides were also investigated and the same trends in coal recovery were observed.

Electrokinetic Studies on Coal

The drop in flotation recovery of coal with pH has been explained in the literature in terms of adsorption of H^+ and OH^- ions in the acidic and basic pH ranges respectively. We conducted electrophoretic mobility measurements on coal in aqueous salt ($NaNO_3$) solutions using a Zeta-Meter. The results showed that coal particles were negatively charged throughout the pH range 3.5 to 10.0, which confirmed the view that a zero point of surface charge is not a criterion for coal hydrophobicity, as advocated in the literature. Our electrophoretic mobility curves were similar to those reported by Campbell and Sun.

Contact Angle Studies on Coal

In order to investigate the effect of polymers on the hydrophobicity (and therefore the floatability) of coal, contact angle measurements were made. The equilibrium contact angles were measured on well polished coal samples in aqueous polymer solutions by contacting free air bubbles at different locations on the surface of coal samples, using the contact angle goniometer. Because of the non-homogeneity of coal samples, about 20 to 30 readings of the contact angles were made for each condition of pH and polymer concentration, and the statistical average was taken as the representative one (with a maximum variation of 5 degrees). The results indicate that the adsorption of high molecular weight (10^6 - 10^7) polymers like polyacrylamides were not very effective in reducing the contact angle and hence satisfactory flotation depression was not achieved. However, Methocel F4M, a cellulose derivative (molecular weight 90,000) was far more efficient and a substantial reduction in contact angle could be achieved with less than 200 mg/l of polymer.

The contact angle measurements also confirmed the pH effect on flotation. That is, the contact angle is reduced as the pH is shifted either direction from neutral pH. In the presence of Methocel, the drop is even faster and at about 166 mg/l and pH of 9.1 the contact angle is essentially zero, which is promising indeed.

The success of the low molecular weight polymer, Methocel F4M, which also contains some hydrophobic groups, suggests that the mechanism depends on either molecular weight or the presence of hydrophobic groups which interact with the hydrophobic surface of coal so that hydrophilic groups are oriented away from the surface.

PLANNED ACTIVITIES FOR 1977

Our plans are to complete the work reported here in order to provide background information for achieving efficient depression of coal by hydrophilic or partially hydrophobic polymers during flotation processing. Further experiments to delineate the important parameters influencing coal depression are therefore needed. More importantly, we plan to direct the work towards the characterization of surface-chemical, electrochemical, and dissolution behavior of pyrite in aqueous environments, because better understanding and more effective control of pyrite removal from coal is essential. In view of the rather meager published work on pyrite characterization and behavior, we plan to conduct a systematic investigation on this important aspect of pyrite removal.

FOOTNOTE

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HIGH PRECISION MASS SPECTROMETRY

M. C. Michel

INTRODUCTION

One of the long-range goals of our geosciences research program is to learn more about the composition and nature of the earth's mantle through the study of volcanic flows. Xenoliths (unmelted inclusions) in these flows may represent materials characteristic of the mantle, with minimal modification during ascent.

The interest in the earth's mantle arises from two sources, 1) the use of geothermal heat in energy production—usable sources are rare compared to the potential resource that may be available if adequate methods for prediction are developed, and 2) many valuable commercial minerals and ore bodies are of geothermal origin. An understanding of basic heat transport and chemistry of the mantle and its interaction with the crust may facilitate the discovery of such widely scattered but potential abundant resources.

As part of the interest in the mantle, we began a program in 1975 to achieve the capability of making state-of-the-art Rb-Sr geochronological measurements. We also planned to make isotopic and chemical measurements by mass spectrometry on rare gases in volcanic xenoliths. Progress on both projects was made in early 1976, but due to funding problems the rare gas work was terminated, and the emphasis of the work was shifted. After considerable reflection and advice of an outside review group, it was decided to emphasize the development of a reliable very-high-precision mass spectrometric technique for the critical $^{87}Sr/^{86}Sr$ ratio, using the special capabilities of the LBL 5-foot-radius isotope separator. This work, if successful, will apply to other areas of research, and in geoscience should hasten the use of other parent-daughter isotope pairs for geochronological measurements, particularly the $^{147}Sm/^{143}Nd$ pair. It should also improve our ability to search for isotopic anomalies due to admixture of, for example, the products of neutron induced fission in a geological setting. This could be pertinent to the problem of nuclear waste disposal.

Work toward the chemical separation and Rb isotopic dilution aspects of Rb-Sr geochronology were pursued during 1976 but will be de-emphasized for the near future. Funding for the high precision mass spectrometry became available in the fall of 1976 and work is now proceeding.

ACCOMPLISHMENTS DURING 1976

The rare gas measurements required reactivation and some modification of an older, bakeable, 6-inch-radius mass spectrometer. We had successfully operated this instrument and had designed and started fabrication of a complex gas release and purification system when the decision to terminate this phase of the work was made. No experimental results are available, but we have simplified techniques and have ideas for technical improvements which we can apply to future work.

The Rb/Sr geochronology is split into two parts; the actual high precision isotopic measurements on Sr, and the chemical analysis of both Rb and Sr in the geological samples. Because the total variation of the $^{87}Sr/^{86}Sr$ ratio in most samples is only a few percent, high precision is necessary to differentiate between samples. Significant differences in geological context can result in isotopic ratio differences of only one part in 10^4 or less. At the inception of our work, reliable reports of data precise to one part in 10^4 were rarely published, and only one laboratory demonstrated an analytic capability as precise as a few parts in 10^5.

As one increases the precision of the isotopic measurements, the chemical analysis precision of Sr and Rb must also increase since inferences are often made from isochron plots of $^{87}Sr/^{86}Sr$ versus Rb/Sr chemical abundance ratios. The appropriate precision in Rb/Sr is less than that required for $^{87}Sr/^{86}Sr$, but the demands increase together. Since most practical chemical methods fail at about the 1% level, isotopic dilution analysis by mass spectrometry is the usual solution. We therefore modified our 12-inch-radius mass spectrometer for use as an isotopic dilution machine for Rb (Sr can be measured by isotopic dilution simultaneously with the $^{87}Sr/^{86}Sr$ measurement), and appropriate techniques were developed to detect and measure Rb in various reagents and vessels in order to check the sources of contamination from the processing. We easily achieved the ability to detect sub-picogram quantities of Rb in solutions of as much as several milliliters. However, "background" Rb from most operations were usually considerably higher. Taking into account the size samples likely to be available, and the limit of 0.3% precision set by the mass spectrometer data readout (improvable only at considerable cost), a "background" of 50 - 100 pg of Rb seemed tolerable as an upper limit. Although there have been problems, a method for doing this, without clean-room techniques, has been developed and tested thoroughly with blank runs. With rare exceptions, the contamination levels are below the chosen limits, although in the absence of completely protected laboratory space there are occasional events somewhat above our desired limits. These should present no problem for most work and the means for further reduction is obvious, but costly, and can be justified only by a more vigorous research program.

The $^{87}Sr/^{86}Sr$ ratio is normally determined by sequential and repetitive measurement of the two ion beam intensities and the results averaged. Because the best ion sources have unavoidable intensity fluctuations, this method has precision limits that are obviously related to the rapidity with which the sequential measurements can be made and how constant the ion beam is at the time of measurement. The method is adaptable to computer control. As simultaneous collection of the two isotopes, which

requires a large radius mass spectrometer, would result in some improvement, our 5-foot-radius isotope separator was adapted to make such measurements. The results with crude readout techniques, indicate that a precision of ~ 6 parts in 10^5 is relatively easily attained. The limitations seem to be purely electronic in the readout process. Measurement times are quite short (~ 10 - 15 min) so that sample preconditioning and pumpdown are critical factors for sample analysis.

PLANNED ACTIVITIES FOR 1977

We have concluded that a precision of one part in 10^5 can be attained through careful attention to noise elimination and other electronic techniques. We are testing these ideas and plan to achieve a reliable system for measurements to this level of precision during 1977. Also, we will learn if any ion-optical or other non-readout limitations exist, and we should be able to test the reliability of the internal linear fractionation correction normally used in Sr/Rb work. Preliminary work on the feasibility of extension to a precision of ~ 1 part in 10^6 should be done in this fiscal year.

ELIMINATION OF ^{248}Cm AS A POSSIBLE PROGENITOR OF CARBONACEOUS CHONDRITE FISSION XENON

D. A. Leich and S. Neimeyer*
and
M. C. Michel†

It has been suggested by various authors that spontaneous fission of ^{248}Cm may be responsible, at least in part, for the heavy-isotope anomalies, known as the CCF component, in xenon extracted from carbonaceous chondrites. In order to test this hypothesis, we have measured the isotopic spectrum of xenon fission products from a 97% isotopically pure ^{248}Cm sample. The products of spontaneous fission of ^{248}Cm were found to be mixed with the products of heavy-ion induced fission reactions. The latter component was produced in a prior use of the ^{248}Cm sample as a target for a heavy-element synthesis experiment. Fortunately, the induced-fission component accounts for only ~ 10% of the observed Xe yields, and its composition can be estimated sufficiently well to allow a fairly precise determination of the isotopic composition of Xe from spontaneous fission of ^{248}Cm.

The data also allow two other estimates of the spontaneous fission yields, the first from a small amount of xenon released at 500 °C from the aluminum foil enclosing the sample, and the second from a reheating performed following a one-month accumulation of new fission products. After fairly large corrections for incomplete decay of precursors to ^{131}Xe and ^{132}Xe, these independent estimates of the spontaneous fission yields are in reasonable agreement with the estimates based on the initial outgassing of the sample, corrected as described for the induced-fission component. The test estimate of the composition of Xe from spontaneous fission of ^{248}Cm is as follows:

$$^{134}Xe/^{136}Xe = 1.066 \pm 0.015,\ ^{132}Xe/^{136}Xe = 0.81 \pm 0.03 \text{ and } ^{131}Xe/^{136}Xe = 0.49 \pm 0.04.$$

These results are totally inconsistent with any of the various estimates of the CCF composition, implying that if spontaneous fission of ^{248}Cm contributed at all to the CCF component, the contribution was relatively minor.

FOOTNOTES

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MODELING OF THERMAL RECOVERY OF OIL FROM THICK, DIPPING PETROLEUM RESERVOIRS

W. H. Somerton

INTRODUCTION

The principal objective of this project is to develop a mathematical model for the thermal recovery of oil from thick, dipping petroleum reservoirs in which gravity override is a major problem. Gravity segregation between injected air and reservoir oil usually occurs in the in-situ combustion process, often giving rise to premature breakthrough of the air into producing wells. The inefficient utilization of oxygen which results necessitates early termination of the burn and thus failure of the project.

Thermal recovery processes, involving heat and mass transfer in porous media, are complex and are difficult to describe physically and mathematically. Development of a mathematical model based on fundamental concepts of mass and heat transfer would seem to give the greatest hope of understanding the roles of the many variables involved. The gravity override phenomenon is probably controlled by many variables such as the ratio between horizontal and vertical permeabilities, oil viscosity and its change with temperature, rate of air injection, magnitude of heat losses of surrounding beds, reservoir thickness and dip, well spacing distance and patterns, etc. The mathematical model currently being developed will be used to study the interrelationships between these variables and their effects on the performance of the in-situ combustion process.

A second very necessary part of this project is to provide supporting information for testing and applying the model. Heat transfer data, knowledge of the effects of temperature on physical properties involved in the model and reliable combustion data are required for this purpose. All but the combustion data are now being generated in the present laboratories. Reliable combustion data will require additional funding to construct an adiabatic combustion tube.

The mathematical model will be tested with field data from such projects as the Cities Service Bodcau Field Trial. However, because of limited instrumentation possible in field projects, a large scale laboratory test facility will be required to test the model completely and to evaluate fully the effects of the variable factors. Additional funding will be required for this purpose.

This project was first started in Spring, 1975, but the first funding was received for FY 76. The initial phase of the work consisted of reviewing the published literature on field case histories and theoretical models describing the in-situ combustion process.

ACCOMPLISHMENTS DURING 1976

Review of the published literature confirmed the importance of gravity override in many in-situ combustion field projects and showed the lack of an adequate theoretical basis to study the problem.

The plan for this year was to develop a 2-D mathematical model to simulate the in-situ combustion process in a thick, inclined oil reservoir. By varying the magnitudes of different parameters in the model, the interrelations between the variables and their effect on the combustion process would be studied.

Laboratory experiments were also planned to provide a basic understanding of the heat transfer mechanisms in porous media in the presence of multiphase fluid saturation and flow.

The basic equations describing the heat and mass transfer process were formulated and expressed in finite difference form. The main subroutine for solution of these equations was developed based on SIP (Strongly Implicit Procedure). The subroutine was tested for a two-liquid immiscible displacement problem, for which the solution was known, and satisfactory results were obtained. Work was started on testing the routine for a gas-liquid displacement process in which gravity override could be expected. Preliminary results again indicate that the solution technique is successful.

Existing steady-state thermal conductivity apparatus was modified to permit the study of natural and forced convection in porous media. With careful guard heating it is possible to make a complete heat balance in the system and thus the combined modes of heat transfer can be studied. Preliminary results show that this apparatus will provide useful data relating heat transfer characteristics to the physical properties of the system.

PLANNED ACTIVITIES FOR 1977

It is planned to complete the mathematical model of in-situ combustion during 1977. A parameter study will be made to evaluate the effects of the variables listed earlier. The model will then be used to optimize the controllable variables such as well spacings and patterns, rates of air injection, and production scheduling for the producing wells. Efforts will also be made to test the model against actual field results.

Laboratory experiments will be continued to provide basic data on flow and heat transfer properties. Final designs will be completed for the adiabatic combustion tube and the large scale laboratory test facility in preparation for anticipated funding in FY 1978.

HIGH-TEMPERATURE PROPERTIES OF SILICATE LIQUIDS: APPLICATIONS TO THE EQUILIBRATION AND ASCENT OF BASIC MAGMA

I. S. E. Carmichael, J. Nicholls,* F. J. Spera,
B. J. Wood,† and S. A. Nelson

High-temperature heat content measurements have been made on a series of silicate liquids, which in conjunction with published data, are used to derive partial molar heat capacities of SiO_2, TiO_2, Al_2O_3, Fe_2O_3, FeO, MgO, CaO, Na_2O, and K_2O in the temperature range 1200-1650 K. Only

Fe_2O_3 appears to be compositionally dependent, and the best evidence suggests that there is no excess heat capacity ($\bar{C}p_i = \bar{C}p$). In combination with calorimetric data and the effect of pressure on the fusion temperature of solid compounds, a consistent set of enthalpy, entropy and volume data have been derived for the liquid compounds $CaMgSi_2O_6$, $NaAlSi_3O_8$, $KAlSi_3O_8$, Fe_2SiO_4 and TiO_2.

By using activities (relative to a liquid standard state) calculated at 1 bar for a range of lavas, the equilibration pressures and temperatures of lavas with a lherzolitic source material are calculated, and for basanites indicate 22-25 kbar and 1310-1360 °C. The regular solution formulation used in these calculations gives estimated errors of 40 °C and 5.7 kbars when compared to experimental equilibria. It is suggested that one of the thermal responses of ascending alkali basalt magma to engulfing cooler lherzolitic nodules could be the precipitation of megacrysts, and the calculated equilibration pressures and temperatures of the megacryst assemblage (16-20 kbar, 1220-1240 °C) are in accord with this.

The importance of viewing volcanic eruptions as the last stage in a sequence of chemical and thermomechanical instabilities is pointed out. Equations expressing the conservation of energy, mass and momentum on a macroscopic scale are given. The high Rayleigh numbers appropriate for even the relatively small magma volumes of erupted alkali basalts indicate turbulent flow-regimes with characteristic thermal convection velocities of the same order as nodule settling velocities. There is a significant partial melting effect in the mantle surrounding an ascending diapir if buoyancy is a significant force acting to drive the magma upwards. The effect of latent heat and convective heat losses on the thermal budget of a rising diapir has been calculated and shows the assumption of adiabaticity is often unwarranted -- even for rapidly ascending magma. Finally, mass transfer rates due to convective diffusion have been calculated for all the major components in a basic silicate liquid. Integral mass exchange depends inversely on the ascent rate and is quite small for the rapidly ascending alkali basalts.

FOOTNOTES

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ASSESSMENT OF THE OFF-SHORE COMMERCIAL SAND AND GRAVEL POTENTIAL ON THE CENTRAL CALIFORNIA CONTINENTAL SHELF*

P. Wilde† and W. B. N. Berry‡

INTRODUCTION

Sand and gravel are the second most valuable non-petroleum mineral commodities produced in California. In 1973, sand and gravel accounted for a dollar value of $162,290,000 or 21% of the value of minerals produced in the state.[1] However, the growth of metropolitan areas, which, on one hand, increases the demand for sand and gravel as aggregate, on the other hand, produces situations which inhibit or will eventually prevent utilization of many land based aggregate resources. The recognition of potentially valuable sand and gravel bars and banks will provide planners for the future with reasonably accessible, recoverable sources of aggregate with which to meet the needs of the urban areas around San Francisco and San Jose. If the potentially useful sand and gravel deposits are identified at this stage of long-range planning, then appropriate consideration of the ecological consequences of mining these deposits may be considered before the real need exists. This project concerns the identification of sand and gravel deposits in the Central California near-shore areas that may be considered for their commercial potential.

The University of California Museum of Paleontology has among its collections a group of about 3,000 samples taken from the California continental shelf and beach areas north of Point Conception. Many of these samples (hereafter referred to as the HEL collection) have been examined for grain size distribution. We will use the HEL collection and the data concerning marine sediment grain size to compile maps showing the distribution of grain sizes on the Central California off-shore and permitting the analyses of this distribution. The maps will also help in defining bodies bearing sand and larger particles of commercial value.

ACCOMPLISHMENTS DURING 1976

As of 1 January 1977, approximately 3/4 of the HEL collection has been checked for punching errors against an initial computer compilation and the sediment descriptions placed in a standardized format. The initial computer compilation (unchecked) has been programmed for map displays, and preliminary maps of sediment location, median grain size, and sorting coefficient have been produced for a selected off-shore strip (see Fig. 1).

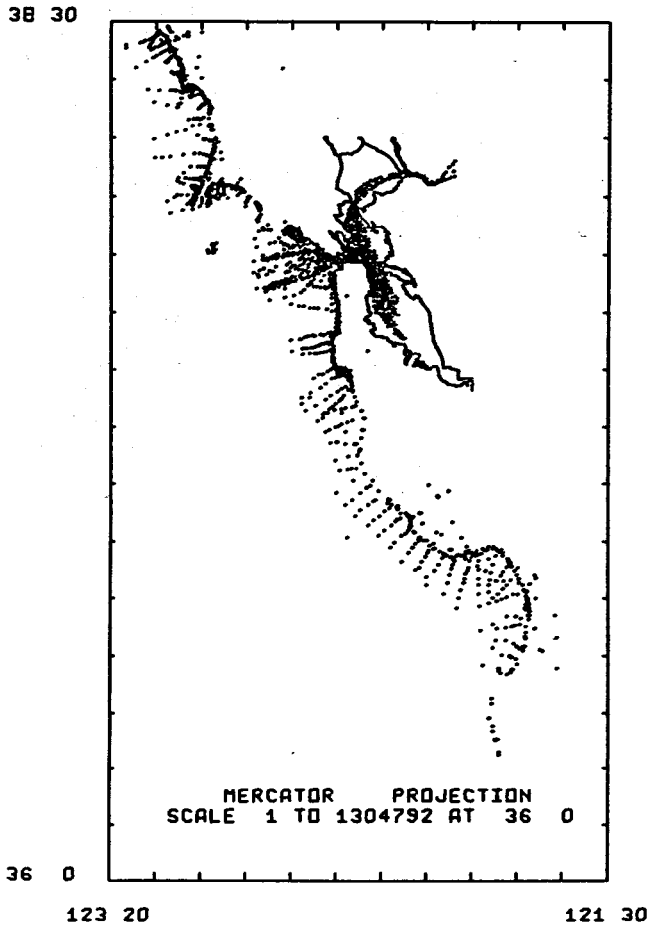

Fig. 1. Selected off-shore strip. (XBL 773-7925)

The project objectives for 1976-77 were to (A) insure that the HEL collection is stored in an orderly manner and that the information in the computer base correlates with the actual sample locations and descriptions, and (B) display four grain size parameters: (1) median grain size, (2) sorting coefficient, (3) skewness, and (4) kurtosis, for stations in the collection where sufficient grain size analytical work has been done. The purpose of these maps is a preliminary delineation of the potential economic off-shore sand and gravel deposits.

At the end of the project year we will have:

I. A corrected computer print-out catalogue of the HEL collection including HEL stations in consecutive order; position in latitude and longitude; sampling device; sampling time in hours, day, month, year; depth; location- intertidal, shelf, beach, etc.; sediment description; key to publication of data; and field number. Raw grain size data will be in an additional section of the catalogue by consecutive HEL number weight of sieve catch in grams; by standard mesh number; millimeters, and phi units.

II. A strip-map atlas showing locations of stations and individual maps of the grain size statistics; median grain size, sorting coefficient, skewness, and kurtosis for the Central California off-shore also will be produced.

1977-78 OBJECTIVES

Under the current Sea Grant project (R/CZ-37), grain size information from the analysed samples is being filed in a computer for processing and generation of computer-plotted maps showing mean grain size, sorting coefficient, skewness, and kurtosis. For the Sea Grant project year 1977-78, it is proposed to (1) complete size analyses of the samples in the HEL collection not yet sieved, (2) up-date the grain size maps generated in 1976-77 with this new data, and (3) produce a map showing the commercial value of the analysed samples in dollars per ton based on grain size/price schedules for San Francisco Bay Area aggregate. From such a map, areas of potential interest for commercial extraction may be identified for environmental impacts. All the data obtained from sample analyses are being processed using computers for eventual retrieval in user-specified formats (maps, charts, listings).

FOOTNOTES AND REFERENCE

*Project funded by Department of Commerce/Sea Grant (R/CZ-37).

†Energy & Environment Division.

‡Department of Paleontology/Paleontological Museum, University of California Berkeley.

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COMPILATIONS OF MARINE GEOLOGIC AND OCEANOGRAPHIC DATA OFF THE WEST COAST OF THE UNITED STATES

P. Wilde,* T. E. Chase,† and W. R. Normark†

Recognizing that the rational utilization and management of the energy resources in or transported through the marine environment depend on adequate but also readily accessible information, LBL in co-operation with the U. S. Geological Survey and other marine data sources on the west coast

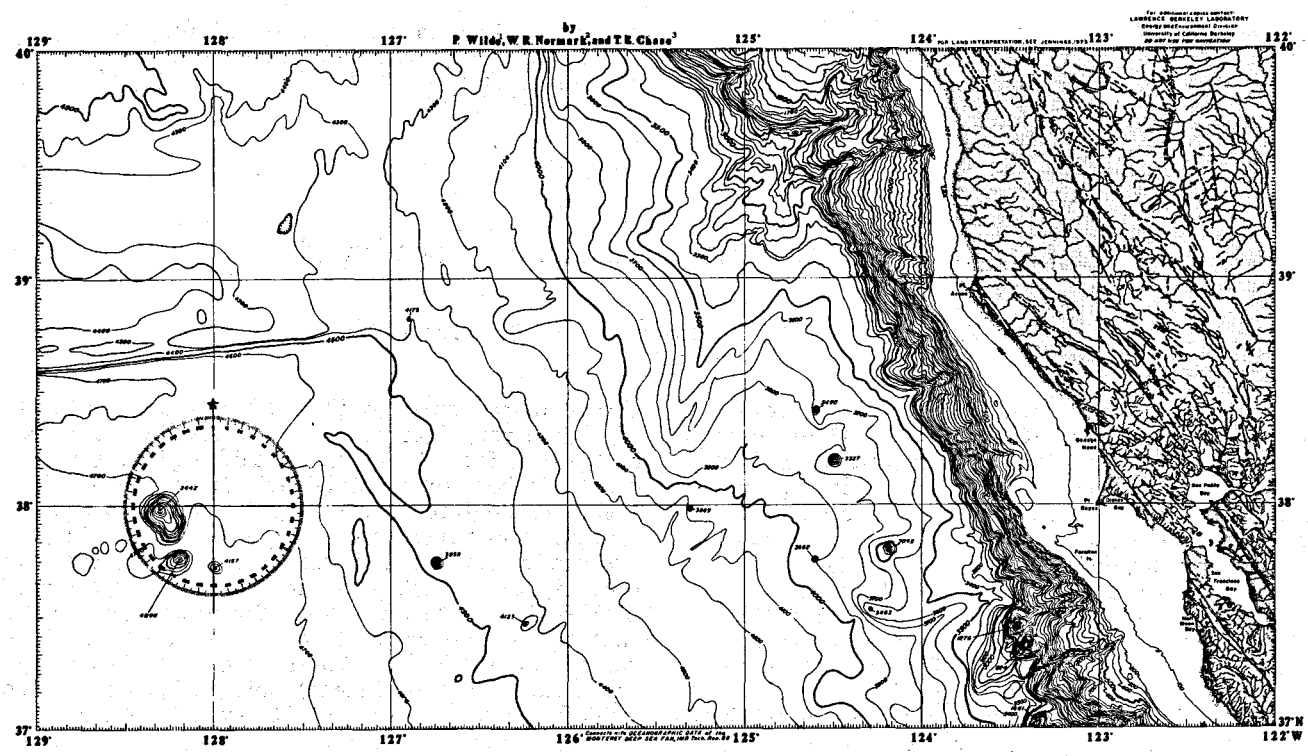

Fig. 1. Oceanographic data off central California 37° to 40° north including the Delgada Deep Sea Fan.

Table 1. Supplementary maps and charts.

Parameter	3000 series Monterey and Delgada	Proposed sub-regional	Proposed regional North pacific
DSDP sites	X		
Earthquake epicenters	X		
Geomorphic features	X		
Gravity	X		
Heat-Flow	X		
Magnetics	X		
Physical Oceanographic stations	X		
Sediment stations	X		
Sub-bottom profile tracks	X		
Surface currents (Monthly)	X		
Surface temperature (Monthly)	X		
Wave direction (proposed)	X		
Commercial fish catch		X	
Geostrophic flow (Monthly)		X	
Mean thickness of surface layer (Monthly)		X	
150 Meter O_2 (Monthly)		X	
Salinity		X	
Temperature		X	
150 Meter 19 year mean O_2		X	
Salinity		X	
Temperature		X	
Pressure systems			X
Profiles (N-S) (E-W) O_2			X
Phosphate			X
Salinity			X
Temperature			X
Thermosteric anomaly			X
Sea conditions (seasonal)			X
Surface currents (seasonal)			X
Surface winds (seasonal)			X
Storm tracks			X

are producing a series of one sheet compilation charts. These charts are map base presentations of bathymetric, marine geologic, and oceanographic data providing summary references to such data available within about 400 km. of the west coast of the United States. A series of five charts will cover the west coast from 34° N (Point Conception, California) to 49° N (U. S. - Canadian border) in 3° segments. The first edition of the two southern sheets, the Monterey and Delgada sheets (see Fig.1 for Delgada base chart), are complete. The bathymetric base is a Mercator projection 3000 series, which will encourage their use at sea. Depths are given in corrected meters and the contour interval is 100 meters. Supplementary maps and charts, at smaller scale, serve as indices to data available on gravity, magnetics, etc. (see Table 1). Other types of data not representable on maps include sub-bottom profiles and columnar sections from the Deep-Sea Drilling Project. References are listed by categories; (1) published papers and books, (2) reports of limited circulation, and (3) academic theses. Sources of navigational information and lists of charts and maps available are included. The major objective of this compilation is to provide a vehicle of convenient size which can be revised and modified as new information is received and which summarizes the pertinent marine geologic and oceanographic data for a given area, with reference to the original data that can be used both as a planning document for upcoming cruises and as a working chart during shipboard operations.

FOOTNOTES AND PUBLICATIONS

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† U. S. Geological Survey, Pacific-Arctic Branch, Menlo Park, California.

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RARE EARTH AND OTHER TRACE ELEMENTS IN HISTORIC AZOREAN LAVAS*

H. Bowman,† M. F. J. Flower‡ and H.-U. Schmincke‡

Rare earth element (REE) and other trace element compositions of 16 lavas from all historic and 2 prehistoric eruptions on 5 islands of the Azores Archipelago show notable intra- and inter-island differences. Fe enrichment and "compatible" element depletion due to fractional crystallization have been superimposed on variations established in the source area. Fractionation of La/Sm, U/Th, K/Na and "large ion lithophile" (LIL) element abundances are probably related to variable fusion of a source periodotite whose LIL element distribution cannot be exactly specified in view of its possible heterogeneity. Relative light-REE enrichment in basalt appears greatest on the "potassic" island São Miguel, the more sodic island Fayal and one lava from Pico, and least in basalts from the "sodic" islands Terceira, São Jorge and Pico. This variation is matched by most other LIL elements, although P shows unexpected enrichment in Terceira lavas, otherwise the least LIL element-enriched and most heavy-REE-enriched. Upper mantle phase chemistry is probably critical in establishing the patterns. In particular, P-REE covariance may reflect phase stabilities of apatite and (P-bearing) garnet in the upper mantle. Distribution patterns of REE in the historic lavas are similar to those of basalts from the Atlantic median rift at the crest of the Azores "platform". Transition to light-REE-depleted rift-erupted basalts to the southwest is believed to be step-wise with increasing water depth, possibly indicating retention of a light-REE-rich phase in the residue from partial fusion as intersection of geotherm and peridotite solidus occur at lower pressures. The source mantle for the Azores basalts is probably light-REE- and LIL element-enriched but we find no evidence so far to suggest its emplacement by thermal "plume" activity.

FOOTNOTES

*Journal of Volcanology and Geothermal Research, 1 (1976).

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Controlled Thermonuclear Research Program

INTRODUCTION

The Plasma Physics and Controlled-Fusion Research Program at the Lawrence Berkeley Laboratory is divided into five projects:

1. Plasma Production and Heating Experiments
2. Plasma Theory
3. Atomic Physics Studies
4. Tormac Project
5. Neutral-Beam Development and Technology.

All of these are parts of the coordinated program of ERDA's Division of Magnetic Fusion Energy. The Tormac Project is in addition partially supported by the Electric Power Research Institute.

The projects are listed here in the order of increasing magnitude, as regards manpower and budget at LBL. By far the largest is the Neutral-Beam Development and Technology Project. It is carried out as a joint program with the Lawrence Livermore Laboratory, and in fact it is administered through LLL and handled as a subcontract to LBL. We are including it here for completeness sake, but we are restricting our report to the work done at LBL. Only very brief summary statements are made because a description of this project appears in the annual report on magnetic fusion energy issued by LLL.

Present and future large tokamak experiments in the U.S. as well as abroad, and the current and future mirror confinement experiments at Livermore depend on powerful and intense, low-divergence beams of neutral hydrogen (or deuterium) atoms for the production of their hot plasma. It is therefore not surprising that the neutral-beam injector problem has been given the highest priority within the Development and Technology category of the MFE program.

In 1976 a large new test stand and associated power supplies were commissioned, capable of handling beam pulses of 20 A ion current and 0.5 sec duration. An accelerating voltage of 70 kV was reached. Eventually the ion energy is scheduled to reach a value of 120 kV, the design figure for the Toroidal Fusion Test Reactor at Princeton. The presently tested pulse length of 0.5 sec is adequate, and the entire approach proved to be promising enough, so that LBL was selected to develop, build, and test the prototype injector system for the TFTR.

The remaining four projects listed above have the following unifying features: Both Plasma Production and Heating Experiments and Atomic Physics Studies are largely serving the function of basic support for the neutral-beam work. The first is concerned primarily with the improvement of our understanding of ion sources and similar matters of relevance to the neutral-beam injectors. In 1976 the effort concentrated on the development of computer models for the source, and on diagnostic work needed to supply experimental input data for these models. The atomic physics is aimed at supplying missing data on fundamental processes, such as certain charge-transfer cross sections or negative-ion production mechanisms. The most striking result here was a surprisingly large negative ion yield for D^+ passing through Cs vapor at energies below 1 keV.

The theoretical effort has been diversified, but as in previous years the emphasis has been on nonlinear processes in plasmas, of interest to controlled fusion because of their relevance to plasma heating schemes.

A substantial fraction of the Plasma Theory is carried out in support of the Tormac Project. The latter is our only direct contribution to the magnetic confinement problem in controlled-fusion research. The Tormac, short for toroidal magnetic cusp, is one of several so-called "alternate concepts." The latter are being worked on in the United States as back-ups, in case unexpected difficulties arise in the mainline developments of tokamaks or magnetic mirrors, or in case a new concept is found leading to a superior or more economical fusion reactor.

The major achievements in the Tormac Project in 1976 have been the completion of and first experiments with the 1-m diameter Tormac V installation. It is too early to quote results from Tormac V. Most of the remaining effort dealt with development and application of new diagnostics. Several of the latter have been used on Tormac IV, which has been yielding very encouraging results.

PLASMA PRODUCTION AND HEATING (ION SOURCE RESEARCH)

C. F. Burrell, J. R. Cary, C. F. Chan, W. S. Cooper
W. B. Kunkel, and K. F. Schoenberg

ION SOURCE MODELING
(C. F. Chan and W. S. Cooper)

The designs and costs of magnetic-confinement CTR experimental devices and reactors that use neutral injection for heating and/or fueling can be greatly affected by the choice of parameters used in the neutral-beam source design. It is therefore important to understand the basic physical conditions of the process controlling the properties of

the plasma ion source. We have developed a computer model for the study of this problem. In an idealized way the model describes a one-dimensional discharge bounded by two insulated parallel walls. The Poisson equation and the ion equation of motion are solved simultaneously with a set of boundary conditions describing neutral gas influx through one wall, local ion generation due to electron-neutral collisions, and ion and neutral loss through the other (partially transparent) wall. Electrons have been described either by a single-component or a two-component Boltzmann distribution. A preliminary comparison between theoretical predictions of the model and available data from an operating LBL plasma source show agreement within experimental errors. The model is also used to do exploratory calculations for situations with various different sets of input parameters. For example, it is found that lengthening the axial dimension can significantly improve the gas efficiency of the device, though we realize that other effects not yet included in the model might cause complications. For a given input neutral flux, increase in the transparencies of the extracting wall for both the ions and neutrals can greatly increase the output ion current if the peak electron density is maintained. For a specified output ion current density, a minimal input neutral flux can be found by varying those transparency factors as well as other parameters.

Further work is planned to include in the model electron energy balance, ion composition, ion-ion scattering, magnetic reflection of ions and electrons on the neutral-flux-entrance wall, etc.

THEORY OF THE ELECTRON DISTRIBUTION FUNCTION IN A PLASMA SOURCE

(J. R. Cary)

The most important parameter in the analysis of any discharge is probably the electron velocity distribution function. In the past it was assumed that the electrons in the LBL plasma source consisted of Maxwellians or monoenergetic primaries plus cold secondaries, as approximations. In order to improve this model, a computer calculation was done during 1976 which predicts the electron energy distribution function in our plasma source. This calculation includes the effects of electron-electron collisions and electron-neutral collisions, but it does not include possible collective effects. The calculation requires five experimental parameters as input: the arc current, the arc voltage, the neutral gas density, and the density and temperature of the cold electrons in the source. From the calculated electron distribution function, the Langmuir probe characteristic is calculated and compared to experimental measurements. The theoretical curves agree with the experimental curve within experimental error.

The success of the calculation described above has allowed two general conclusions to be drawn. The first is that collective effects are not needed to explain existing experimental data regarding the electron distribution function in the plasma source. The second conclusion has to do with determining electron distribution functions from Langmuir probe characteristics. Although the calculated distribution function was highly non-Maxwellian, the associated theoretical Langmuir probe characteristic agreed well with an experimental probe characteristic which had been interpreted as being due to the superposition of two Maxwellian distributions. Evidently inferring electron distribution functions from Langmuir probe characteristics can be very unreliable.

The calculation has not yet been made self-consistent so that power balance and particle balance cannot be used to determine the electrical characteristics of the discharge. Eventually, however, such computed energy distributions must be incorporated into ion source models as discussed in the preceding section.

EXPERIMENTAL MEASUREMENTS ON THE LBL PLASMA ION SOURCE

(C. F. Burrell, W. S. Cooper, and K. F. Schoenberg)

The computer model of the plasma ion source used in our neutral beam systems requires the electron density and the neutral atomic temperature as input parameters. An experimental investigation of the LBL 10-ampere ion sources has been undertaken using spectroscopy and electrostatic probes. The objectives of this experimental program are to provide the input data required by the computer model, to serve as a comparison for the predictions of the computer model, and to provide insight into the processes in the source which control the efficiency and the atomic/molecular particle mix in the source.

Spectroscopic measurements of Doppler-broadened line profiles in the source were made using a scanning Fabry-Perot interferometer. The plasma source was observed through the accelerator slots on an optic axis at a slight angle with the neutral beam axis. From the Doppler broadening of the atomic deuterium Balmer-Beta (D_β) line profile, the neutral temperature in the source can be determined. The neutral temperature is a required input to the plasma source computer model and is also required to estimate the neutral gas density in the source.

The observed D_β profiles were corrected for Stark broadening and fine structure as well as instrumental broadening. The atomic deuterium temperature was observed to increase from ~0.29 eV to ~0.4 eV as the arc power was increased from 10 kW to 55 kW at a gas flow rate of 6 Torr • ℓ/sec. For comparison, operation of the plasma source with a helium discharge (and observation of the HeI 4922 Å line) yielded neutral helium temperatures ranging from 0.1 eV to 0.15 eV as the arc power was increased from 20 kW to 50 kW. It seems likely that the higher temperature of the deuterium compared to the helium is due to the fragmentation energy of the deuterium molecule. When D_2 is dissociated, each atom carries off approximately 2 eV in kinetic energy; however, multiple wall collisions reduce the atomic temperature to less than 0.4 eV.

Molecular ions (D_2^+ and D_3^+) in the plasma source are also accelerated by the high voltage on the extractor grids and contribute to the neutral

beam current. The molecules fragment in the neutralizer section producing one-half and one-third energy components of the neutral beam. A high priority of source development is to reduce the molecular content of the neutral beams because the fractional energy neutrals penetrate less deeply into a target plasma than does the full energy component and tend to heat only the surface. In order to understand the processes which determine the molecular-to-atomic ratio in a plasma source, it is necessary to know the molecular temperature as well as the atomic temperature.

We have used the same Fabry-Perot system discussed earlier to measure the molecular temperature from Doppler-broadened molecular lines. We find the neutral molecular temperature to be in the range 0.09 eV to 0.15 eV or very similar to the results for atomic helium.

Langmuir probe measurements have been made in the plasma source to measure electron density and temperature. These are input and output parameters, respectively, for the computer model of the source. The electron temperature is especially important because the ionization rate in the source is a sensitive function of the electron temperature.

On a single shot we sweep the voltage on a standard Langmuir probe and display the probe current and voltage on a X-Y oscilloscope display. When the probe data is transferred to a semi-log plot we find the curves are well fit by a broken straight line, indicating a "two-temperature" distribution with most of the electrons at the lower temperature. If we fit the data in this manner by two straight line segments, each characterized by its own "temperature", we find that for a gas flow of 6 Torr • ℓ/sec the low temperature component went from 4 eV to 5 eV as the arc power was increased from 10 kW to 50 kW, and the high temperature component increased from 5 eV to 7 eV. The electron density was observed to increase linearly with the arc power.

Because the Langmuir probe integrates over the electron velocity distribution function it is difficult to distinguish between different electron velocity distribution functions which produce similar current versus voltage characteristics. In order to resolve this ambiguity work is in progress to double-differentiate and amplify the probe signal to directly determine the distribution function from the relation

$$f(V_\phi) = -\frac{1}{2\pi}\left(\frac{Me^2}{e^3}\right)\frac{d^2 j(V_\phi)}{dV_\phi^2}.$$

PLASMA THEORY

B. I. Cohen,* J. H. Hammer, S. Johnston,† A. N. Kaufman,
H. A. Mynick, N. R. Pereira, A. M. Sessler, and G. R. Smith

INTRODUCTION

Our studies in plasma theory continue to be concentrated in the area of nonlinear plasma waves and their interactions. The waves considered may be thought of as being externally launched, as in heating schemes; or produced by instabilities; or due to wave-wave interactions.

The phenomena studied may be classified according to the role played by resonant particles. Three of our studies pertain to situations where this role is dominant:

- The stochastic motion, induced in tokamak trapped particles by the overlap of resonances between wave frequency and particle bounce frequency, acts as a saturation mechanism for wave instability.

- A wave destabilized by a resonant-particle beam traps the beam and undergoes self-consistent modulations in amplitude and phase.

- A large-amplitude wave, excited by an applied field, traps particles and undergoes modulation at the nonlinear mismatch frequency and simultaneously at the trapped-particle bounce frequency.

When resonant particles play a less dominant role, two nonlinear effects become significant: three-wave coupling and nonlinear propagation.

- A general expression was obtained for the coupling of three normal modes in a nonuniform magnetized Vlasov plasma, such as in a tokamak. This coupling manifests Manley-Rowe symmetry.

- The class of exactly solvable nonlinear wave equations was studied by the use of scaling transformations.

As a separate study, we have analyzed the conditions for and stability of interior poloidal rotation of plasma in the Tormac configuration. The following sections describe each of these studies in more detail.

STOCHASTIC PARTICLE MOTION AND THE TRAPPED-ION MODE

(G. R. Smith)

Anomalous transport in large tokamaks is probably caused by fluctuating electric fields which occur when the dissipative trapped-ion instability is present. The amplitude of the fluctuating fields is determined by that nonlinear mechanism which saturates the instability at the lowest level.

We are studying[1] a nonlinear process not previously considered--the overlap of bounce resonances. The frequency of bouncing between magnetic

mirrors depends on the magnetic moment μ and the longitudinal action J. Resonance occurs when the frequency of the trapped-ion mode ω is an integer multiple of the bounce frequency $\omega_b(J,\mu)$. A mode of finite amplitude causes overlap of bounce resonances and, in the vicinity of the boundary (in velocity space) between trapped and untrapped particles, destruction of the invariance of J. A relatively small mode amplitude causes a large fraction of the ions to move stochastically, with low-energy ions most strongly affected. We expect the stochastic motion to have a strong effect on the nonlinear growth of the trapped-ion mode.

The dynamical system studied here is also of interest in research on the disruptive instability in tokamaks and on the general theory of stochasticity.

A TRACTABLE MODEL FOR NONLINEAR BEAM-PLASMA INTERACTION[2]

(H. E. Mynick and A. N. Kaufman)

The interaction between plasma waves and resonant particles is a frequently occurring phenomenon in many areas of plasma studies, including plasma heating. In heating the plasma with a beam, the beam causes growth of modes with phase velocity near the beam velocity, while in heating with a large-amplitude externally applied wave, the resonant particles are in the plasma distribution itself. Many workers have studied variants of this wave-resonant-particle problem, in experiments, simulations, and analytic work. We have concentrated on developing a fuller explanation of the results of a particular study: a simulation of a beam-plasma system done by O'Neil, Winfrey, and Malmberg.[3]

We use a simple picture of the two-dimensional phase-space trajectories of the beam particles, namely that the phase space motion of the particles trapped in each wave trough can be decomposed into two parts; an average motion of the particles as a whole (sloshing in the trough) plus a revolution of the bar-like shape which the particles form in phase space about that average phase point.

We formalize this picture by applying a novel reduction procedure to the Hamiltonian for the full N-particle problem, to obtain a reduced Hamiltonian, having only two degrees of freedom.

The reduced problem is simple enough to be analytically tractable and yet captures enough of the essential physics of the full problem that it describes well many aspects of the previously unexplained results of Ref. 3. For example, the simulation presented in that paper yielded an instantaneous growth rate having a sawtooth shape, and a frequency shift having a characteristic superposition of components at the bounce frequency and its second harmonic. Our reduced theory gives explicit expressions for these functions, which show each of these features. Moreover, these features now have a simple physical explanation.

In principle the technique is applicable to other wave-resonant particle interaction problems, such as the post-saturation behavior of a linearly unstable mode.

NONLINEAR WAVES EXCITED NEAR RESONANCE[4]

(B. I. Cohen and A. N. Kaufman)

When a plasma wave is excited by an applied field of given frequency and wave number, its amplitude is inversely proportional to the mismatch between the frequency and the eigenfrequency of a freely propagating wave of the same wave number. Further, the amplitude modulates with a frequency given by that mismatch. An important complication arises from wave nonlinearity– for a Langmuir wave, a sufficiently large amplitude causes electron trapping. This has two effects: first, the eigenfrequency develops nonlinear contributions to the magnitudes of its real and imaginary parts (frequency shift and damping, respectively); secondly, the bouncing of the trapped electrons produces further modulation, at the bounce frequency (and its harmonics), of the complex eigenfrequency, and thereby of the amplitude.

This process has been studied by computer simulation and has been interpreted analytically by a dielectric formulation. If one considers the applied field as due to beating of two primary waves, the phenomena studied apply directly to three-wave interactions.

OSCILLATION CENTER THEORY OF THREE-WAVE INTERACTIONS

(S. Johnston and A. N. Kaufman)

The three-wave coupling coefficient is important in many nonlinear plasma problems. Heretofore this coefficient has been calculated for specific physical situations. Our aim is to obtain a more general expression, which is concise and which exhibits the symmetry leading to the Manley-Rowe relation.

The basic concept used in this work is the oscillation center, defined as the orbit about which a particle executes wave-induced oscillations. Just as the center of particle gyration, or guiding center, in a magnetic field is subject to a quasi-static averaged magnetic force, an oscillation center is subject to a "ponderomotive" force due to nonlinear effects of the waves on the particle.

In our formalism an oscillation-center Hamiltonian, that is trilinear in the wave amplitudes is derived for a nonresonant particle, using canonical perturbation theory. Summing this Hamiltonian, over the unperturbed particle distribution, leads to a form for the three-wave coupling coefficient that has the desired symmetry.

The formalism at present is general enough to describe the electromagnetic normal modes in any nonuniform magnetized collisionless plasma. Since no restrictions are placed on the magnitudes of wave frequencies, the results may be applied to such problems as the coupling of drift waves and lower-hybrid waves in tokamaks.

SCALING INVARIANCE OF THE MOTION OF HELICAL CURVES AND SOLITON EQUATIONS[5]

(N. R. Pereira)

At present there is much interest in plasma physics and in other areas of physics where nonlinear wave phenomena are important, in exactly solvable nonlinear wave equations (soliton equations). Various stages of lower-hybrid heating of large tokamaks are described by two such equations: the nonlinear Schroedinger and the modifed Korteweg-de Vries. Lamb[6] has shown how to relate these two equations to the motion of helical curves. Our research shows that the invariance properties of this motion, under a scaling transformation, restrict the class of nonlinear equations that can be solved exactly to only those that scale as the ones already found by Lamb.

THEORY OF TORMAC INTERIOR

(J. H. Hammer and A. M. Sessler)

To restrict motion due to guiding-center drifts, it has been proposed to make the interior region of Tormac, containing only toroidal field lines, rotate about the minor axis. During 1976 we have investigated problems related to the equilibrium, stability, and damping of the rotation.

The equilibrium analysis has been further improved by the techniques of Eli Hameiri (Courant Institute of Mathematical Sciences, New York University), in which the exact general solutions of the two fluid equations are found for density, pressure, magnetic field profiles, and a single nonlinear partial differential equation is evolved for the stream function Ψ. A sufficient condition for existence of solutions to the equation for Ψ is found to be $d\Omega/d\Psi \equiv 0$, where $\Omega \equiv$ the vorticity $(\nabla \times v)$ to lowest order in $\epsilon \equiv r/R$, the inverse aspect ratio.

A stability analysis, employing an inverse aspect ratio and examining flute modes $k \cdot B = 0$, yields a sufficient condition for stability of Kelvin-Helmholtz (velocity shear) modes: $d\Omega/d\Psi \leq 0$, identical to the equilibrium condition above.

The possibility of a damping of the rotation has been suggested by Boozer, Rosenbluth and others. In the presence of classical collisions or some anomalous process, the anisotropic pressure of the plasma will tend to relax toward isotropy. As flux tubes are convected around due to the rotation, the perpendicular and parallel components of the pressure are driven apart as a result of the compression and decompression of the tubes. When the frequency of compression-decompression ($\omega_{rotation}$) is on the order of the isotropization rate ($\nu_{collision}$), the process is nonadiabatic and energy is extracted from the rotation and converted into heat.

Calculations of the damping rate and constraints on possible driving mechanisms provide restrictions on the parameters of the device, specifically the inverse aspect ratio $r/R \lesssim 1/30$ for bulk rotation if the electrons are classical. A thin layer ($\Delta r \sim \rho_i$, the ion gyro-radius) of rotating plasma may be a possibility if the electrons are isotropized by classical collisions.

In 1977, studies of the interior should include investigation of Rayleigh-Taylor (centrifugal) instabilities in the presence of velocity shear, further analysis of the ramifications of rotational damping, and possible isotropization mechanisms for the electrons.

FOOTNOTES AND REFERENCES

*Present address: Lawrence Livermore Laboratory, Livermore, CA 94550.

†Present address: Columbia University, School of Engineering and Applied Science, New York, NY 10027.

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ATOMIC PHYSICS STUDIES

K. H. Berkner, W. G. Graham, D. Leung, R. V. Pyle, S. E. Savas, A. S. Schlachter, P. J. Schneider, K. R. Stalder, and J. W. Stearns

PRODUCTION AND DESTRUCTION OF H^-

The atomic physics section of the CTR group is continuing to study the formation and destruction of H^- ions,[1] a topic of considerable interest to the neutral-beam injection program.

FORMATION OF H^- BY BACKSCATTERING FROM CLEAN METALLIC SURFACES

The study of backscattered negative ions from clean metal surfaces bombarded by H_2^+ and D_2^+ ions was continued during the year. The negative-ion production coefficient (backscattered negative ions per incident H or D nucleus) vs energy for a molybdenum substrate coated with Li, K, Na, Cs, and Rb is shown in Figs. 1a and 1b. These preliminary results show a strong energy dependence of the negative-ion production coefficient for all the alkali targets, with the maximum yields occurring at the lowest incident energy. There is also evidence of an isotope effect. As yet the negative ions have

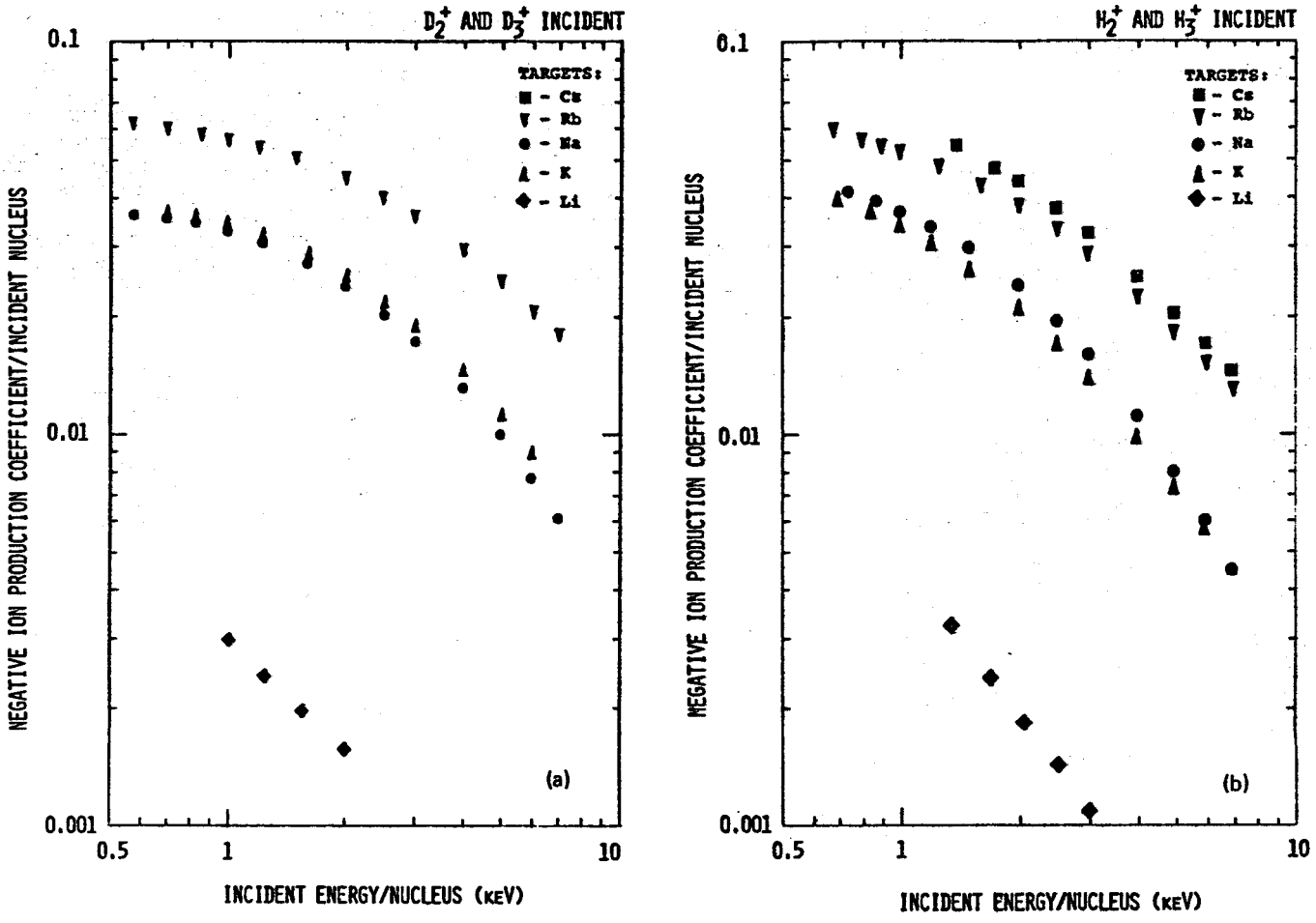

Fig. 1a & 1b. The yield of negative ions (backscattered negative ions per incident H or D nucleus) produced by backscattering when H_3^+ or D_3^+ ions bombard a molybdenum substrate coated with Li, K, Na, Cs, or Rb.

not been identified. During the next year a quadrupole mass analyzer will be used to analyze the backscattered negative ions. The negative-ion yield as a function of substrate temperature will also be investigated.

LOW-ENERGY SURFACE-SCATTERING EXPERIMENT

Construction of the low-energy surface-scattering experiment[1] has been completed. In this experiment atomic hydrogen produced in a hot tungsten tube will be used to bombard a hot, cesiated tungsten surface. A quadrupole mass spectrometer will be used to analyze backscattered H^- ions. Preliminary experiments are scheduled to begin in March.

CHARGE EXCHANGE OF H^+ IN METAL VAPORS

As part of a continuing effort to explore negative-ion production by charge transfer in metal vapors, we have measured the equilibrium charge fractions that result when 3.3- to 35-keV deuterium beams emerge from a "thick" target of Sr vapor. Preliminary results are shown in Fig. 2.

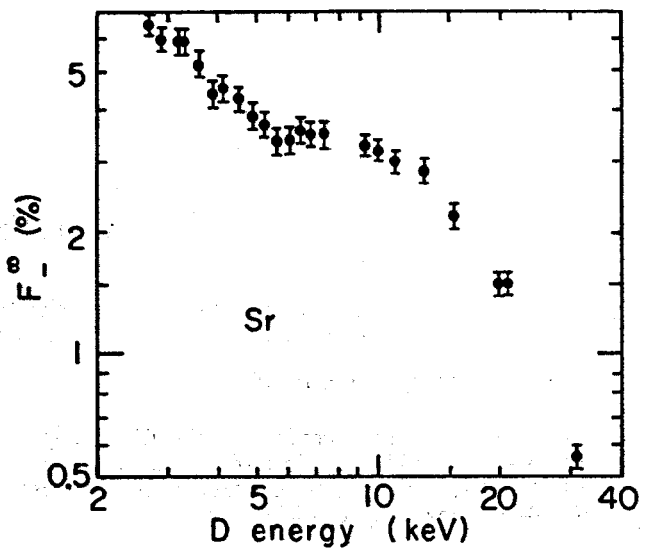

Fig. 2. Equilibrium yield F_-^∞ for D in strontium vapor target. (XBL 773-570)

Charge exchange of deuterium in cesium vapor is a promising way to make intense negative deuterium ion beams for the injection of neutral atoms into tokamaks and mirror machines. Cesium was believed to have the highest negative conversion efficiency of any target medium known, but at low energies there were discrepancies of greater than a factor of two in the previously-measured values (the maximum being between 10 and 21%). To resolve these discrepancies a special apparatus for low-energy measurements was constructed. The main features are: close spacing between the accelerator, vapor cell, electrostatic analyzer, and detectors to minimize beam loss due to scattering; a recirculating cesium vapor target designed on the same principle as a heat pipe--this permits use of a large-aperture target; detection of the atomic beam with a large acceptance-angle pryo-electric detector; and detection of charged particles with large acceptance-angle, magnetically-shielded Faraday cups. The negative-ion conversion efficiency for deuterium ions in cesium vapor, or the equilibrium D^- yield, was found to be 35% at a deuterium energy of 300 eV, dropping smoothly to 27% at 1 keV and 2.8% at 10 keV (see Fig. 3). This large conversion efficiency at low energies is being applied to large-scale negative-ion systems at Livermore and elsewhere.

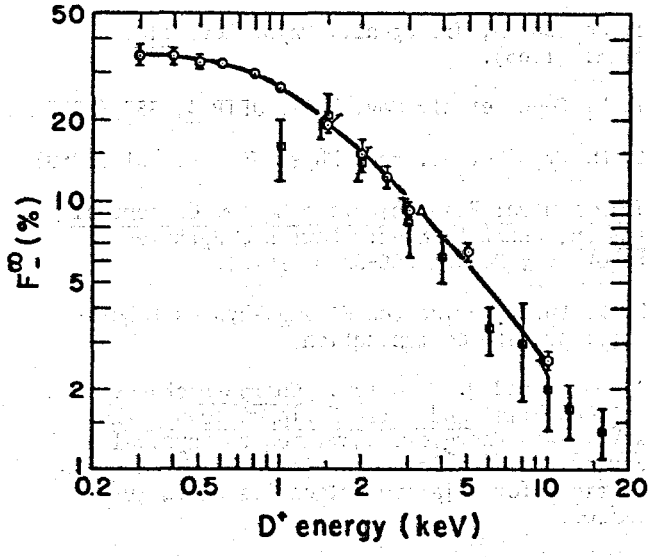

Fig. 3. Equilibrium yield, F_-^∞, of D^- for D^+ in cesium vapor target. ○ Present experiment; □ Schlachter, et al. (1969); △ Schlachter and Stearns (1975), unpublished. The curve is drawn for clarity. (XBL 772-410)

H^- INTERACTIONS WITH A PLASMA

The plasma target to be used in converting 100- to 150-keV H^- ions to neutral atoms is still being developed. Work is continuing in producing a dense ($n\ell \approx 10^{15}$ ions/cm^2) hydrogen plasma in a pulsed, high-current, hot-cathode arc discharge in a magnetic field.

CROSS SECTIONS FOR CHARGE-CHANGING COLLISIONS OF 20- to 120-keV OXYGEN IONS AND ATOMS IN HYDROGEN

High-Z impurities may have a very detrimental effect on the behavior of fusion plasmas. One possible source of these impurities is in the neutral hydrogen or deuterium beams used for plasma heating and fueling. In order to measure the impurity-atom content of these beams, it is necessary to know the charge-changing cross sections for the impurity ions in the neutralizer gas. Since oxygen is a possible impurity both in positive[2] and negative[3] ion sources, we have measured the charge-changing cross sections for O^+ and O in H_2 at energies from 20 to 120 keV. Preliminary results are shown in Figs. 4 and 5. Cross-section measurements for O^- ions are planned.

ELECTRON-CAPTURE AND -LOSS BY HIGHLY-STRIPPED IONS IN HYDROGEN TARGETS

The primary plasma-heating method in controlled-fusion magnetic-containment devices, such as tokamaks, is the injection of 80- to 150-keV deuterium atoms;[7] the atoms penetrate the magnetic field and are ionized (and hence trapped in the containment region) by a target plasma. A crucial question in determining the penetration depth (trapping profile) of the injected D beam is the effect of impurity ions, which in a tokamak plasma exist in very high charge states (e.g., Fe^{+26}).[8] These impurity ions can attenuate the

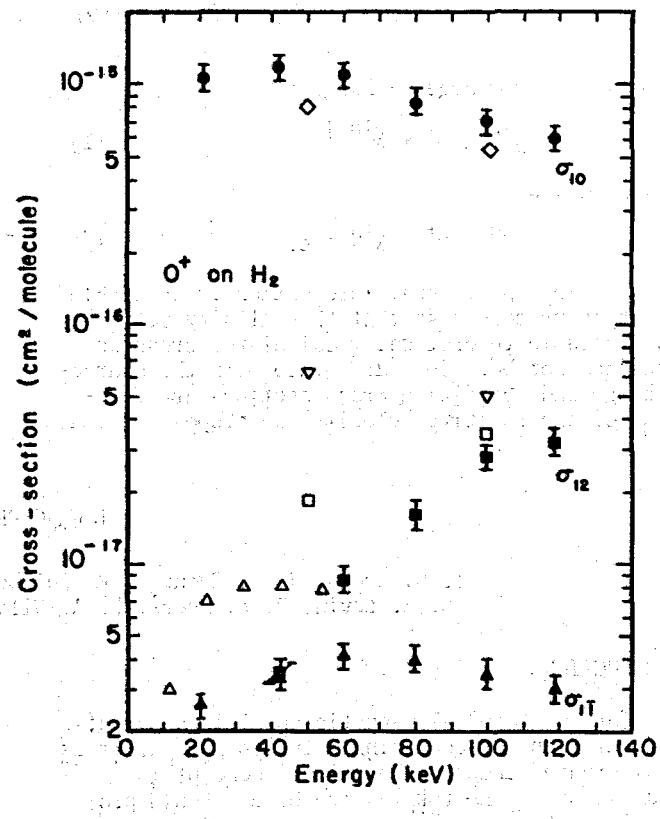

Fig. 4. Cross sections for O^+ on H_2. σ_{10}: ●, present; ◇, Ref. 3. σ_{12}: ■, present; □, Ref. 3. σ_{1-1}: ▲, present; ▽, Ref.3; △, Ref. 4. (XBL 773-490)

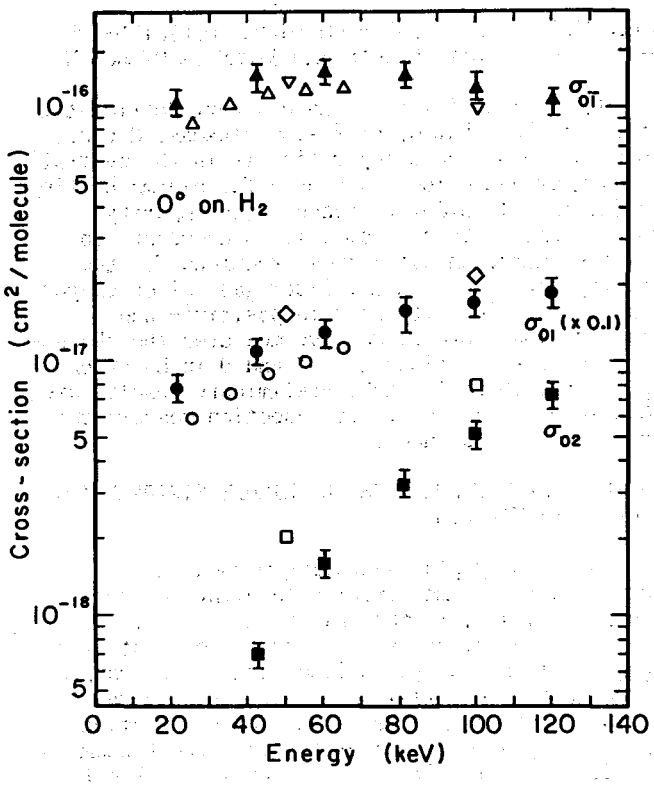

Fig. 5. Cross sections for 0° on H_2. σ_{01}: ●, present; ◇, Ref. 3; ○, Ref. 5. σ_{0-1}: ▲, present; ▽, Ref. 3; △, Ref. 5. σ_{02}: ■, present; □, Ref. 3.

(XBL 773-489)

beam by either charge exchange

$$D + X^{+n} \rightarrow D^+ + X^{+n-1} \quad (1)$$

or ionization

$$D + X^{+n} \rightarrow D^+ + X^{+n} + e. \quad (2)$$

Very little experimental information is available for these processes so that the validity of the few available theoretically calculated cross sections has not been tested.[9] Since both the charge-exchange and ionization cross sections are functions of the relative velocity, we propose to measure these cross sections with SuperHILAC beams of highly-stripped heavy ions impinging on a deuterium target.

The general experimental arrangement consists of an analyzer magnet to select one particular ionization state (X^{+n}), a differentially pumped gas target, and another magnet to analyze the charge states produced in the target cell by sweeping the beam across a slitted Faraday cup or an array of solid-state detectors.

The apparatus for the charge-exchange measurements was built and checked out with an 8.5 MeV/amu beam of Ar^{+18} and Ar^{+17} ions. The first experiments with iron beams are scheduled for the latter part of January 1977. The apparatus can be readily modified for ionization measurements, which are scheduled for the second half of 1977.

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TORMAC PROJECT

I. G. Brown, J. W. Coonrod, B. Feinberg, M. J. Greenwald, W. B. Kunkel, M. A. Levin, B. R. Myers, R. A. Niland, W. M. Sharp, and R. S. Shaw

INTRODUCTION

Tormac (toroidal magnetic cusp) is a magnetic configuration for confining a fusion plasma. It is an alternate concept. The primary concept is tokamak, and using tokamak the U. S. should produce a breakeven fusion reactor by 1984. Unfortunately, there is concern that tokamak may not be suitable as a commercial reactor. It is pulsed; it has a minimum size larger than most currently used power installations, and it requires magnetic fields of size and intensity awesome to contemplate and expensive to build. Tormac as an alternate concept looks more economically practical as well as technically simpler. If Tormac works, it can be operated in steady state, it can be of relatively small size, and it requires magnetic fields of a size and intensity currently obtainable without superconductors.

To determine if the Tormac concept can be made into a fusion reactor, LBL has embarked on an experimental and theoretical program to test the several postulates about plasma behavior on which it is based. These include questions of MHD stability, collisionless containment of particles and wave heating of plasma.

TORMAC IV EXPERIMENT

The basic magnetohydrodynamic stability of cusps has long been known and understood. On the other hand, the problem with cusps has been that in the classical geometry there is a rapid loss of plasma along open field lines. The Tormac geometry was developed in an attempt to solve this problem by the use of symmetry. The toroidal symmetry of Tormac creates a canonical invariant which helps to trap particles on magnetic field lines between collisions.

In effect, what happens in Tormac is that the basic stability of cusps is combined with a surface mirror containment to give Tormac, at least in theory, an adequate containment time for a fusion reactor. As in a mirror device, high temperatures are needed to see and study this problem; however, all the problems of Tormac are not in the sheath, the internal structure is also of concern. Of particular interest is the boundary of the sheath with the internal plasma and the insulating properties of this system. The study of this boundary is being carried out in Tormac IV.

Tormac IV is a small relatively low temperature experiment. It has a Tormac shape (Fig. 1) but its sheath plasma is too cool and too collisional to be mirror contained. In Tormac IV flow along magnetic field lines is stopped by the wall itself. Wall stoppering is enhanced by increasing the magnetic field near the wall. This region of intense field narrows the contact surface so as to reduce thermal conductivity that would otherwise cool the sheath. Measurements indicate that the bulk of the sheath has a temperature near 30 eV; however, near the wall the gas would necessarily be cool.

Pressure equilibrium along magnetic field lines would then create high density gas near the wall. This high density gas recombines and serves to insulate the hotter gas from the wall. Surprisingly the rate of loss of the cool gas near the wall is very slow because of the high collision rate with trapped ionized particles. Thus, with a relatively stable warm sheath held in place by wall stoppering it is possible to study the internal structure in Tormac IV.

One detail of interest in Tormac is the insulation of the bulk of the plasma from the sheath. The sheath in a high temperature Tormac reactor would be mirror contained. This fact imposes special conditions on the electron temperature and the ion distribution function. It is then at least desirable and probably necessary to insulate the central region from the sheath. Without insulation, thermal conductivity and propagation of the special mirror distribution function into the central region could degrade the containment properties of the geometry. One method of plasma insulation is with an internal poloidal magnetic field (see Fig. 2).

A poloidal magnetic field can be established internally in Tormac IV by trapping. To accomplish this a tokamak-like discharge is first produced. In this mode helical field lines are formed within the plasma; and, at the same time, the plasma is heated to trap these field lines. The cusp magnetic field is then applied to form the configuration shown in Fig. 2.

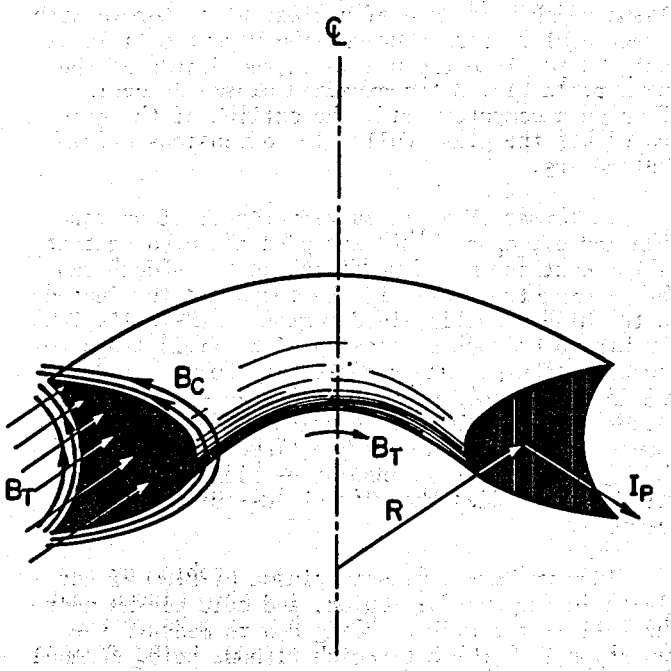

Fig. 1. Outline of a high-density plasma magnetically confined in a bicusp. (CBB 754-2804)

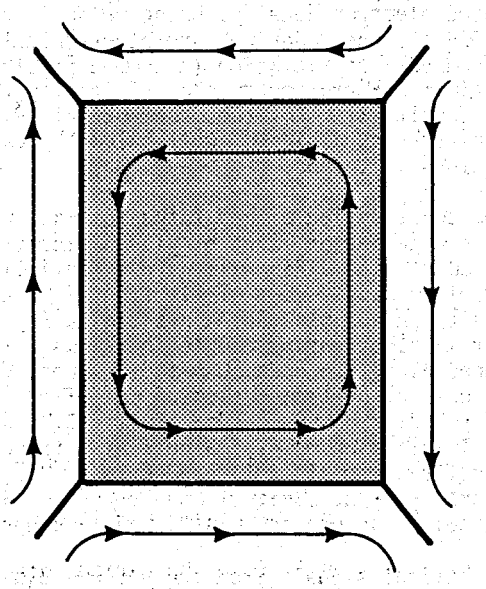

Fig. 2. Schematic representation of a plasma confined in a four pole cusp magnetic field with an internally-trapped poloidal field. Note the reversal of magnetic field direction across the boundary. (XBL 773-649)

Experimental measurements in Tormac IV using the above technique have given relatively high plasma temperatures in the center of the plasma with a relatively long time constant. A typical result is $n \simeq 3\times10^{14}$, T_i = 100 eV, τ = 50 μsec. The mean free path for ions in such a plasma is long compared to the size of the plasma. The time constant is also long compared to the ion collision time and the ion electron collision time for cold electrons. The implication of these results is that it is possible to form a stable Tormac configuration with thermal and particle isolation between an internal hot region, and a relatively cool sheath.

DIAGNOSTIC TECHNIQUES

The principal diagnostic tools currently used in the Tormac IV and Tormac V experiments employ light in the visible spectrum in one way or another. Since the vacuum vessels in these devices are glass, ready access to view virtually the whole interior region is available. On the other hand, many of the conventional plasma diagnostics (Langmuir probes, magnetic probes, etc.) cannot be used because of the high plasma temperatures and densities achieved in the Tormac experiments.

Spectroscopic techniques are heavily relied upon, particularly the Doppler and Stark broadening of spectral lines as measurements of plasma temperature and density. A number of polychromators (devices whigh split plasma light into many narrow wavelength increments and convert the light intensities in each "channel" into electrical signals) have been designed and constructed by the Tormac Group. Typical parameters of these devices are a separation between channels of 0.3 Å, with a total of 16 adjacent channels, and time resolution ~1 μsec.

A number of laser interferometers have also been designed and constructed in-house. These devices sense plasma electron density averaged over the path of the laser beam and hence give a line-integrated electron density. Using He-Ne lasers (λ = 6328 Å), these devices are electronically stabilized against vibration (a common problem with optical interferometry that limits its resolution). Sensitivities of the order of 5×10^{13} electrons/cm^2 are achieved, well below typical measured values in Tormac.

The construction of apparatus to measure Thomson scattering of light by plasma electrons is nearing completion. This will give a spatially and time-resolved measurement of electron temperature and density in the plasma. A particle energy analyzer is also nearing completion. This will be positioned along the open cusp field lines, where it will collect particles flowing out of the main body of the plasma and measure their energy distribution. Information on plasma currents, trapped magnetic flux, etc. is collected by a number of flux loops, current monitors and Rogowski coils at various points around the plasma and windings.

Electrical signals from the various diagnostic devices are collected, digitized and stored in a PDP-11 computer. The computer typically samples the output of each diagnostic every 1/2 μsec for the duration of the experiment. This data is then immediately displayed after a shot and stored on magnetic tape for later use. Some data analysis is performed immediately on the PDP-11 and displayed, such as the calculation of spectral line profiles, correction for instrument calibrations, etc. Large-scale data analysis, such as the spatially resolved spectral line emission calculations described in the next section, is carried out at the LBL computer center with a CDC 7600 computer, using the taped data. Permanent records of all data taken on the Tormac experiments are stored at the computer center, where they remain available for analysis.

SPECTRAL LINE RECONSTRUCTION

A technique for spatially resolving spectral line profiles in two dimensions as a function of time from a set of one-dimensional projections for an arbitrary plasma shape has recently been developed as a plasma diagnostic tool for the Tormac devices. Light emitted from the plasma is collected in a light pipe with a narrow acceptance angle at various positions around the plasma, and is transmitted to a polychromator where it is broken up into wavelength increments. Amplitudes are recorded by the computerized data acquisition system. A computer code using the data from about a hundred light-pipe positions calculates the self-consistent point-by-point emission of light from the plasma as a function of time and wavelength interval. This allows the reconstruction of spectral line emission at points within the plasma. These spatially resolved Stark and Doppler broadened line profiles then give plasma temperature and density as a function of position and time. A further refinement of the technique unfolds plasma drifts and rotation by Doppler shifts of spectral lines.

RECONSTRUCTION FOR TORMAC IV

Tormac IV makes an almost ideal subject for developing the reconstruction technique. It has a reasonably hot plasma and good visibility. The plasma chamber is made of a clear glass toroid with a rectangular cross section. The magnetic field is designed to place the plasma in the center of the chamber. In Fig. 3 the expected plasma shape is drawn on a computer grid. The outline of the grid represents the glass walls. The dimensions are in centimeters.

In Tormac IV a plasma temperature of no more than 150 eV, $n_e = 5\times10^{14}$ has been measured so that mirror containment of particles in the sheath can not be expected. However, the cusps are terminated in the high magnetic field region on the wall. Thus the plasma escapes by flowing along field lines to the wall. The plasma is cooled at the wall and recombines. The cold neutrals can then flow into the vacuum regions. The only problem is that the counterstreaming neutrals are trapped by the incoming gas to form an insulating blanket near the wall which reduces the rate of loss of plasma from Tormac IV.

Thus we have a classic plasma problem of hot plasma in the central region, and cold plasma near the wall -- the problem being how to measure the radiation from the hot region without being swamped by light from the cold gas. To solve this the reconstruction technique is used.

Figures 3 and 4 were made using the 16-channel spectrograph ($\Delta\lambda \sim 0.3$Å) using four sweeps of the plasma at 45°, 90°, 135°, and 180°, each at 18 positions; however, for these pictures the light has been integrated over wavelength to give the total emission of 4686 from the 10% helium in hydrogen plasma.

In order to determine the temperature of the plasma in the central region, it is necessary to perform spatial and time integrals to collect enough light to make a measurement.

Approximately 50 line shapes corresponding to each point in the shape in the central region is Doppler broadened, reflecting ion temperature. A simple routine has been incorporated into the computer program which gives the temperature if the line were Gaussian.

The advantage of the reconstruction method is that it discriminates so that light from the low emission region is separated from the more luminous cool regions. Unfortunately, this separation of light is not perfect and the low emission regions do have some "scattered light from more intense regions." An examination of the line shape and averaging over time and space helps to to reduce the ambiguity introduced by the scattered light. A set of temperatures has been arrived at for the entire plasma over the entire time period. It should be pointed out that this represents measuring radiation from a plasma probably in Saha equilibrium with a 60-70 eV electron temperature. Since electron temperatures are not expected to go much above 100 eV in Tormac V, it is expected that this technique will be able to help with diagnostics on Tormac V.

As an illustration of the power of the reconstruction technique, a set of measurements was taken in Tormac IV with the interior region of the plasma near 100 eV. Under these circumstances the emission intensity in the plasma interior is about 1% of the intensity in the surrounding region. In Fig. 5 the line shape with error bars is shown. This result indicates the power of this technique which should give definitive results in Tormac V above 300 eV.

TORMAC V

Tormac V is designed around a 1-m by 1-m glass system shown in Fig. 6. Unlike Tormac IV, which has a wall supported plasma, the Tormac V plasma is designed to be fully collisionless with the cusps mirror contained. Thus, Tormac V represents a first test of the Tormac Concept of sheath

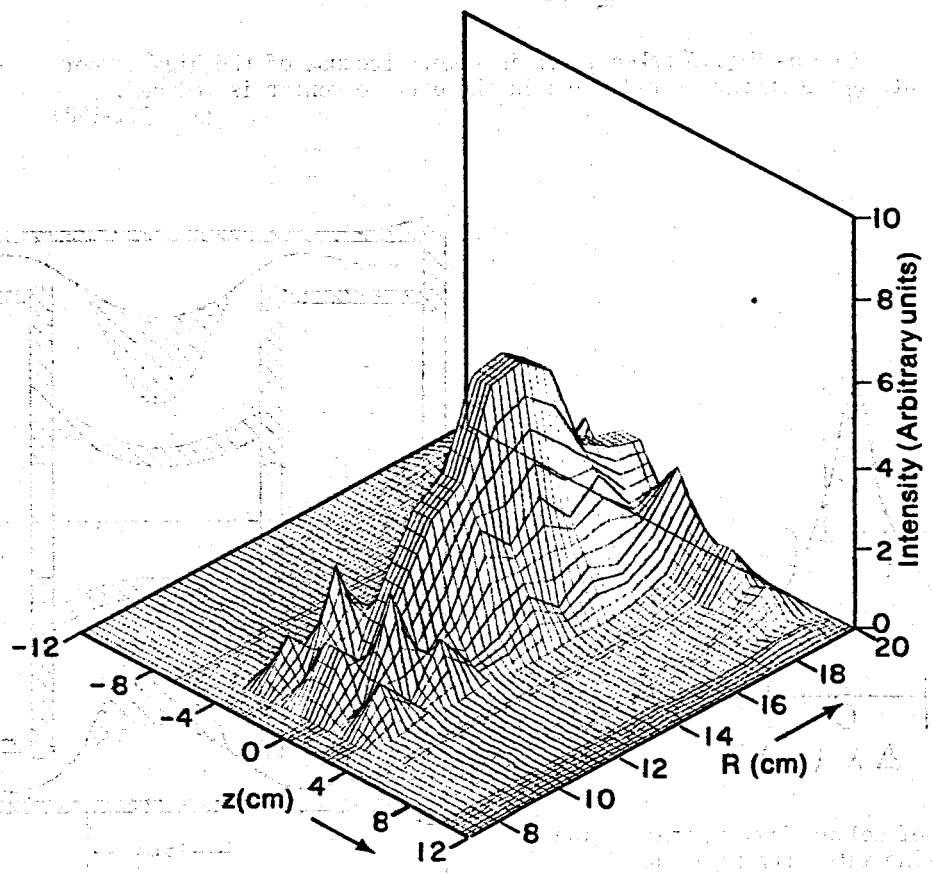

Fig. 3. Reconstruction of the line radiation from ionized helium in a bicusp. Taken soon after compression, the intensity of radiation tends to be high in the center. (XBL 771-199)

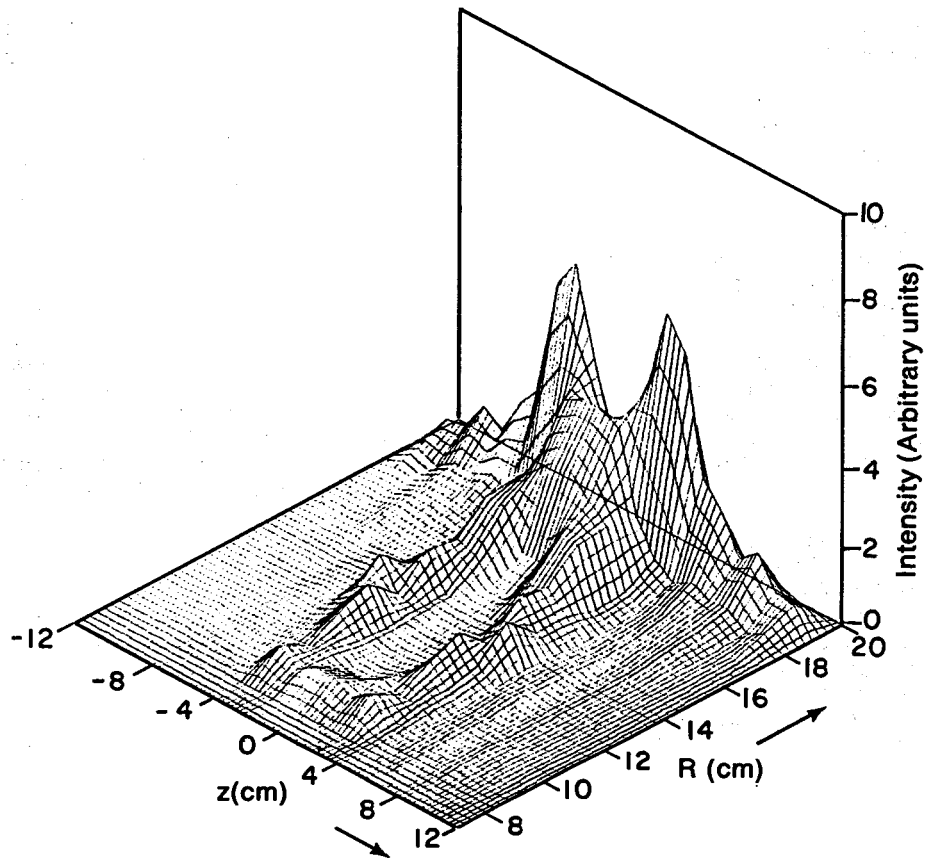

Fig. 4. Same as Fig. 3 taken later in time. Because of the high temperature the amount of radiation in the extreme center is reduced.
(XBL 771-198)

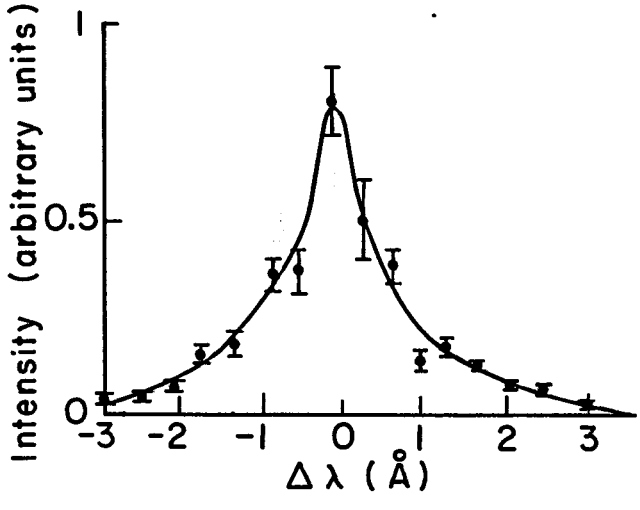

Fig. 5. 4686 Å line of helium from central region of plasma. Line intensity is about 1% that of surrounding region but is recovered from data with relatively small error bars using reconstruction technique.
(XBL 771-186)

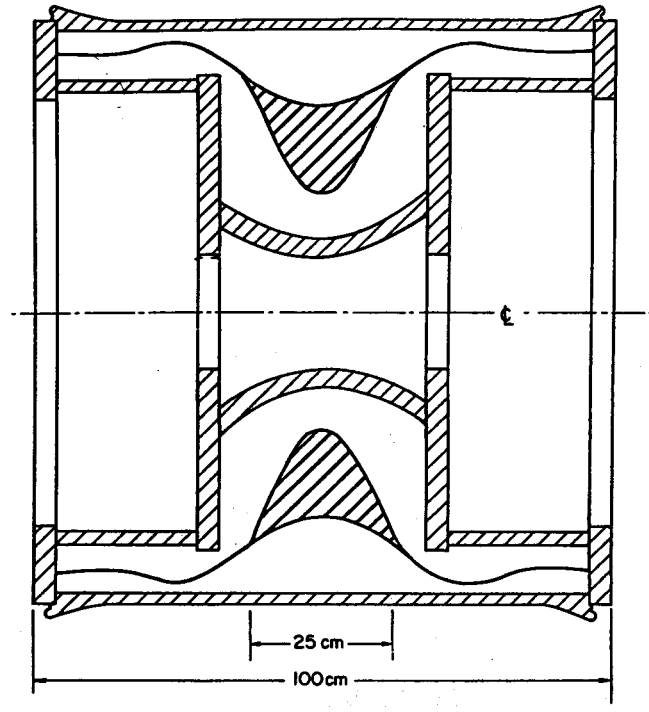

Fig. 6. Tormac V glass cross section with plasma outline in center. (XBL 757-4469)

containment of plasma. In order to do this, the plasma must be collisionless to the extent that the particle mean free path is long compared to the size of the plasma.

ferometer. The results of this measurement are shown in Fig. 8. A three-dimensional plot of the interferometer measured electron density is shown as a function of position and time. On the back

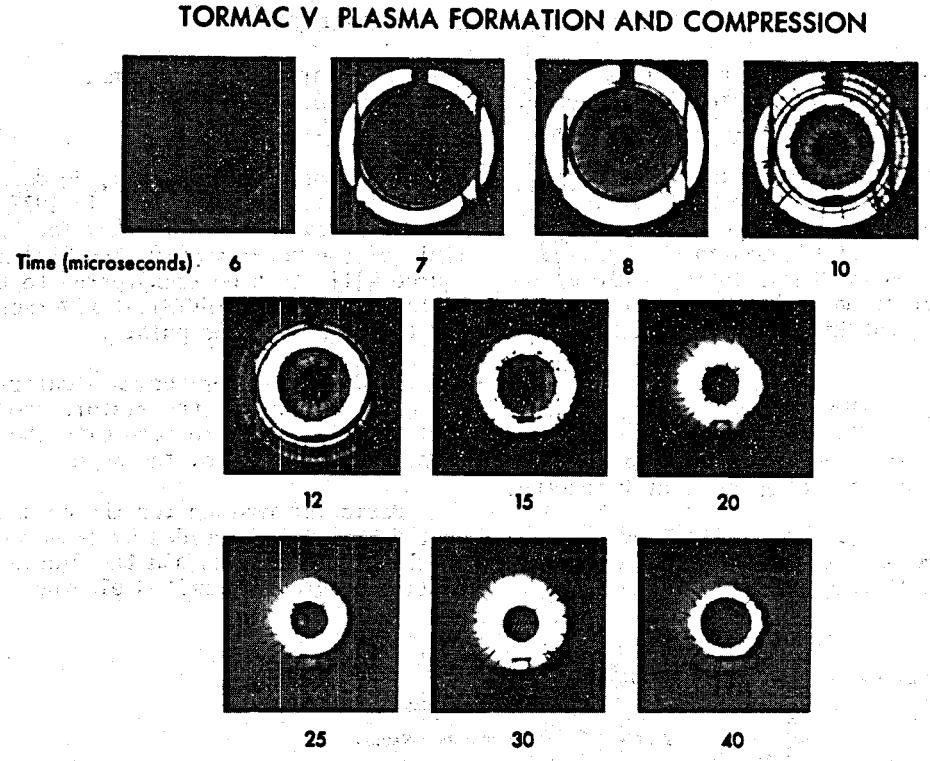

Fig. 7. Image converter picture of preionization phase in Tormac V. (XBL 763-2263)

The production of a collisionless plasma in Tormac V represents one of the more difficult problems of the experiment. This is because magnetic field trapping and plasma currents from an important part of the overall magnetic field design. This means that the plasma density must be sufficient to hold the magnetic pressure; it also means that the particle gyroradius must be small compared to the size of the plasma. Thus, in order to create a collisionless plasma, the plasma ion temperature must be at least 300 eV.

To produce the high temperatures in Tormac V a combination of "Shaker" heating and magnetic compression is used. A series of image convertor pictures showing the plasma formation and compression is shown in Fig. 7. In this picture the plasma is shown being radially compressed during the preionization period. In Fig. 8, a current trace with a record of the electron density is shown as measured by an interferometer. In Fig. 8 one sees the formation of the plasma at about 30 μsec with the preionization and then the further compression of the plasma at 60 μsec when the cusp bank is turned on.

In order to examine the shape of the plasma and follow its time history, a "reconstruction" was performed by moving the position of the inter-

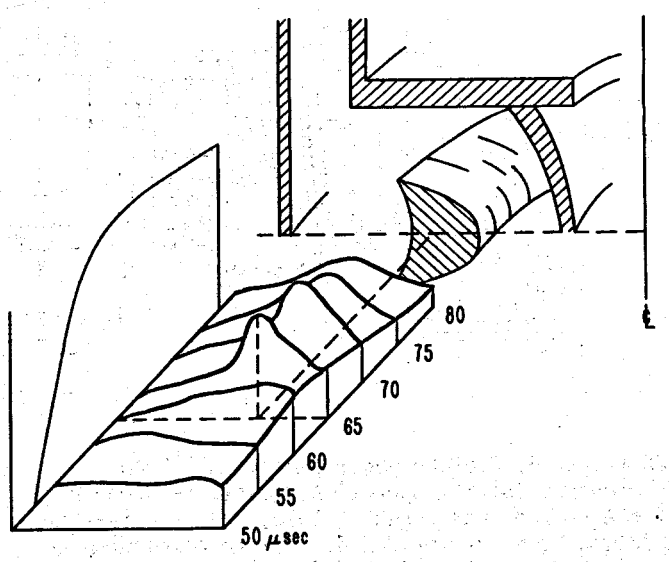

Fig. 8. Foreground represents interferometer record of $\int n_e d\ell$ as a function of time and position. In the background is a model plasma in the apparatus. The curve on the side is a plot of applied magnetic field intensity. (XBL 773-632)

plane is shown a record of the current waveform as a function of time. The outline of the vessel with the bicusp plasma is shown so that the density profile might be better interpreted. These results were obtained with plasma temperatures of about 200 eV. In order to raise the temperature of the plasma to the required 300 eV a larger higher frequency heating system is being developed.

NEUTRAL-BEAM DEVELOPMENT AND TECHNOLOGY*

W. R. Baker, K. H. Berkner, W. S. Cooper, K. W. Ehlers, D. B. Hopkins, J. M. Haughian, W. B. Kunkel, H. M. Owren, J. A. Paterson, B. A. Prichard,† R. V. Pyle, and J. W. Stearns

The objective of this program is the development of the technology and hardware required for the production of multi-megawatt beams of hydrogen and deuterium atoms to heat plasmas in CTR confinement devices and fusion reactors. There is close cooperation and interaction with fusion experimenters at Livermore, Oak Ridge, Princeton, and General Atomic.

The pulsed-beam development in 1976 was oriented toward the development of a 120-keV, 65-ampere, 0.5-second neutral-beam injection module for the Tokamak Fusion Test Reactor being built at Princeton.

The test facility described in the previous annual report[1] became operational in 1976. A one-fourth-area test source (Fig. 1), as well as a 120-kV, 20-A, 0.5-sec power supply, has been fabricated. Initial operation, mostly "shakedown" of the system, was begun in 1976, and 7-A, 70-kV hydrogen beam were produced. Work is continuing to obtain beams at the 120-keV design energy. During 1977 this test facility will be computer controlled with a system developed by the LBL Real Time Systems Group and Draper Laboratories.

A full-scale (65A, 120 kV) neutral-beam source was designed and construction has begun. At the same time a 65-A, 120-kV, 30-msec power supply has been under construction. In 1977 this system will be operated by to 120 keV for 30 msec, the limit of the power supply. The 65-A neutral-beam source will then be transferred to the High-Voltage Test Stand (HVTS) at Livermore to complete the tests for 0.5-sec pulses.

To diagnose these beams a calorimeter system was built. Arrays of thermistors are linked to a MODCOMP II computer to determine the beam-produced temperature profile of the beam.

Basic information for the neutral-beam development activity is provided by research carried out in the Atomic Physics and the Plasma Production and Heating programs described elsewhere in this report.

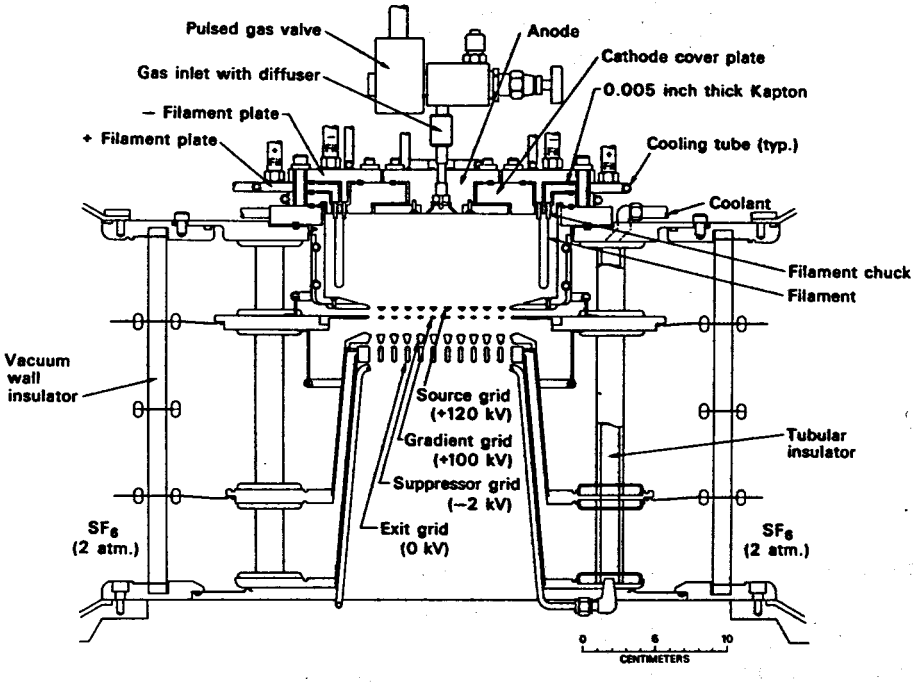

Fig. 1. Cross section of the 120-kV, 15-A, 0.5-sec module. (XBL 764-2747)

FOOTNOTES AND REFERENCE

*This work is part of a program of neutral-beam development being conducted jointly by the Lawrence Livermore and Lawrence Berkeley Laboratories. It has also been reported in the LLL Annual Report series UCRL-50002.

†Permanent address: Princeton Plasma Physics Laboratory.

1. Energy and Environment Annual Report (1975) Lawrence Berkeley Laboratory Report, LBL-5299.

Solar Energy Program

INTRODUCTION

The national solar energy research and development program has goals ranging from immediate demonstration of existing technologies to the development of future technologies. The solar efforts at LBL span this range in various time scales for potential application. Research in a variety of disciplines and at a variety of levels of technological development are included. Current programs include: the solar heating and cooling of buildings; solar thermal, photochemical, and photoelectric conversion; chemical energy storage; environmental and economic analysis; solar data collection and assessment; and ERDA support efforts.

The immediate application of existing solar technologies is being supported by a data collection and assessment project. This effort focuses on the California solar resource and will provide input for present and future designers of solar systems. Another program provides technical support for an FEA/ERDA/HUD plan to retrofit several houses with solar heating systems. Basic definition and design of these systems has been carried out at LBL. A program to develop a controller for residential solar heating and cooling systems has led to a prototype unit which is entering a test and evaluation phase. This controller is intended to be commercially viable and provide performance tailored to the needs of the individual residential users.

Several projects are directed toward the near-term application of the solar energy resource. A solid state heat engine driven by the temperature dependent properties of shape memory alloys has gone through several prototype stages. A working model, capable of using the low-grade heat from flat plate collectors, is currently being evaluated. Flat plate collectors are also expected to power an ammonia-water absorption air conditioning system currently under development at LBL. Technical feasibility has been established and the air conditioner has reached the prototype state. A project devoted to the measurement of the amount of circumsolar radiation may be especially important in the near-term demonstration of solar thermal electricity production via central receivers. These measurements will help to determine the expected thermal output of these plants and can also be used in atmospheric aerosol research.

Finally, there are two projects in more basic solar energy research and one program in the assessment of the effects of application of solar technologies. These three projects share a common time scale; their potential benefits lie in the future. One of these research efforts involves studying the feasibility of storing energy as the heat of reaction in certain reversible chemical processes. Appropriate reactions have been defined and their applicability to and integration with future solar thermal electric generation facilities are being investigated. The second basic research program is investigating photochemical conversion of solar energy. We are attempting to understand both the mechanisms by which hydrogen is produced in processes driven by photosynthesis and how certain chemical systems demonstrate the ability to generate photoelectric potentials. Experiments are being performed which demonstrate these effects and allow initial assessment of the concepts. The project studying the environmental and economic impact of the wide scale application of various solar technologies has concentrated thus far on the effects of central receiver solar thermal concepts. The primary efforts include studies of the redistribution of industrial activities, atmospheric effluents and climatic alterations resulting from a solar based electric generation capacity.

NITINOL ENGINE DEVELOPMENT*

Ridgway Banks and Michael Wahlig

INTRODUCTION

Temperature-dependent changes in the elastic properties of certain Shape Memory Alloys make possible the conversion of relatively low temperature heat to mechanical work by means of 'solid state' heat engines. Such machines show promise of having competitive conversion efficiencies and capital costs, when compared to other types of engines for low-temperature energy conversion, and have possible advantages in simplicity of practical installation. The current project deals with the use of such a solid-state heat engine for driving a vapor compression air conditioner using solar-heated hot water. Other potential applications for this type of engine include the generation of mechanical power (and, in turn, electricity), from solar thermal, ocean thermal, geothermal, or industrial waste heat sources.

A prototype heat engine based on a nickel-titanium alloy known as 55 Nitinol[1] has been in operation at the Lawrence Berkeley Laboratory since August 1973. Since that time the mechanics of the shape memory properties of Nitinol have been studied, as have the thermodynamic properties of engine cycles using Nitinol wire as the working element. Several iterations in engine design have led to an improved understanding of the important practical considerations in Nitinol engine operation and have led to the development of an improved prototype engine.

Design Criteria for Solid State Heat Engines

Use of a crystalline solid as the working 'fluid' in a heat engine imposes special consider-

ations in mechanical design. As the solid lacks the flow and compression characteristics of conventional fluids, special attention must be paid to the thermal and mechanical properties of the working material as well as to the dynamics of the cycle in which it is used.

Of the Nitinol materials commercially available, the most effective have proven to be wires approximately 0.5 mm in diameter. Tests[2] conducted at LBL during 1975 indicated that wires of this size, when strained axially at 3% elongation, have an output potential of $\geq$ 1.0 watt/gram at a cycling rate of 60 cpm. It was also found that if the wires were not uniformly heated during the transformation, or if the stresses developed during shape recovery were allowed to peak at a point of minimum mechanical advantage, excessive stress concentrations would develop. This would lead to progressive fatigue and eventual failure of the wires. Other investigations into the details of Nitinol wire behavior under cyclic conditions revealed that the time response of the wire's shape change was quite different when heated (rapid response) than when cooled (slow response).

During 1975 a new engine design was developed to accommodate these unique wire properties. This is known as the Cam-Track Nitinol Engine and is shown in Fig. 1. In this design, 0.5 mm diameter wires are supported between movable trolleys mounted on continuous tracks. The tracks are supported by a multiplicity of standoffs from the ends of a cylindrical tank. While the ends of the tank are parallel, the lengths of the standoffs differ so that the distance between the tracks may be varied. In practice, the tracks converge along approximately 20% of their complete length, diverge during approximately 50%, and run parallel for the balance of their length.

In the part of the cycle that the tracks diverge (outer diameter in Fig. 1) the wires are immersed in cold water and, because of the divergence of the tracks, are elongated by approximately 3%. Following this part of the cycle, the tracks run parallel as the direction of travel is reversed to approach the concentric hot water bath (inner diameter). Immediately at the point where the wires enter the hot water, the tracks begin to converge, and recovery stresses in the Nitinol wires are relieved as shortening of the wires drives the trolleys forward along the track. Following this part of the cycle (the power stroke), the tracks again run parallel as the wires leave the hot bath and re-enter the cold bath.

Each of the twenty working elements of the engine contains 240 feet of Nitinol wire, wound to form 80 parallel 3-foot lengths. These elements are joined by a continuous linkage incorporating sprocket teeth that engage a flexible belt leading to the power take-off. The full load of Nitinol in the prototype is 4800 feet. At an elongation of ~ 3%, with an anticipated cycling rate of $\geq$ 60 cpm and parasitic (frictional) losses of ~ 50%, output is expected to be in the neighborhood of 0.5 horsepower.

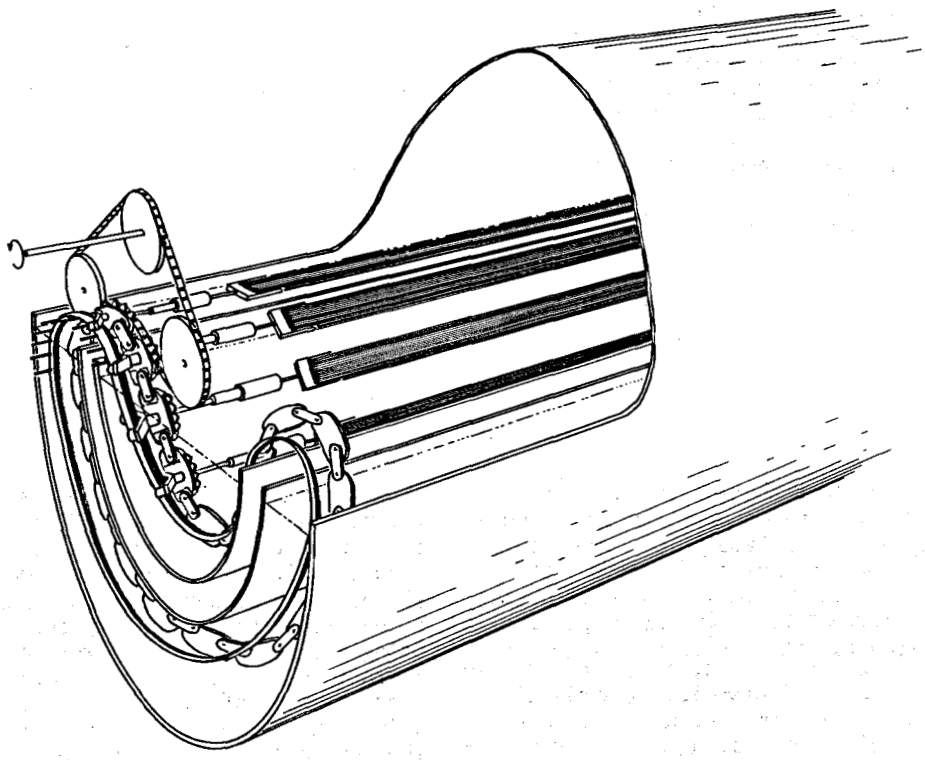

Fig. 1. Cutaway view of the Nitinol Cam-Track engine. One end of the tank is pictured, showing concentric water baths, typical power elements, one of the pair of cam-tracks and power take-off.
(XBL 767-3131)

ACCOMPLISHMENTS DURING 1976

Preliminary tests were run on a hand-cycled apparatus that simulated the mechanical cycle of the Cam-Track design. These tests indicated that wires could be reproducibly elongated to > 3.0% without fatigue or non-recoverable strain. The critical part of the cycle proved to be the mechanics of unloading the recovery stresses developed in the wires on heating. In the first tests recovery loads were so extreme that the ball bearings of the trolley mechanism failed. Following these tests pairs of compression springs were introduced between the trolleys and the Nitinol wires. The next series of tests revealed that test elements containing 240 feet of Nitinol wire fully compressed the springs. Strain gage measurements indicated that the test elements readily developed a net increase in force of approximately 350 pounds.

With the springs in place, 1000 cycles were made on this apparatus with no detectable permanent elongation of the wire. Since progressive elongation is normally detectable well below 100 cycles, this test established a conservative lower limit for reproducibility. In this configuration, however, the output of the engine would be essentially limited to the energy output of the springs. Therefore it was decided to direct future efforts towards increasingly 'hard' mechanical cycles.

After a series of iterations it proved possible to eliminate the springs by redesigning the contours of the Cam-Tracks. In the improved design, rate of convergence (axial displacement of the wire on heating) is not linear, but follows approximately the form of an exponential decay curve. With this configuration (which essentially matches the rate of heat transfer into a wire of cylindrical cross-section) 1000 cycles were successfully completed.

Construction of the new engine began in August 1976 with major components and assembly essentially completed by November 1. The engine was run without power take-off to check the timing (phasing of thermal and mechanical cycles on the power stroke) and to confirm potential for net torque. It was necessary to make slight modifications in the track contours and in the level of the hot water bath to achieve continuous operation, and afterwards the machine was run free at very moderate hot-bath temperatures. Following assurance that the design was operable, further testing was delayed until the power take-off could be completed, so that power output could be directly measured. In addition a flywheel was installed to ensure smooth operation. This work was completed by the end of December 1976, and initial testing of the engine as a whole is anticipated early in 1977.

The heart of the Cam-Track design is its unique mechanical cycle which allows broad control of the stresses induced in the Nitinol wires on both heating and cooling and provides maximum thermal uniformity of the working elements at dynamic points in the cycle.

PLANNED ACTIVITIES FOR 1977

If tests to be conducted during the coming year show the mechanical treatment of this design to be compatible with the thermodynamic behavior of commercially available Nitinol wire, it will serve both as an experimental apparatus for measuring the practical conversion efficiency of this type of engine and as the basis for design refinements leading to mechanical simplification and scale-up. The device itself is designed to provide adjustment in the percent of elongation of the working elements and in the length of wire in each element so that output can be increased with no increase in the physical size or number of moving parts in the engine. If this machine is shown to have future commercial potential, features presently incorporated to provide experimental flexibility will be replaced by simplified and standardized components.

FOOTNOTE AND REFERENCES

*Much of the information in this article was presented at the International Solar Energy Society Meeting, Winnipeg, Canada, August 1976, and is contained in LBL report "Nitinol Engine Development," Ridgway Banks and Michael Wahlig, LBL-5293, August 1976.

1. The name of the alloy is derived from the chemical symbols for nickel and titanium, and the abbreviation of the Naval Ordnance Laboratory (now the Naval Surface Weapons Center) in White Oak, Maryland. It was here that the alloy's shape memory properties were first observed in the late 1950's.

2. H. P. Hernandez, et. al., Nitinol Engine Project Test Bed Report, Lawrence Berkeley Laboratory Rept. UCID-3739 (1975).

ANALYSIS OF THE CALIFORNIA SOLAR RESOURCE*

Paul Berdahl, Donald Grether, Marlo Martin, and Michael Wahlig

INTRODUCTION

Lack of adquate solar data would seriously limit development of solar energy as an alternative energy source. This project was designed to help the California Energy Commission to evaluate the current extent of this limitation, and to plan to avert such limitation in the future.

The objectives, then, of this project are to:

1. Consider all reasonable options and make a recommendation to the California Energy Commission, detailing the role it should fulfill to ensure availability of adequate solar data for California;

2. Carry out an interim program to meet immediate needs for solar data by

   a. Locating and gathering present and potentially available California solar radiation data,

   b. Evaluating the quality of these data, and

   c. Publishing these data with relevant background information in manuals that can be used by Californians.

The project plan for meeting these objectives consisted of 1) determination of user's needs for solar data by direct questionnaires and other methods, 2) determination of available solar radiation data, 3) formulation of a plan to satisfy needs for solar data, including the use of available data and plans for new data if necessary, and 4) recommendation of the roles that the Energy Commission should play in implementing this plan.

This project began on April 1, 1976 and is scheduled for completion on January 31, 1977.

ACCOMPLISHMENTS DURING 1976

Assessment of Solar Data Requirements

Two basic approaches were used to determine data requirements. One approach was to poll current and potential data users, asking them what their needs were. Telephone calls, meetings, and questionnaires were used. A great variety of data types were suggested. Of primary interest were averages of daily totals for each month of the year for:

1. Total radiation received on a horizontal surface (which has been measured for a number of locations in California);

2. Direct component of radiation (which has recently begun to be measured at a few locations in California);

3. Diffuse component of radiation;

4. Total radiation received by surfaces of various orientations.

Data users who intended to perform detailed computer simulation computations generally requested hourly rather than daily time resolution for the data. Furthermore, hourly data for direct and total radiation (items 1 and 2) can be used to produce fairly reliable values of the diffuse component of radiation and the radiation received by tilted surfaces (items 3 and 4).

A second approach to determining data requirements was the analysis of solar energy systems which have potential for widespread applications. These analyses provided definition of the data types and the accuracy necessary for economically reasonable system design. The data types listed above were determined to be adequate when supplemented by non-solar climatological data such as temperature, wind velocity, and humidity. Domestic space and water heating, as well as solar thermal electric conversion, were analyzed in some detail to assess data accuracy requirements. For some applications it was found that relatively inaccurate (± 20%) solar data can be tolerated for system design and sizing, without incurring large (± 5%) economic penalties. In some cases more precise data may be required; e.g., power plant siting, or deciding whether or not to install solar systems where competing technologies have similar energy costs.

Identification and Evaluation of Available Solar Radiation Data

A survey of past, present, and planned insolation monitoring programs in the state has been made. Approximately 140 sites have been identified where systematic measurements have been taken of total radiation received by a horizontal surface. No other type of solar radiation measurement has been common in the past. Nine sets of measurements were taken with photovoltaic cell instruments, and 39 sets of data were obtained with bi-metallic strip instruments. Most useful for the present work are the 87 data sets produced by thermopile-type instruments, as these instruments are capable of producing monthly totals of radiation with ±10% accuracy. Of these 87 records, however, only 22 have lengths of 5 years of more, and are thus useful for accurate estimates of climatological averages (see Fig. 1). Finally, evaluation of the data shows numerous problems with instrument calibration in these 22 climatological stations. The China Lake (Inyokern) record is known to be too high for a period of years.[1] The two San Jose stations show major discrepancies. Other problems with the data are evident from even a cursory inspection of the data records.

The records of solar data have been evaluated by direct examination of clear-day readings produced by the stations, by comparison with the data of nearby stations, and by visiting 25 selected stations.

The edited and corrected data sets are being used to generate summary information regarding solar radiation availability for California. This information will be published in California Solar Data Manuals.

Development of a Program to Coordinate and Manage Solar Data

In addition to the 22 solar data stations with climatological (5 year) data sets, there are approximately 30 new high-quality data stations with less than 2 years of data. Approximately 8 pyrheliometers, which measure the direct component of radiation, have recently been installed. Thus the solar data base for California is rapidly expanding. In view of the large quantity of data now becoming available and in view of the historical difficulties with solar data acquisition systems, it is important to develop a coherent program for data management.

The results of these project tasks (including user's data requirements, data collection, and determination of the plans of various agencies for data collection) will be incorporated into recommendations to the California Energy Commission

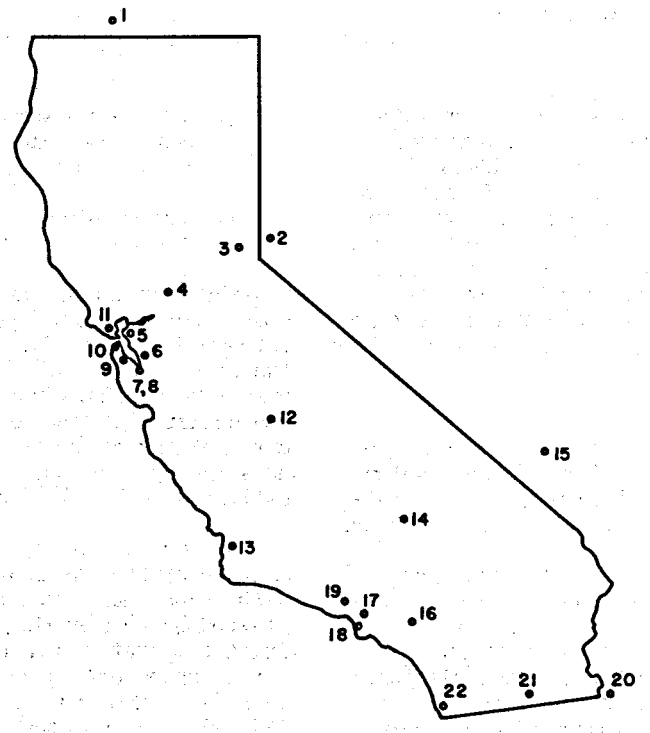

Fig. 1. Solar radiation measurement stations (Thermopile-type pyranometer sites with more than 5 years of data). 1) Medford, Oregon, 2) Reno, Nevada, 3) Soda Springs (Elev. 6885 ft.), 4) Davis, 5) Richmond,* 6) Fremont, 7) San Jose, 9) Redwood City, 10) San Francisco, 11) San Rafael, 12) Fresno, 13) Santa Maria,* 14) China Lake (Inyokern), 15) Las Vegas, Nevada, 16) Riverside, 17) Los Angeles (Urban),* 18) Los Angeles (Airport),* 19) Northridge, 20) Yuma, Arizona, 21) El Centro, 22) La Jolla.* (*Indicates a station no longer in existence).
(XBL 773-640)

which will detail a data management plan for California.

PLANS FOR 1977

During January 1977 (the final month of the project) the recommendations for solar data management will be formulated. Recommendations also will be made regarding station planning, instrument calibration and maintenance, and data processing and evaluation. In addition, the solar data manual and final report will be completed.

FOOTNOTE AND REFERENCE

*Work supported partially by ERDA and partially by the California Energy Resources Conservation and Development Commission (Energy Commission).

1. R. W. Durrenberger and A. J. Brazel, Science, 193, 1154 (1976).

DEVELOPMENT OF ABSORPTION AIR CONDITIONER FOR SOLAR HEATING AND COOLING SYSTEMS*

Kim Dao, Melvin Simmons, Richard Wolgast, and Michael Wahlig

INTRODUCTION

An ammonia-water absorption air conditioner that can be driven by solar-heated hot water is being developed for residential cooling applications. The air conditioner is being designed for operation at temperatures $\lesssim 200°F$ and is therefore compatible with the use of flat-plate solar collectors. An important aspect of the design is the use of air cooling for the condenser and absorber coils, thus

avoiding the use (and maintenance problems) of water cooling towers.

The condenser, absorber, precooler, evaporator, and solution pump from an Arkla gas-fired ammonia-water absorption water chiller (Model ACB-60-00, which had a nominal cooling capacity of 5 tons) were used as a base for the fabrication of the new prototype air conditioner. The following components were added to this base: generator (a packed tower counterflow heat exchanger), preheater and rectifier (both shell-and-tube, one pass, counterflow heat exchangers), storage tanks, adjustable expansion valves and measurement instruments.

ACCOMPLISHMENTS DURING 1976

The first phase of the air conditioner development program was completed and 22 test runs, totaling about 60 hours of operation, were carried out on the prototype unit.

The instrumentation used to monitor the performance of the experimental unit consisted of:

1) Twenty copper-constantan thermocouple junctions silver soldered to the external surface of the tubing and covered with thermal insulation. The locations of the junctions are shown on Fig. 1. The digital voltmeter, used for direct reading of the temperatures, was calibrated to an accuracy of ±0.1°C at the ice point and ±0.2°C at the boiling point of water.

2) Four Bourdon pressure gauges calibrated to ±1 psi.

3) Two rotameters, calibrated to ±2% accuracy, for the measurement of the flow rates of the weak solution and of the ammonia.

4) Two sampling chambers for the measurement of the concentrations of the solutions.

The heat inputs to the generator (Q_G) and to the evaporator (Q_E) were calculated from the water flow rates and the temperature drops of the water through the heating coils of the generator and through the evaporator coils. The flow rates of the hot water and chilled water were measured by calibrated mercury columns (±2% accuracy). The temperatures were measured by thermocouples. The total errors were estimated to be ±4% for Q_G and ±5% for Q_E.

The system was charged with 65 lbs. of solution with an ammonia concentration of 55%. The unit was started by pumping hot water, controlled at constant inlet temperature, through the generator. The condenser-absorber fan and the solution pumps were turned on when the generator pressure reached about 150 psig. Flow rates of ammonia and of the weak solution were then adjusted to the desired values using expansion valves. Experimental data were taken 30 to 45 minutes after establishing the desired running conditions. This ensured that the system had reached steady state.

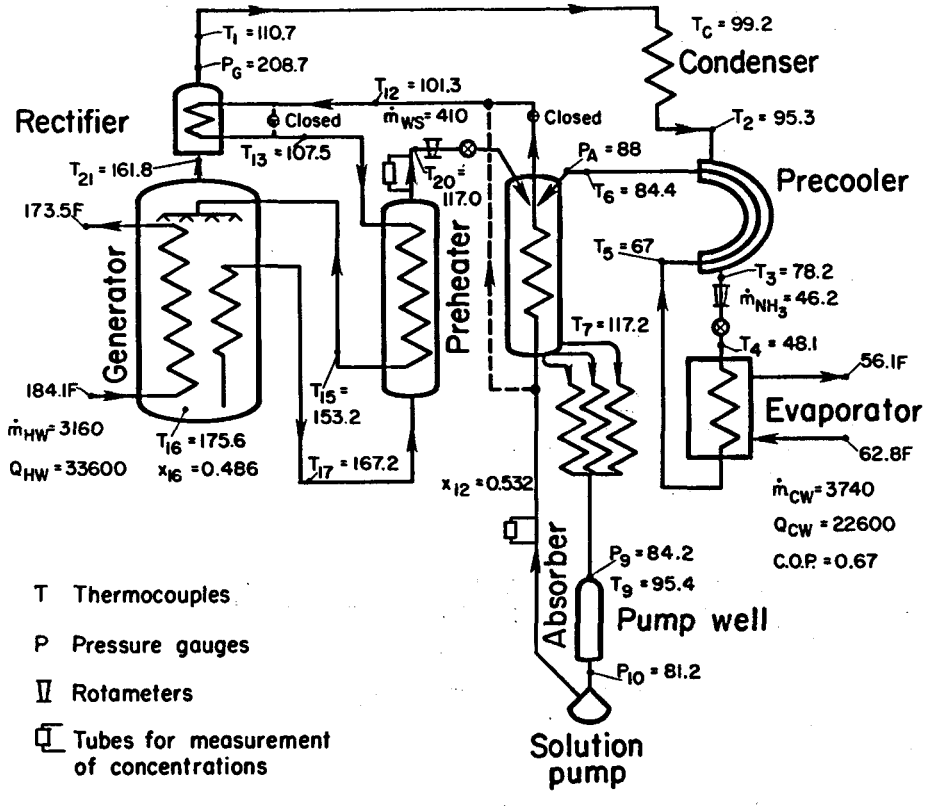

Fig. 1. System configuration and state points of a typical run. (XBL 767-3132)

TEST RESULTS

The tests produced the following results:

1) The operation of the ammonia-water absorption refrigeration cycle is very stable close to the cut-off conditions; i.e., stable up to circulation ratios of the order of 30 and possibly higher.

2) The validity of the analytical cycle calculations based upon the assumption of equilibrium states is confirmed within experimental errors of ±5%.

3) The pressure drop across the absorber is important for operation near the cut-off temperature since its effect is to increase the evaporating temperature T_E. A pressure drop of 8 psi increases T_E by 5°F.

4) The overall heat transfer rate of the packed tower type of generator is poor (of the order of 120 Btu/hr-ft^2-°F), even with Linde high flux coating on the water tubing. Therefore another type of generator must be developed to improve the heat transfer characteristics for a smaller size generator.

5) Coefficients of performance (COP) of 0.4 to 0.7 were obtained. These values agreed with the calculations to within ±5%.

CONCLUSIONS

For acceptable cooling and dehumidification of the conditioned air using reasonably-sized chilled water coils, the evaporator temperature is limited to $T_E < 47°F$. Inexpensive flat plate collectors may reasonably limit the generating temperature to $T_G < 195°F$. These practical constraints combine to require condensing and absorbing temperatures (T_C and T_A, respectively) below 110°F. The constraint $T_C < T_A < 110°F$ can be met by doubling both the cooling air flow rates and the size of the condenser-absorber compared to those used in conventional gas-fired systems using finned-tube condenser and absorber. (These conditions are essentially satisfied already for our experimental chiller since we are using the condenser, absorber, and fan from a conventional five-ton chiller for our three-ton solar unit.) Doubling the cooling air flow rates is a must, but new designs of more efficient condenser-absorbers may reduce the requirement of doubling the size (and cost) of these heat exchangers. Doubling the cooling air flow rates typically increases the power of the fan from 1/140 to 1/70 watt per Btu/hr of cooling, making the total power consumption equivalent to 35 Btu/hr of cooling per watt of electrical power input (as compared to a rating of about 8 Btu/hr per watt for a mechanical compressor unit).

The COP depends strongly on the preheater effectiveness (ϵ_{PH}) and the difference in concentration (Δx) between the strong and weak solutions, and is quite insensitive to the values of the remaining parameters. To have a COP > 0.65 with $\Delta x = 0.03$, the preheater effectiveness ϵ_{PH} must be at least 90%. This value is not expensive to achieve since there is sufficient pressure in the weak solution line to promote high heat transfer coefficients. A high value of ϵ_{PH} is a must in order to avoid dumping into the absorber the heat contained in the weak solution.

The first phase of the ammonia-water absorption air conditioner development has demonstrated experimentally that it is technically feasible to use the ammonia-water absorption cycle for cooling with a heat source temperature below 200°F and a heat sink temperature (using air cooling) below 110°F.

PLANNED ACTIVITIES FOR 1977

The next phase of this project will involve redesign and retest of the generator and preheater, with combined objectives of lower-cost and higher-efficiency for both of these components. Additionally, the absorber, condenser, and evaporator coils will be modified or replaced with more efficient units. All components must realize their full performance potential in order to achieve the project goal: operation with air-cooling and solar-heated hot water temperatures of 200°F or less. When the performance goal is attained, an assessment of the commercial potential of the air conditioner will be made with the assistance of project consultants. Assuming a favorable result, steps will be initiated to transfer this technology to the commercial sector.

FOOTNOTE

* Test results were reported at the International Solar Energy Society Meeting, Winnipeg, Canada, August 16-20, 1976, and are also contained in the LBL Report , "Performance of an Air-Cooled Ammonia-Water Absorption Air Conditioner at Low Generator Temperatures", Kim Dao, Melvin Simmons, Richard Wolgast, and Michael Wahlig, LBL-5224, August 1976.

CHEMICAL STORAGE OF THERMAL ENERGY

A. S. Foss and S. Lynn

INTRODUCTION

A means of storing energy economically would be of considerable value to both nuclear and solar power production. One means of storing energy is by carrying out a reversible chemical reaction that absorbs heat at a high temperature as the reaction proceeds in one direction and, on controlled reversal, releases the heat at a somewhat lower temperature. To be useful in modern steam-cycle power

generation, the heat-release reaction must occur at temperatures of 500-600°C. Two reaction systems appear to be of particular interest:

$$2SO_3 \rightleftharpoons 2SO_2 + O_2 \quad (1)$$

and

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2 \quad (2)$$

This project has concentrated on studying the first reaction. However, thus far most of the effort has been devoted to flowsheet development, and it has been found that the basic approach that must be taken to achieve the highest possible energy efficiency is the same for either system.

The primary advantage of using a chemical reaction for energy storage is that the storage temperature can be near ambient. However, an inevitable requirement of near-ambient storage is the need for extensive heat exchange between the streams being taken from storage temperature to reaction temperature and back. Since a large fraction of the total heat of reaction is the sensible heat associated with this change in temperature of the chemical streams, efficient heat exchange between the hot reaction products and cold chemicals feeding the reactor is desirable. This heat exchange results in higher plant efficiencies through decreased rejection of heat from the hot products to the environment and through decreased thermal demands placed on the plant by the storage system. In addition, the latent heat of condensation and vaporization must also be exchanged. The latter effects arise if one is to take advantage of the reduction in storage volume afforded by condensing SO_3 and SO_2 in the one system or H_2O in the other.

Funding for this project began in November, 1975. Initially the project was directed toward storage of energy obtained from nuclear power. During 1976 the emphasis changed to storage of solar energy. However, most of the work to date is independent of the assumed source of energy. The objective of the project has been to develop a technically feasible flowsheet for the chemical storage of thermal energy that, as the result of analysis and modification, has the highest practical energy efficiency.

ACCOMPLISHMENTS DURING 1976

The work first proposed for the current year was to continue the flowsheet development for the sulfur oxide system in an effort to improve the initial flowsheet studied by Bhakta.[1] Second, a study of the methane system of Kugeler et al.[2] was initiated in order to obtain a comparison of the two systems based on similar assumptions. A third goal was to seek other reversible reactions for study. Finally, the possibility of using non-cyclic reactions was to be considered.

The first study led to a major improvement in the thermal efficiency of the flowsheet by recognizing the need for integration of the storage system with power production. Reference was made in the Introduction to the large quantities of sensible and latent heat that must be exchanged in both the heat-absorption and heat-release processes. It is not possible to achieve a thermal storage efficiency much greater than 50% if the thermal storage process is operated independently of the power production system. This is because the heat capacities of the streams change as the result of the chemical reactions, and heat of condensation is released at a temperature lower than that needed for heat of vaporization. In an independent storage system these mismatches require heat dissipation to the environment. The presence of a power plant allows the use of this low-level heat to preheat boiler feed water and raises the attainable thermal efficiency to 65-75%. Achieving maximum efficiency requires the generation rate of the power plant to be no less than a certain multiple of the storage rate of the storage system. This multiple varies from 2.5 to 5, depending upon the system used and the design details. The overall thermal efficiency of a storage system for solar plants is less than that for a nuclear plant because of less favorable opportunities for integration in the solar plants.

Because many different definitions of thermal efficiency may be used, comparisons of different systems by different investigators may be confusing. In this project a more general definition of efficiency is being developed. This efficiency is based on comparison of the electric energy obtained from the storage system to that obtainable from the associated power plant in the absence of the storage system. While doing this it has become apparent that the use of modern steam-cycle technology is very important to the future use of solar energy in power generation. Any storage system should therefore be compatible with this technology.

Two other chemical systems have been proposed as possibilities for thermal energy storage:

$$2NH_3 \rightleftharpoons N_2 + 3H_2 \quad (3)$$

and

$$COCl_2 \rightleftharpoons Cl_2 + CO\ . \quad (4)$$

The ammonia system is undesirable because presently available catalysts are not active enough to drive the heat-release reaction (ammonia formation) to equilibrium at temperatures below 400°C. At that temperature the equilibrium conversion is only about 20% at a pressure of 200 atm.

The phosgene-forming reaction, in contrast, proceeds at a measurable rate without catalysts at room temperature. One would therefore expect a substantial rate of recombination in the heat exchangers following the heat-absorption step, which would lead to low efficiency.

No other suitable reactions are known that do not involve solids. (Solids have been excluded because of disadvantages such as attrition, low thermal conductivity, change of density during reaction, and so forth.) It is not surprising that the number of suitable reactions is small since the temperature of reaction is above the limit of stability of most organic compounds, and the desire to avoid working with solids rules out most of the lighter element compounds.

No progress has been made on the use of non-cyclic reaction systems for energy storage. Initial investigations have proven unfruitful, and this approach to energy storage will not be actively pursued.

ACTIVITIES PLANNED FOR 1977

In the coming year flowsheet development efforts will continue. The sulfur oxide and methane systems will be compared under roughly optimum conditions for each. The compatibility of potential materials of construction with SO_3, SO_2, and O_2 at 1000-1200° C will be determined experimentally.

A close working cooperation with the ERDA group overseeing contracts in the area of solar energy storage has been established. It is expected that support services, including reviews of reports and proposals, will be provided to them during the coming year.

Finally, it is of interest to compare chemical energy storage to the more conventional storage of sensible or latent heat. Comparisons and evaluations of these storage techniques will be initiated.

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2. K. Kugeler, H. F. Niessen, and M. Röth-Kamat, Nuc. Eng. and Des. 34, 65 (1975).

MEASUREMENT OF CIRCUMSOLAR RADIATION

Donald F. Grether, Arlon J. Hunt, and Michael Wahlig

INTRODUCTION

The objective of this project is to provide detailed measurements of the direct component of the solar flux at the surface of the Earth. The "direct" component usually measured includes radiation from around the solar disc (circumsolar region) in addition to the "true" direct component from the solar disc. The circumsolar radiation is produced by small-angle scattering of sunlight from atmospheric aerosols with dimensions on the order of or greater than the wavelength of light. Under some circumstances these aerosols can cause a significant fraction of the solar flux to be deviated to angles of several degrees or more. Solar energy conversion techniques using high concentration ratios, such as the central receiver concept, only collect light from the solar disc and a small portion of the circumsolar region. Pyrheliometers, the instruments normally used to estimate the direct solar radiation, typically have a field of view of 5-6°. The pyrheliometer measurement includes a large portion of the circumsolar radiation and thus overestimates the amount of direct sunlight that would be collected by a concentrating system. The detailed angular distribution of the circumsolar radiation is important, as it affects the radiant energy distribution on the surface of the receiver in solar thermal power plants. Circumsolar radiation measurements will be used in calculating the performance of solar power plants and will determine the conditions under which pyrheliometer data are adequate for estimating this performance.

This project was started in 1974 with feasibility studies leading up to the design and construction of the prototype instrument. During 1975 the prototype instrument was completed and work was initiated on three more fixed site instruments. This year the three new instruments were completed, debugged, and deployed. They began operation between May and July of 1976 at the following locations: 1) near the 5 megawatt (thermal) solar test facility in Albuquerque, N. M.; 2) at the site of a total energy system pilot plant in Ft. Hood, Texas; 3) currently at China Lake, Ca., to be located at the site of a 10 megawatt (electric) central receiver pilot plant.

CIRCUMSOLAR TELESCOPE

The basic instrument was designed and fabricated at LBL and consists of a "scanning telescope" that is mounted on a precision solar tracker. A digital electronics system provides control for the tracking and scanning mechanisms. A photograph of the three instruments near completion is shown in Fig. 1. The design has been described in more detail elsewhere.[1] The telescope uses as its basic optical element an off-axis mirror of 7.5-cm diameter and 1-m focal length. A fused silica window protects the mirror from the environment. The mirror forms an image of the sun and sky around it on a plate to the side of the telescope axis. A small hole in this plate, the detector aperture, defines the angular resolution (1/20 of the solar diameter), and the amount of light passing through the aperture into the detector assembly constitutes the fundamental measurement. In the detector assembly the light is mechanically chopped, optically filtered, and focused onto a pyroelectric (thermal) detector. This type of detector was chosen for its uniform wavelength response in the 0.3 to 2.5 μm region and its wide dynamic range.

The telescope scans through a 6° arc with the sun at the center and measures the brightness of the solar and circumsolar radiation as a function of angle. The instrument scans in declination so that at sunrise and sunset it travels nearly parallel to the horizon and at noon it moves in a vertical plane. A number of precautions are taken to reduce the levels of scattered light inside the

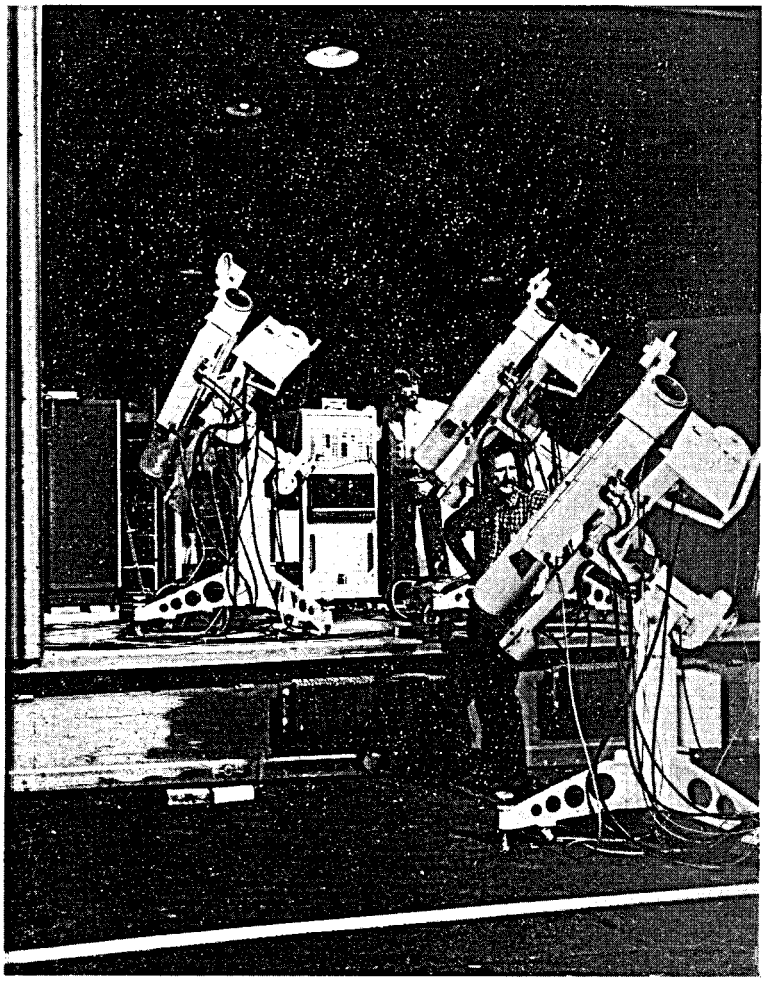

Fig. 1. Circumsolar "scanning telescope". The photograph shows the three instruments near completion. (CBB 763-2422)

telescope to less than 10^{-7} at 3°. This, in conjunction with a total dynamic range of nearly 10^7, effectively solves the problem of measuring the very large intensity differences between the sun and aureole region.

Each 6° scan requires one minute of time. The brightness is digitized every 1.5' of arc. Within 0.5° on either side of the sun an aperture of size 1.5' of arc is used, and outside this region the aperture is increased to 5' of arc. A set of measurements consists of one scan at each of 10 "filter positions". There are eight optical filters, one open (or "clear") position, and one opaque position. The opaque position is used to monitor the detector noise. The absolute determination of the normally incident flux (within 2.5° of the sun center) is provided by an active cavity radiometer.[2] This device is self-calibrating and has an accuracy of 0.5%. This pyrheliometer is provided with a matched set of filters that rotate synchronously with those on the scanning telescope. Thus an absolute calibration of the normally incident flux along with the detailed solar profile in eight wavelength bands provides enough information to determine both the atmospheric turbidity and the scattering phase function. Two pyranometers are used, one mounted in the conventional horizontal position, and one tracking the sun.

The telescopes are capable of unattended operation for up to a week, although they typically receive a daily inspection during the work week. During the night the solar trackers run backwards and automatically initiate operation at the beginning of each day. The data is recorded on magnetic tape and processed at the laboratory's computer center.

Figure 2 is a computer-plotted graphical display of a clear filter scan made by SCOPE 1 at Berkeley at 1313 hours on June 1, 1976. The computer code proceeds as follows. A search is made for the peak brightness point of the sun. (This peak point is close to, but not always exactly at, the center of the sun.) The "edges" of the sun (defined as the angles at which the brightness is down by a factor of 30 from the peak) are then determined. These edges are indicated on the graph by the two vertical dotted lines. The center of the sun is taken as the angle midway between the two edges and is indicated by the solid vertical line. Next an ef-

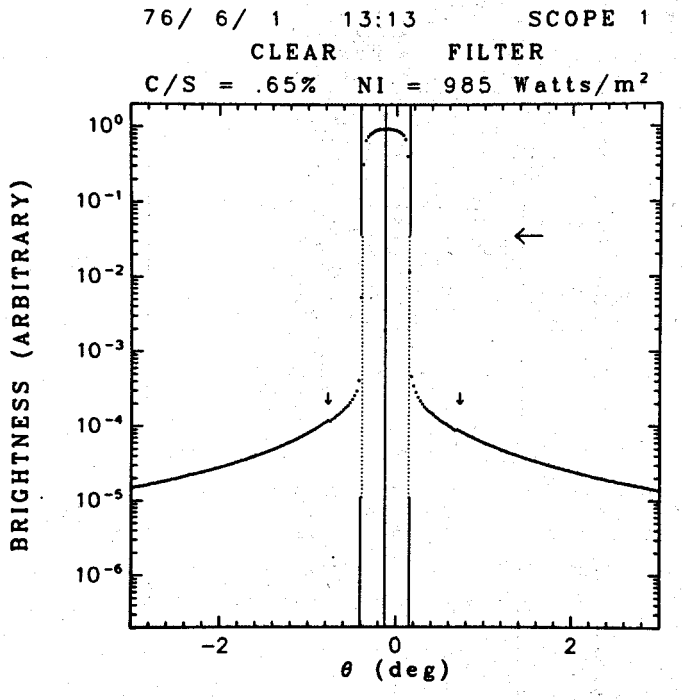

Fig. 2. Computer-plotted graphical display of a clear filter scan made by SCOPE 1 at Berkeley at 1313 hours on June 1, 1976. The dots are the individual scan digitizations. The scan started at +3, as indicated by the large horizontal arrow, crossed the sun near 0°, and ended at -3°. The small vertical arrows indicate the angles where the aperture was switched from 5' of arc to 1.5' of arc, and then back again. (XBL 7611-9866)

fective radius is defined as the true radius of the sun (approximately 16' of arc; the exact value is calculated for the specific date, as it changes during the year because of the varying earth-sun distance) plus the radius of the detector aperture (0.8' of arc). The effective radii are indicated by the solid vertical lines at the top and bottom of the graph, and in this case are nearly coincident with the edges of the sun. The brightness is then integrated from the center of the sun to the effective radius and from the effective radius to the end of the scan to give the intensities of the direct and circumsolar radiation respectively. The ratio of circumsolar to solar radiation is then calculated and is given at the top of the graph (C/S =). The normal incidence measurement provided by the pyrheliometer (NI =) is also indicated. This particular scan is for a clear day, with a circumsolar to solar ratio of only 0.65%, and a normal incidence value of 985 W/m^2.

Figure 3 illustrates measurements from the instrument at China Lake, California. Though taken on a clear day, substantial circumsolar levels are observed. The diagrams are similar to Fig. 2, but taken through band pass filters in two consecutive minutes near noon. The pass bands of the filters are indicated above the graph. The data contain several interesting features. Note the rather severe limb darkening in the short wavelength scans, in contrast to the nearly flat solar profile in the infrared scan. Another observation

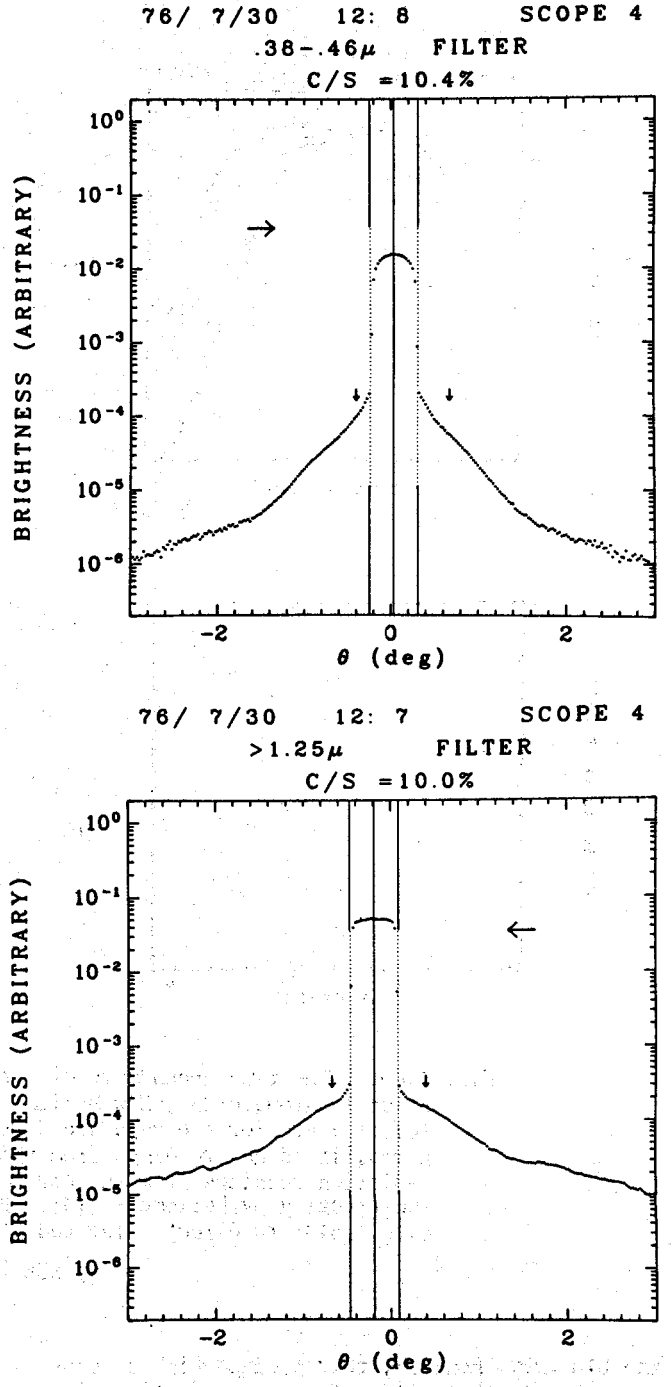

Fig. 3. Measurements taken from the instrument at China Lake, California. The pass bands of the filters are indicated above the graph. (XBL 772-7487;7488)

is that the circumsolar to solar ratios are approximately equal but the aureole (circumsolar) profiles differ. There is also a distinct shoulder about one degree from the center of the sun. The shoulder indicates the presence of large particles which produce a sharp forward diffraction peak. From weather observations taken that day it is most likely that the scattering was produced by thin cirrus clouds containing ice crystals. Clouds of this type are common in desert regions on "clear" days but are so tenuous that they are not usually noticed against

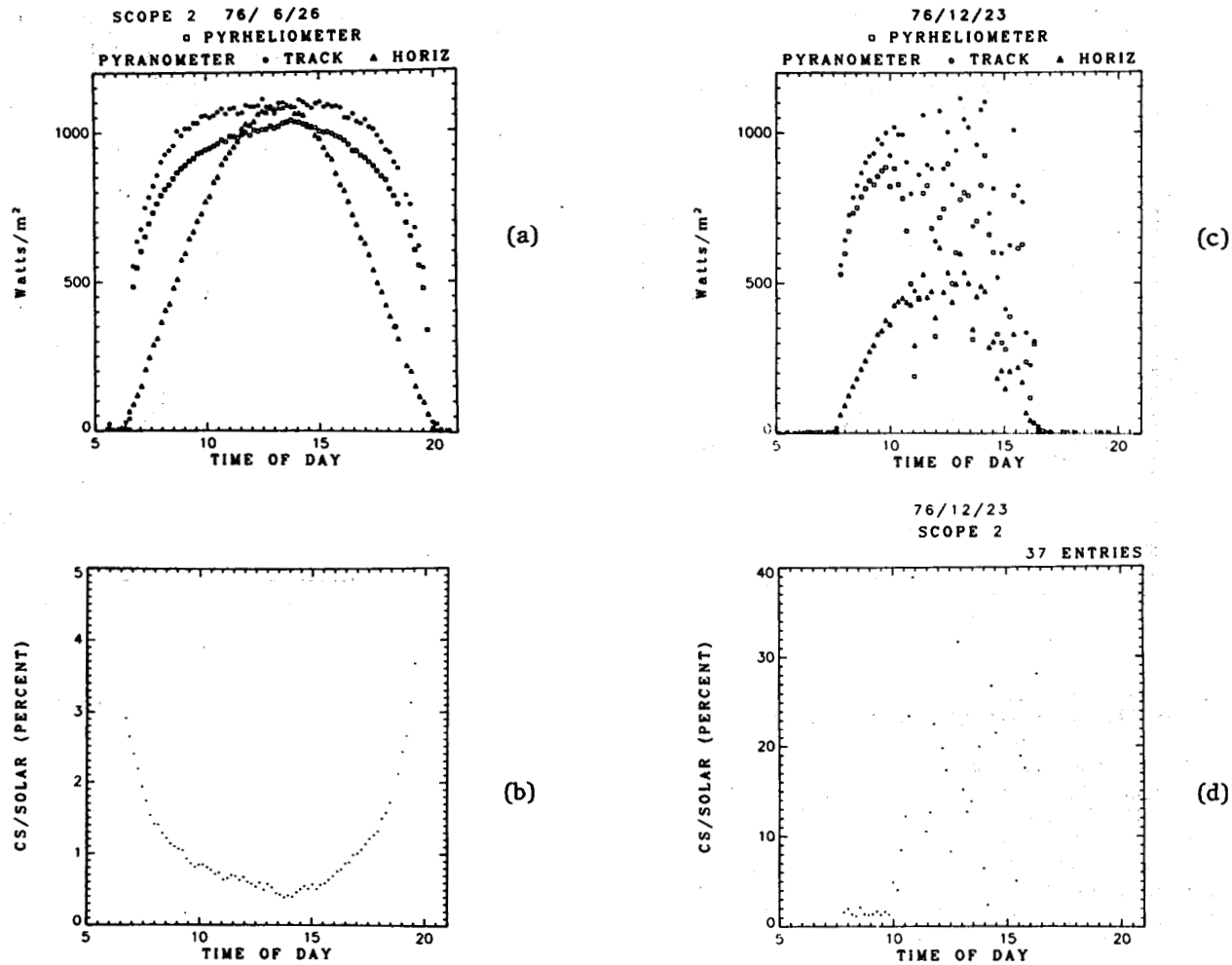

Fig. 4 a-d. The time dependence of various parameters of the solar radiation in Albuquerque, New Mexico. The pair of graphs (a), (b) and (c), (d) are for two separate days. Figures (a) and (c) show the normal incidence readings from the pyrheliometer (□), and the total radiation readings from the horizontal pyrheliometer (Δ) and from the sun-tracking pyrheliometer (0). Figures 4b and d show the ratio of circumsolar to direct solar radiation for the same day.

[(a) XBL 772-7483; (b) -7482; (c) -7464; (d) -7463]

the blue sky. However, they produce high circumsolar levels that will affect the operation of a solar power plant.

Figures 4a-d display the time dependence of various parameters of the solar radiation for two separate days. These measurements were taken by SCOPE 2 which is located in Albuquerque, New Mexico. The total losses that would be experienced by a highly concentrating collector due to circumsolar radiation can be calculated by integrating the product of the normal incident radiation and the circumsolar to solar ratio. If the collector system fills the receiver with the solar disc, the total integrated losses for the day in Fig. 4a and 4b would be equal to 1.2%. Figures 4c and d illustrate a day that probably had a blue sky slightly whitened by cirrostratus cover. (Note the difference in scale for the circumsolar graphs in Figs. 4b and 4d.) The normal incidence readings are moderately high throughout the day. The circumsolar to solar ratio is low early in the morning but from 10 a.m. onward its average is very high (many points are above the top of the graph). The pyrheliometer data indicates sufficient flux for plant operation most of the day but the integrated losses due to circumsolar radiation for the whole day are calculated to be over 17%. Thus the errors in utilizing pyrheliometer data for this kind of day would be considerable.

It is anticipated that solar power plants will be operated whenever the solar input exceeds the radiative losses from the receiver. In order to accurately assess the effects of circumsolar radiation for a given location and type of collector, therefore, it is necessary to determine the circumsolar to solar ratio throughout the year for all

but completely overcast days. For very clear days in the desert it appears that circumsolar radiation losses will be small even for highly concentrating collectors. However when considering plant operation under real conditions it is not yet clear how important a role that circumsolar radiation will play; it may be substantial and it certainly will have considerable geographic variation. The quantitative answer to the question of the importance of circumsolar levels to solar collection will become clearer as the data base increases.

ACCOMPLISHMENTS DURING 1976

This year the three new telescopes were completed and set up at the three sites mentioned earlier. Local personnel were trained at each site and the telescopes were maintained by them with the help of occasional visits by LBL employees.

The prototype instrument has been used for making measurements in Berkeley and as a test bed to aid in debugging the electronics for the new telescopes. After the new instruments were installed, the prototype was automated by including the night retrace feature for automatic morning acquisition of the sun, modifying the declination drive for continuous operation, and adding a rain sensing and protection system as well as a blower supplying ultrafiltered air for maintaining a dust free window.

Automatic weather stations were added to two of the telescopes. A digital interface system was obtained to access the weather measuring instruments that will be installed by Sandia at the 5 MW test facility. The weekly data from each site was processed and reviewed using data summaries stored on microfiche. Work began on the verification and transfer of raw data from tapes to permanent storage files. Various requests for data were filled for a variety of interested workers.

PLANNED ACTIVITIES FOR 1977

The collection of data will continue until a two year data base has been established. A reduced data base will be developed to make the processing and manipulation of solar and circumsolar information more convenient. When established, this base will be used for a variety of statistical studies, such as determining the percentage of time that pyrheliometers are able to predict the performance of various collector systems.

The remaining weather stations will start operation as soon as the telescope now at China Lake is moved to the site of the 10 MW solar thermal electric pilot plant and the weather system at the 5 MW solar thermal test facility is completed. A program of field measurements by the portable instrument will begin early in the year and measurements will be made at a number of new locations.

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ENERGY TRANSFORMATIONS USING CATALYSTS FROM CHLOROPLASTS, CYANOBACTERIA AND HALOBACTERIA

L. Packer, E. Tel-Or, L. Luijk, W. Cullingford, P. K. Shieh, T. Konishi and S. Tristram

INTRODUCTION

Through evolution, photosynthetic and phototrophic organisms have evolved highly efficient catalytic systems for solar energy conversion. The mechanisms producing these energy transformations have long been a subject of inquiry by investigators in various areas of bioenergetics. Two characteristics of living organisms have recently attracted particular attention as possible biological sources for photoelectrical potentials and currents. The catalytic systems in chloroplasts from higher plant leaves and light-triggered catalysts in certain microorganisms such as the cynaobacteria (also known as blue-green algae) and halobacteria (salt-loving organisms) are being studied. These systems may provide either practical solar energy converters or may serve as patterns for artificial converters based upon their principles.

ACCOMPLISHMENTS DURING 1976

H_2 Gas Production by Photosynthetic Preparations from Chloroplasts and Cyanobacteria

The photosynthetic process is a highly specialized light-energy transducer which at ordinary temperature photolyzes water into protons and electrons. The protons and low-potential electrons in the living plant are coupled to the reduction of carbon dioxide to form carbohydrates and other carbon substances by metabolism. It is possible, however, to construct a similar in vitro system composed of chloroplasts, a low-potential electron mediator, and a hydrogenase enzyme. When these components are combined, they produce H_2 gas driven by photolysis of water, i.e., biophotolysis. Such

a system has been under study.[1,2,3] It has been found that the system efficiently (80%) couples photolysis of water into H_2 gas production. However, coupling the photolytic process to hydrogen gas production suppresses the water photolysis rate by an order of magnitude. The system is short-lived and survives at 30°C for about 8 hours. It produces approximately 10-15 micromoles H_2 gas per mg. chlorophyll per hour. The total production of H_2 is 60-70 micromoles per mg. of chlorophyll under continuous illumination in a hydrogen gas generator.[1]

Although this is a model system that is expensive and unstable and therefore not in itself practical it identifies two steps in the process which need further study. These are the stability and the mechanisms of the water-splitting reaction. Better understanding of the mechanism is needed at the sites where (1) light energy is absorbed and (2), where transference of the low-potential electrons generated by the photosystems is coupled to the hydrogenase catalyst for H_2 production. Improved understanding of the water-splitting reaction will be useful in designing an efficient and stable hydrogen gas producing device.

Based on experience with the processes described above, an investigation of a system in cyanobacteria was initiated. This system has the photosynthetic capacity and a catalyst for H_2 production in a single, naturally occuring organism.

Cyanobacteria are perhaps the most highly specialized of the primitive microbial organism. When grown aerobically in the absence of combined nitrogen, they develop a few specialized cells known as heterocysts which are capable of fixing atmospheric N_2 into ammonia. The rest of the cells, called vegetative cells, carry out normal photosynthesis. The system is thought to work as follows: photosynthesis in the vegetative cells produces reducing power in the form of carbon substances which are transferred to the heterocysts. There the substances are used to reduce N_2 into ammonia which, in turn, is transferred back into the vegetative cells where it is used to make proteins. Unfortunately, up to half of the reducing power or energy for N_2 fixation is lost as H_2 gas by the catalyst nitrogenase. This loss of hydrogen in N_2 fixing organisms is quite common in nature.[4] Studies have shown that purified preparations of heterocysts indeed produce H_2 gas. They do so by means of their nitrogenase catalyst and in addition, they have been found to possess a hydrogenase catalyst which is present in the same cells.[1,2,5]

Experiments have demonstrated that isolated heterocysts from Nostoc muscorm or Anabaena cylindrica, can produce H_2 via hydrogenase continuously for as much as a day at a rate of about 1-4 micromoles/mg chlorophyll per hour. If H_2 is present in the atmosphere, the rate of H_2 consumption can be 10-20 fold faster than this rate of H_2 production. Also H_2 consumption is virtually an exclusive property of the heterocysts (i.e., very low activity is present in the vegetative cells). The existence of two catalytic systems for H_2 production, only one of which (the hydrogenase) is reversible, suggests that hydrogenase provides a way to recapture the energy loss in heterocysts. In these organisms H_2 gas utilization by hydrogenase may therefore be a means for enhancing the N_2 fixing productivity of the cyanobacteria. A scheme depicting this process is shown in Fig. 1. In support of this proposal, recent studies have shown that hydrogenase activity can be induced by providing growing cultures of cyanobacteria with hydrogen gas; this results in a ten-fold enrichment of H_2 uptake activity.

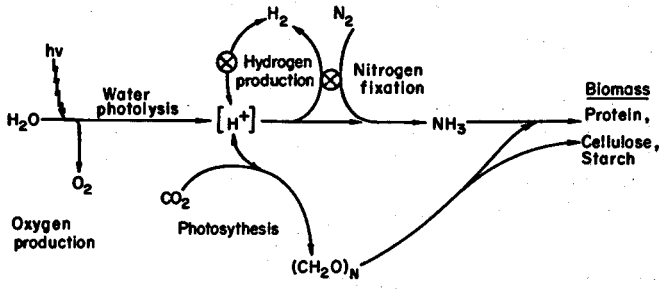

Fig. 1. This diagram suggest the possibility that the wasteful loss of H_2 gas known to occur in nitrogen fixing organisms might be corrected by using hetrocysts to recycle the hydrogen gas. The result would be an increased N_2 fixing productivity by cyanobacteria.
(XBL 767-9129)

Photoelectrical Potential Generation by Bacteriorhodopsin, a Catalyst from Halobacteria

Halobacteria growth requires concentrations of salt many times higher than sea water. When these organisms are transferred to ordinary water, they burst. This causes most of their enzymes and catalytic systems to be destroyed. An exception, however, is a very stable patch derived from their outer envelope (the purple membrane) which contains a protein pigment. This protein has been termed bacteriorhodopsin and is similar to the pigment present in the eye. When this protein pigment absorbs solar energy in the visible region it causes the vectorial movement of an H^+ ion across the dimensions of the molecule. When the molecule is oriented in the membrane of the halobacterial cell photoelectrical potentials are developed. These potentials provide pumping ions, thus enabling the organisms to thrive in a high salt environment.

In this laboratory membrane preparations containing this light-sensitive pigment have been partially oriented in planar membranes. Upon illumination photoelectrical potentials of the order of 250 mV[6,9] have been obtained, (Fig. 2). In particular, it has been shown that a pigment can serve as a stable catalyst for the generation of photoelectrical potentials over a period of approximately half a year (although the activity declines during this period); this was accomplished by having the pigment trapped in a lipid impregnated plastic filter.[10] This is prototype of a device (Fig. 3) capable of generating large photoelectrical potentials and photocurrents. These may be developed for the construction of a biochemical fuel cell, or for H_2 gas production by photolysis

Photoelectrical Responses Generated by Bacteriorhodopsin Across Lipid-Impregnated Filter Membranes

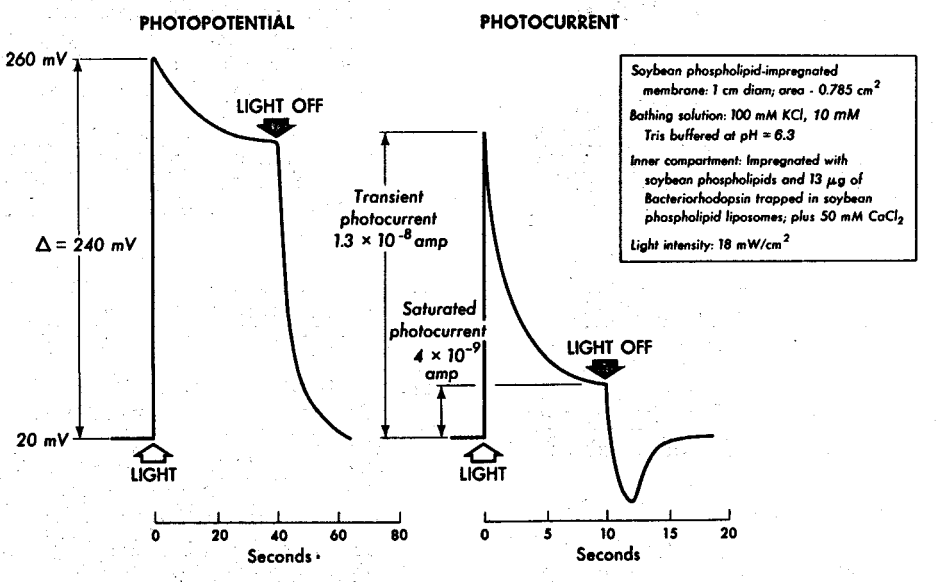

Fig. 2. Photoelectrical potential and current generation catalyzed by bacteriorhodopsin as measured across a lipid-impregenated millipore filter membrane. (XBL 7612-11184)

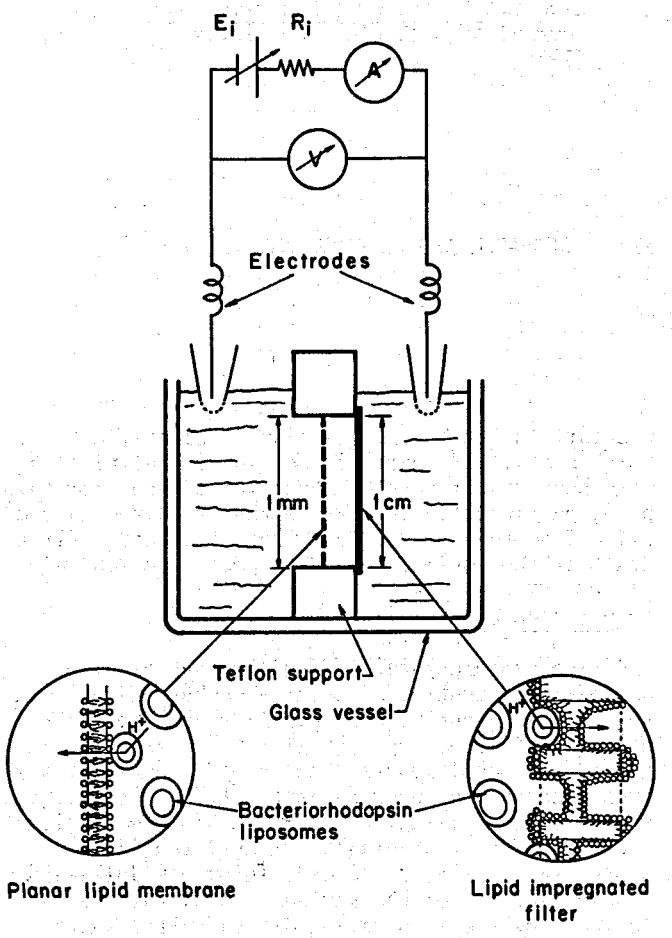

Fig. 3. Schematic of the method used to measure the electrical characteristics of the light sensitive pigments of halobacteria. (XBL 7610-9374)

of water if the voltage can be built up by connecting several membranes in a series.

PLANNED ACTIVITIES FOR 1977

There is much interest in how the photochemical cycle of the protein pigment is capable of causing the release and uptake of a proton. This catalyst is perhaps the best biological example of an ion pump.[11,12,13] The understanding of how an ion pumps work is a primary research interest of membrane bioenergeticists. In halobacteria, the action of bacteriorhodopsin serves to set up photoelectrical potentials and acts as a driving force for the exchange of other ions, in particular salt transport. It has been suggested that this type of catalytic system could be used in the design of a practical system for desalination of sea water. Hence this laboratory plans to further study the mechanism of bacteriorhodopsin action and how it may be coupled to sodium salt transport.

Efforts in the study of H_2 gas reactions via photosynthetic processes will continue. In particular, the possibility of improving the N_2 fixing efficiency of cyanobacteria, as described above, will be explored.

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SUPPORT ACTIVITIES FOR ERDA HEATING AND COOLING RESEARCH AND DEVELOPMENT PROGRAM

M. Wahlig

INTRODUCTION

Several of the ERDA Laboratories, including LBL, have been engaged in support activities which provide assistance to ERDA Headquarters in planning, implementing, and monitoring the solar heating and cooling R&D program. These activities have included program planning, preparation of solicitations for proposals, proposal reviews, project monitoring, and overall coordination. The areas in which LBL has had primary responsibility have been those of Controls (i.e., electromechanical control subsystems) and Non-Engineering Aspects (e.g., legal, economic, legislative, etc.) of Solar Heating and Cooling. LBL has had a supporting role in the area of Solar Cooling.

ACTIVITIES DURING 1976 AND FUTURE PLANS

Program Planning

A comprehensive plan was formulated during 1976, and is described in the recently released document "Program Plan for Research and Development in Solar Heating and Cooling", ERDA 76-144. The major support role in the preparation of this plan was carried out by the Los Alamos Scientific Laboratory (LASL). LBL participated in several planning workshops that generated much of the input for this plan, participated in reviews that resulted in modifications to the plan, and wrote the entire first draft of the Non-Engineering Aspects section.

Preparation of Solicitations

The implementation of the program plan requires the execution of a large number of tasks in several different technological areas. The technologies affected include collectors, storage units, air conditioners, heat pumps, controls, systems, and non-engineering aspects (economic, legal, regulatory, legislative, architectural, educational, social and environmental). LBL assisted in assigning priorities and in defining schedules and funding levels for the various tasks. This was followed by the preparation of draft Statements of Work that will be contained in RFP's (Request for Proposal) or other solicitations to be issued by ERDA. Most of the effort involved in implementing the R&D plan will be expended by the non-ERDA

organizations (i.e., private industries, universities, etc.) who respond to these solicitations. It is expected that during 1977 LBL will participate in evaluating the proposals received from the interested institutions.

Proposal Reviews

LBL has been participating in the peer-review of unsolicited proposals received by ERDA. During 1976, LBL solar researchers participated in two panel sessions set up for this purpose, and several proposals were also forwarded to experts outside of ERDA for additional individual reviews. These activities have primarily involved the areas of controls and solar cooling.

Project Monitoring

Project monitoring provides technical evaluation of ongoing projects, including site visits, review of progress reports, and the conduct of contractor meetings when necessary. Reports of findings and activities are provided, when appropriate, to Program Managers at ERDA Headquarters. Work carried out during 1976 included one site visit and review for a controls project. It is expected that activity in this category will increase significantly in 1977 as additional projects resulting from RFP responses are initiated.

Overall Coordination

An inter-laboratory committee has been established for coordination of all support activities of this type. LBL has participated in several of these committee meetings in 1976, and it is anticipated that this participation will continue in the future.

CONTROLLER DEVELOPMENT FOR SOLAR HEATING AND COOLING SYSTEMS

M. Wahlig, E. Binnall, J. Dillworth, C. Dols, R. Shaw, W. Siekhaus

INTRODUCTION

A prototype of a modest-cost electronic controller was designed and fabricated. This instrument will serve as the control element for solar energy heating and cooling systems. It is analogous to the simple thermostat control utilized today in most conventional heating and cooling systems. By energizing proper valves, pumps, and other devices in the solar system, the controller will optimize system performance with the use of operating algorithms that have been pre-programmed into the unit. The experimental solar heating and cooling system at LBL will be used to test the controller's effectiveness under various solar collector input and heat load conditions. This testing and operating experience may indicate the desirability of changes in the controller's electronic circuity in order to affect the desired degree of system optimization. However, the overall goal of this effort is to develop a controller with a cost that is compatible with acceptance and use of the unit in the commercial market.

ACCOMPLISHMENTS DURING 1976

Controller Unit

The electronic circuit design of the controller was completed and a prototype unit was fabricated and debugged. Currently it is being linked to the valves and pumps of the solar system. A functional verification of the various heating and cooling algorithms is underway.

The prototype controller was built emphasizing experimental flexibility and circuit accessibility. It possesses extra operational features and displays, not necessary for a commercial model, for experimental testing and development.

The circuit design of the prototype unit is shown schematically in Fig. 1. The following circuit components are included:

1) Standardizer: This permits voltage offset and gain calibration through an amplifier stage that processes the output signal from each temperature sensor. It allows standardization of the response curves from all of the temperature sensors and therefore permits precise inter-comparisons between any two sensor outputs. This improves the quality of the decision-making process taking place as the heating and cooling algorithms are implemented. This stage is required only because the currently available temperature sensors being used (LX5700A) are not sufficiently accurate. Perhaps future commercial development of these sensors will make available sensors accurate enough to eliminate the need for the electronic standardizers.

2) PPIM (pin-programmable input matrix): This permits selection of those input signal pairs to be compared in the subsequent comparator stage. With the use of PPIM the operator can easily select the options of interest. This is primarily an experimental tool; in a commercial model, this pin board would be replaced by a simple matrix card with pre-selected options for signal comparisons.

3) Comparators: Each provides an output binary logic signal indicating which of the two input signals is greater. The inputs to the comparators are analog signals from the temperature sensors and from pre-set temperature levels. These pre-set levels are set using potentiometers on the front of the controller chassis. Adjustable resistors in the comparator circuitry allow variable voltage offsets and hysteresis bands for the two inputs.

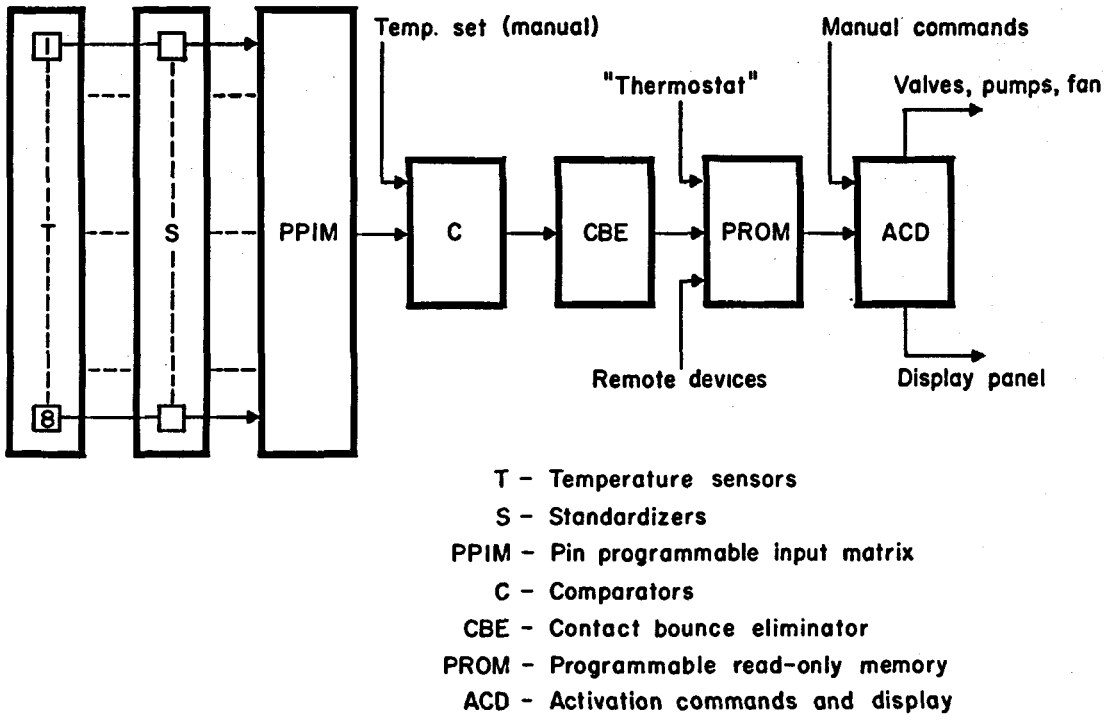

Fig. 1. Block diagram of the controller ciruit.

The prototype controller contains ten comparator circuits.

4) CBE (Contact bounce eliminator): This component tests the stability of the comparator output, therefore controlling system sensitivity. The purpose of the CBE is to prevent momentarily unstable decisions resulting from electronic noise or short-term temperature fluctuations of the sensors. The CBE requires that a changed output binary level from a comparator remain constant for four "periods" before this change is passed on to the PROM. The duration of the "period" is adjustable over a wide time range (from milliseconds to minutes).

5) PROM (programmable read-only memory): The PROM contains the algorithm that maps the signals from the input sources (temperature comparators, thermostat, etc.) to the various output devices (solenoid valves, pumps, and fans). All input and output signals are binary. The prototype controller contains three PROM chips which can generate up to twenty output signals.

6) ACD (activation commands and display): ACD provides the necessary AC power to activate the solar system valves, pumps and fans, while displaying these commands on a control panel. The AC power is transmitted to these flow control devices through a relay driver board. It is possible to override the controller generated commands by manually activating any one of the relays on the driver board. The display of all the ACD functions on the controller display panel permits monitoring of the entire system operation.

Domestic Hot Water Heat Exchanger Study

The study of the effectiveness of alternative control algorithms began by considering the domestic hot water (DHW) system. The coupling of the solar heat supply to the DHW takes place via heat exchange with the main 3000-gallon hot water storage tank. This is typical of systems that use liquid collectors to supply both space heating and domestic hot water heating.

Prior to beginning the controller performance evaluation it was necessary to consider various options for physically extracting heat from the main storage tank. The options studied included various types of DHW heat exchangers installed within the main storage tank; namely, a copper coil, a stripped (of insulation) 30-gallon DHW tank with a large surface-to-volume ratio, and a similar 40-gallon DHW tank with a significantly smaller surface-to-volume ratio. During the tests of relative heat-exchange effectiveness, each of the heat exchangers was positioned near the center of the main storage tank, providing comparable experimental conditions of heat transfer from the water in the main tank. The water inlets to the immersed DHW tanks were modified to produce a tangential swirl to the incoming water. As expected, it was determined experimentally that this geometry improved the heat transfer effectiveness, especially at higher flow rate.

The results of these heat exchange tests are presented in Fig. 2. The swirl appreciably improves the heat transfer rate. With this swirl the heat transfer rates of the immersed 30 and 40 gallon

tanks are comparable or better than that of the 100 foot copper coil. The tank with the higher surface-to-volume ratio is superior at higher flow rates.

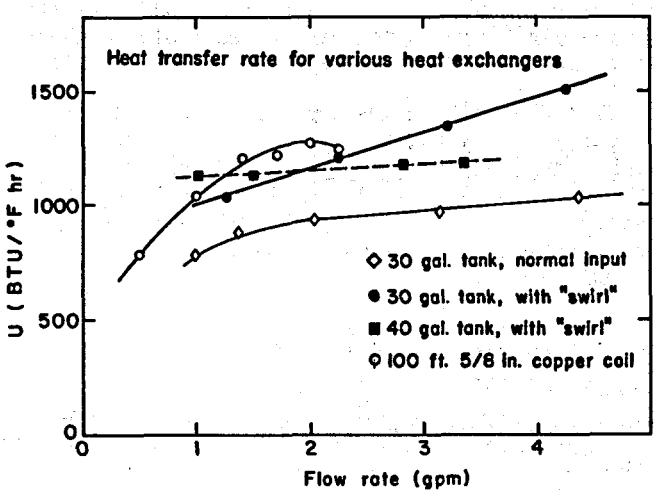

Fig. 2. Results of experimental heat exchange tests. (XBL 771-61)

In practice, the main storage tank heat exchanger is only one part of the DHW system. It must be coupled to an external conventional DHW tank, or to a flash heater coil, to allow the use of auxiliary back-up energy. In some existing solar installations, two external DHW tanks have been used, with one serving as a solar preheater tank. The overall optimum DHW system must be selected by considering the most cost-effective combination of: a) main storage tank heat-exchanger; b) external, conventionally-heated DHW coil or tank; and c) operating algorithm. This experimental program will continue and will investigate the relative economics of complete DHW systems using all practical combinations of components and operating algorithms.

Other Studies and Modifications to the Solar Heating System

During a period when the main storage tank was not being used, a series of temperature readings were taken over a two week period in order to investigate the degree of temperature stratification under no-flow conditions. The results are shown in Fig. 3. Although the average temperature of the storage tank dropped from approximately 62°C to 44°C during this period, very little mixing occurred. The initial condition of temperature stratification persisted throughout the test period, with all regions of the tank experiencing nearly uniform temperature decreases.

Since copper tubing is used throughout the plumbing system, corrosion of the aluminum collector panels represents a potential problem. Measures were taken to minimize the extent of the corrosion: a getter (consisting of aluminum shavings) and filters were installed between the copper and aluminum components, and an anti-corrosion compound (Nalco 39L) was added to the water system. The rate of aluminum corrosion was monitored using aluminum test coupons. Measurements of the weight loss of these test coupons indicated an aluminum corrosion rate of 0.1 mils (2.5 μm) per year, attesting to the effectiveness of these corrosion-inhibition measures.

The experimental solar heating and cooling system contains a "pseudo-collector" unit (actually, a hot water boiler) that can substitute for real solar collectors by providing input energy to the solar system. Under typical operating conditions about 1/3 of the heat input would come from the real collectors and 2/3 from the pseudo-collector. A commercial temperature control unit was installed to ensure that the pseudo-collector output temperature matched that of the water in the return line from the real collectors on the roof. This commercial control unit permitted errors of the order of 6°C in the pseudo-collector output temperature. Through modifications to the control unit, its plumbing connections, and the gas-fired heating stage in the boiler, this temperature error was reduced to the extent that the pseudo-collector output now tracks the real collector outflow temperature to within ± 0.5°C.

Finally, modifications were made to the air vent lines between the collectors and storage tank to avoid pump start-up problems associated with air entrainment in the water flow lines.

PLANNED ACTIVITIES FOR 1977

Now that the controller fabrication has been completed and most of the start-up bugs have been worked out of the solar heating and cooling system, the main experimental effort during 1977 will concentrate on the determination of relative system performance and economics as a function of the control algorithms being used.

FEA/HUD/ERDA REGIONAL SOLAR ENERGY RETROFIT OF LOW AND MODERATE COST HOMES

T. Webster

INTRODUCTION

This project is a cooperative effort undertaken by HUD, FEA, and ERDA within the Region IX area common to these agencies. As stated in the Memorandum of Understanding,[1] the general objectives of the project are the same as those of the National Demonstration Program; that is, promotion of solar energy to reduce demand on conventional fuel supplies. However, unlike other programs,

this effort is directed to the demonstration of retrofitted solar heating systems on low and moderate cost homes. The basic objectives are, (1) to evaluate the social and economic impact of this application of solar technology, (2) to assess the savings resulting from various energy conservation measures, and (3) to publicize the efforts of the agencies in developing energy efficient homes in the low and moderate price range.

Two houses in each of two locations (Sacramento and Las Vegas) were selected for retrofitting; all houses are to be well insulated and one house in each location will be equipped with a solar space and domestic hot water heating system.

The responsibilities of the agencies involved are as follows:

1) FEA

FEA has responsibility for overseeing the project, i.e., collecting utility bills and questionnaires, doing periodic analysis and a final report as well as taking care of publicity. FEA will monitor the houses for three years and will conduct a review of financial limitations, reaction of owners and neighbors, and will fund all passive energy conservation measures such as insulation and weatherstripping.

2) HUD

The houses were provided by HUD from a stock of repossessed houses. HUD will 1) sell the houses, 2) assess the degree of conformity to existing solar standards,[2] 3) determine marketability by annual appraisal of the properties for five years, and 4) fund all rehabilitation work to bring the houses up to minimum property standards. New owners will be required to submit utility bills and other information to FEA as a condition of sale. The houses will be placed up for sale using established HUD procedures.

3) ERDA

ERDA will fund the design and installation of one solar heating system for each location. After this installation ERDA will transfer ownership to HUD.

This project was originally conceived by FEA in October 1975. LBL became active in the project in March 1976 at the request of ERDA/SAN (the ERDA San Francisco Operations Office) for technical assistance. LBL Plant Engineering has responsibility for administration and technical management during the design and installation of the two solar systems. Technical assistance is being provided by the Solar Energy Group in the Energy & Environment Division.

ACCOMPLISHMENTS DURING 1976

When LBL became involved in the project the scope had been reduced from the original 6-8 retrofitted houses in each of 3 locations (Sacramento, San Jose, Phoenix) to 2 in each location. Additional budget limitations eventually reduced the scope of the project to two retrofitted houses in each of two locations: Sacramento and Las Vegas. The selected houses were tract type homes of 1000-1200 square feet of floor area. An attempt was made to select houses that were constructed after 1970, were physically near each other and of similar construction, were in relatively desirable neighborhoods, and would be easily available to the public.

A number of calculations were made to determine the savings resulting from various levels of insulation. The schemes investigated were not required to be cost effective or to conform to existing codes. The final decision was to insulate as follows:

Sacramento:

Ceiling	R28
Walls	R11
Floors	R11

Weatherstrip doors and windows, storm/screen front door, insulate ducts and hot water piping, water restrictors.

Las Vegas:

Same as Sacramento except R38 in ceiling and none in floor (i.e., concrete slab).

Early in the project it became apparent that there were unresolved questions about what the specific objectives of the project were and how these objectives were to be accomplished. Given the limited monitoring and instrumentation available, it appeared that an energy-use comparison between the houses was not feasible. Two actions resulted: 1) LBL agreed to produce a Conceptual Design Report to better fix the scope, costs, and schedule for the solar heating systems; and 2) the project objectives were formulated in a Memorandum of Understanding between the three agencies. Both of these documents were completed in July. In September 1976 ERDA approved $43,300 for the design and construction of the two solar systems.

Solar Heating Systems

Several architect-engineering-consultant firms were evaluated by a panel and a mechanical engineering consultant, Koepf and Lang, was contracted to do detailed design of the solar systems. These systems were designed in accordance with the HUD standards, the LBL conceptual design, and the following criteria:

1. They were to be constructed from standard commercially available components and installed by local heating and plumbing contractors;

2. They were designed for simplicity of operation, minimal maintenance, and a service life of 10 years;

3. They were designed to minimize damage due to vandalism.

The systems were sized using the Beckman-Duffie simplified sizing procedure known as

TABLE 1. Design and Performance Parameters for Solar Heating System.

	Latitude	Collector Slope	Collector Area	House Load	DHW Load	Storage Capacity	Solar Fraction
	Deg	Deg	ft^2	Btu/hr- F	Gal/ Day	Gal.	%
SACRAMENTO	38.5	20°	300	500	60	600	65
LAS VEGAS	36	7°	200	459	60	450	60

"f-chart",[4] as shown in the HUD standards. Table 1 summarizes the parameters used in the calculations and the expected annual performance of the systems. The calculations were based on a standard performance curve for single glazed, non-selective surface collectors.

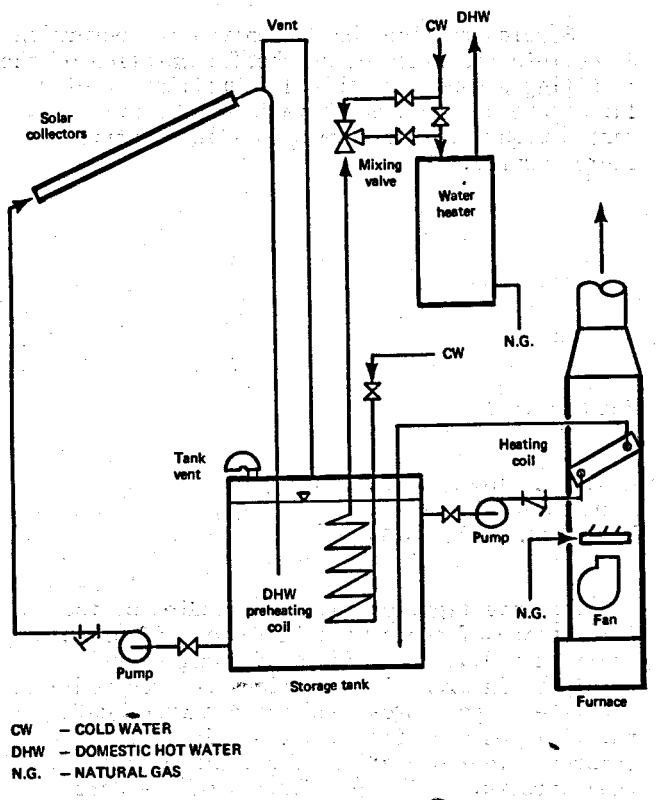

Fig. 1. Solar Heating System Flow Diagram. (XBL 773-637)

Figure 1 is a flow diagram for the systems. The final design included the following features:

1. Single-glazed (w/plastic), liquid-type copper tube collectors mounted flat on roof (patio cover in Las Vegas),
2. Insulated steel storage tanks in outside enclosure,
3. Self-draining collectors,
4. Copper coil in storage tank for preheating domestic hot water,
5. Heating coils located in existing furnace plenum,
6. Two-stage thermostatic control.

PLANNED ACTIVITIES FOR NEXT YEAR

In December local contractors were asked to make bids for the installation of the systems. The bids were due on January 4, 1977 and installation should be completed by May 1, 1977. When the systems have been completed, checked out and accepted LBL's responsibility in the project will be discharged.

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2. Intermediate Minimum Property Standards for Solar Heating and Domestic Hot Water System, NBSIR 76-1059, April 1976.
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Chemical Process Research and Development Program

INTRODUCTION

In the area of chemical process development, research on processes that might result in the development of substitute fuels to replace petroleum and natural gas has been emphasized. The limited reserves of petroleum and natural gas make the development of improved processes for the liquefaction and gasification of coal increasingly attractive. Part of the economic disadvantages of these processes arise from the extreme conditions of pressure and temperature which must be used for conversion. We are studying the fundamental processes involved in the liquefaction and gasification of coal to determine whether milder operating conditions might be feasible. Studies are being conducted on various types of catalysts that might lead to liquefaction at low pressures and low temperatures and on the development of some new and unusual catalysts. These studies are being made with model compounds as well as with bituminous and sub-bituminous coals.

Filtration of ash from the hydrogenated coal stream supply has proved to be a difficult and expensive component of solvent-refined coal production processes. Another project involves an exploratory study for an improved method of ash agglomeration for the filtration process.

A project is underway involving a study (1) to ascertain the tertiary-mode efficiencies of flooding acidic California crude oils with dilute aqueous bases and (2) to devise laboratory screening tests which will elucidate the governing recovery mechanisms and permit development of an improved mobility-reactive tension agent flooding package.

Short term energy storage can increase the efficiency of present energy systems by providing a means of smoothing peak loads with respect to minimum loads. Chemical systems are one means of energy storage. A study of the SO_2-O_2- SO_3 system for energy storage has been started, and a preliminary design for use of that system has been made.

Studies continue on the enzymatic conversion of cellulose to glucose and the fermentation of the resulting glucose to ethanol. Utilization of a large part of the biomass that is presently wasted might well be developed into an attractive energy source.

SELECTIVE HYDROGENATION OF COAL

A. T. Bell, E. A. Grens, E. E. Petersen, T. Vermeulen, G. S. Booras, T. T. Derencsenyi, G. P. Dorighi, R. R. Holten, J. B. McLean, E. Mendizabel, S. Salin, M. Seth, K. I. Tanner, N. D. Taylor, G. H. Zieminski

INTRODUCTION

Existing technology for coal liquefaction is based on thermal decomposition of the coal, or pyrolysis, with subsequent hydrogenation of the initial pyrolysis products. Such nonselective thermal bond breaking yields a wide range of products including light hydrocarbon gases and is, therefore, not efficient in hydrogen utilization. This project seeks to establish a basis for conversion of coal to liquids, with minimum hydrogen addition, by selective scission of certain bond types in the coal structure below pyrolysis temperature. Bonds linking conjugated hydroaromatic groups in the coal, including aliphatic bridges and noncarbon links (e.g. ether, carboxylic, and disulfide bridges), are being attacked by hydrogenolysis or hydrolysis in the presence of homogeneous catalysts. The use of these dissolved catalysts in a liquid reaction medium permits access to reaction loci on the extensive interior surface of the coal.

The investigation involves studies of the interaction of coals with inorganic and organic reaction media, the effects of homogeneous catalysts in promoting reactions in such media at moderate temperatures, and the action of catalyst materials on specific bond types in model compounds representative of certain aspects of coal structure. The interaction of the pore structure of the coal with the progress of reactions and the influence of transport on reaction rates in this structure are included in this study.

The project was initiated in January, 1974. During the first two years of the program, equipment and laboratory procedures were developed and studies undertaken of the interaction of sub-bituminous coal with several organic solvents and with zinc chloride melts, phosphoric acid, and sodium hydroxide. Hydrogenolysis of model compounds with Lewis-acid catalysts was also investigated as were the changes in coal pore structure caused by interactions with organic solvents.

ACCOMPLISHMENTS DURING 1976

The project activities planned for 1976 included investigation of coal interaction with polar, especially basic, organic solvents, and with inorganic phases including zinc chloride melts and phosphoric acid. Catalysis of hydrogenation of model compounds by homogeneous catalysts, particularly strong Lewis acids and transition metal carbonyls, was another area of emphasis for this period. In addition previous work in characterization of coal internal surface structure, and changes in this structure with coal treatment, were to be expanded. The sub-bituminous coal used in most of this work is from the Roland Seam, Wyodak Mine.

INTERACTION OF COAL WITH ORGANIC SOLVENTS
(E.A. Grens, G.P. Dorighi, G.H. Zieminski)

The interaction of coal with polar, nitrogen containing organic solvents, was studied in the temperature range 150°C to 350°C. The coal was extracted, nearly to completion, in pure refluxed solvents, and the extracts were analyzed for elemental composition, average molecular weights, aromaticity of their hydrogen content (by proton NMR), and fractional solubilities in standard solvents (cyclohexane and benzene at their normal boiling points). For all solvents the yield of dissolved material increased significantly with increasing temperature, by roughly a factor of two between 150°C and 300°C. The soluble material yield increased dramatically with increasing amine character of the solvent, as shown for 250°C, 4 hr extractions in Table 1. Over 60% of the sub-bituminous coal dissolved in ethylenediamine at 250°C, compared to only about 16% in pyridine and 7% in tetralin, a commonly studied solvent material. These findings are consistent with the existence of an extensive acid (-OH)/base (amine) linkage structure in the coal, a structural concept that is now becoming widely accepted. The relatively low hydrogen/carbon ratios found in the dissolved materials (.95-1.35), even when a large fraction of the coal was dissolved, suggest the opportunity for obtaining considerable conversion of coal to liquids at quite moderate hydrogen expenditures.

An interesting aspect of the interaction of these solvents with the sub-bituminous coal studies is the nature of the gases evolved during the process. Although these gases may account for 5 to 10% of the mass of the coal involved, they contain very little methane or other hydrocarbons, consisting almost entirely of CO_2 and CO. Thus at least a significant fraction of the high oxygen content of the coal (18% by weight) can be eliminated without hydrogen consumption.

This work is now being extended to investigate interaction of coal with mixed solvents and to study rate limitations in coal solvent interactions.

TREATMENT OF COAL WITH ANHYDROUS PHOSPHORIC ACID
(J.C. McLean, M. Seth, T. Vermeulen)

Phosphoric acid, investigated as a homogeneous medium for coal liquefaction, has been used to treat Illinois No. 6 coal at 250°C under hydrogen at 35 bars. Na_3PO_4, added to the extent of 5% of the water-free H_3PO_4, was found to suppress foaming when the water in the coal feed is discharged.

Phosphoric acid is found to "activate" the coal but not to convert it to useful products. The pyridine-extractable content of untreated coal (dry ash-free basis) is 19.2 wt-%. Treatment with H_3PO_4, alone or with Na_3PO_4, reduces this level to about 11.0 wt-%; while use of H_3PO_4 with 10% anhydrous H_2SO_4 further reduces the solubility to about 7.0 wt-%. Despite these reductions, the reactivity of coal at 250°C which has thus been demonstrated is considered as a potential asset for coal liquefaction under mild conditions of treatment, and a search is under way for co-reactants which may lead to favorable results.

Table 1. Yield of dissolved material for coal/solvent contact at 250°C-4hr

Solvent	Yield of dissolved material (DAF basis)	Dissolved material H/C ratio[a]
Tetralin	8.4%	1.35
Pyridine	15.9%	1.29
Quinoline	31.7%	0.94
Piperidine	36.6%	0.95
Ethylenediamine	65.1%	——

[a]Coal H/C ratio (DAF basis) = 1.07

TREATMENT OF COAL WITH ZINC CHLORIDE MELTS
(R.R. Holten & T. Vermeulen)

The hydrogenolysis of Wyodak sub-bituminous coal, Illinois No. 6 bituminous coal, and solvent-refined coal (SRC) with molten zinc chloride solutions has been studied at the mild conditions of 250°C and 35 bars H_2 pressure in a Parr autoclave. Because pure $ZnCl_2$ melts at 316°C, approximately 9.0 wt-% water was added to the zinc chloride to form a liquid melt. Various inorganic (and organic) additives were used to determine their ability to promote catalysis by zinc chloride.

The extent of conversion of the three feed materials to soluble products for several experiments is given in Table 2, along with extraction yields for the raw feeds. The one and three hour runs with Wyodak coal indicate that conversion to pyridine solubles is slow at 250°C and that further conversion might be attained by using reaction times longer than three hours. Equivalent runs with the three feed materials show that the Illinois No. 6 coal, which is bituminous, is more susceptible to the $ZnCl_2$ treatment than the Wyodak coal, which is sub-bituminous. SRC showed no change in total solubility (it was completely soluble to begin with), but its benzene solubility actually decreased. This could have been the result of polymerization reactions.

Exploratory runs involving zinc chloride with concurrent use of organic compounds (which were potential hydrogen donors) were conducted as part of a related project. These studies show that zinc chloride remains an active catalyst for coal conversion at relatively low temperatures. Other areas to be investigated include (a) the possible improvement of melt properties and economics by admixture of other chlorides (K, Na, Li, Ca), and (b) introduction of co-catalysts which might enhance the conversion rate at a given temperature and pressure ($CuCl_2$, $FeCl_2$, $SuCl_2$, and perhaps metal carbonyls).

SELECTIVE HYDROGENATION OF FUSED-RING AROMATICS
(T.T. Derencsenyi & T. Vermeulen)

Ligand-substituted transition metal carbonyls have been investigated as potential catalysts or co-catalysts in coal conversion by experiments on model compounds (anthracene, phenanthrene, and naphthalene). New combinations of known metal carbonyls and known co-ligands have been synthesized and investigated for both chemical stability and catalytic activity. These new catalyst materials all have improved stability at any given temperature and given CO partial pressure and are therefore suitable for investigations in the range of 15 bars of CO partial pressure or less, and temperatures of up to 300°C, at which carbon-carbon bond breaking may begin to occur.

Because of the small scale of the experiments, the catalysts were used in a concentration of 10 mole-% based upon the reactant (1 mole-% based on the solvent). The co-ligand was added to the reaction mixture, in a 2:1 mole ratio to catalyst, but proved to be so firmly bound that it would not dissociate if added in a pretreatment. The results are shown in Table 3. Among the co-ligands tested, tri-ethyl phosphine gave the best combination of activity and selectivity; both its cobalt complex and its iron complex appeared to give near-equilibrium conversions of anthracene to dihydro-anthracene. Tri-ethoxy phosphine with cobalt on anthracene was less active, and with iron yielded tetrahydroanthracene which is a less desirable product. Tri-butyl phosphine with cobalt was more active for phenanthrene, probably equally active for anthracene, and very weakly active for naphthalene. Tri-ethoxy phosphone with cobalt was less active on anthracene than tri-butyl; and with iron it yielded tetrahydroanthracene (which

Table 2. Extraction yields of coals and treated coal materials (DAF basis-wt-%)

Test material	CycloC_6	Benzene	Pyridine	Total	Increase over feed
Wyodak Coal	0.7	1.1	11.0	12.8	
Illinois No. 6 Coal	0	0.5	17.7	18.2	
SRC (Pamco)	3.1	36.5	60.4	100.0	
TREATED COAL MATERIALS					
Wyodak - $ZnCL_2$ (1 hr)	0	4.6	16.8	21.4	8.6
Wyodak - $ZnCl_2$ (3 hr)	2.1	3.2	22.2	27.5	19.7
Illinois No. 6 - $ZnCl_2$ (3 hr)	0.3	3.7	41.4	45.4	27.2
SRC - $ZnCl_2$ (3 hr)	3.6	16.9	79.5	100.0	-

Table 3. Hydrogenation tests with carbonyl catalysts, using equimolar CO/H_2 gas feed and anthracene as reactants, in decane or similar solvent.

Metal in carbonyl	Ligand	Temp. C	Pressure, bars	Time, hr.	Conversion, % Dihydro	Tetrahydro
Cobalt	Et_3P	175	30	1.0	99	0
	$Bu_3P + Ph_3P$	175	29	0.5	92	0
	$(EtO)_3P$	200	39	1.0	73	0
Iron	Et_3P	240	44	4.0	35	0
	Ph_2ClP	300	51	2.0	21	0
	Bu_3P	225	36	2.3	4	0
	$(EtO)_3P$	200	38	4.0	0	33

is a less desirable reaction for coal-conversion sequences). Tri-phenyl phosphine with cobalt decomposed below 250°C (with iron it was inactive). Chloro-di-phenyl phosphine with iron remained active to 300°C; at this temperature it displayed some tendency to incorporate CO into anthracene, but it may not be unique in this regard. Sulfide ligands with iron had lower activity, but were not inert. Carbonyls of chromium, molybdenum, wolfram, vanadium, and manganese appeared disadvantageous, forming tetrahydroanthracene and also large proportions of carbon monoxide derivatives.

Iron carbonyls are preferred to cobalt carbonyls because of both their lower cost and their ease of handling (they are liquid rather than solid). For iron, in terms of our present knowledge, the ligands are rated in the order of tri-ethyl phosphine first, then tri-butyl phosphine, then chloro-di-phenyl phosphine. These iron catalysts may point the way to a successful homogeneous hydrocracking catalyst.

CATALYTIC HYDROGENATION AND HYDROGENOLYSIS OF ORGANIC STRUCTURES RESEMBLING THOSE FOUND IN COAL

(A.T. Bell, S. Samlin, K.I. Tanner, N.D. Taylor)

Strong acid catalysts are being investigated for their ability to promote the cracking, hydrogenation, desulfurization and denitrogenation of organic structures similar to those found in coal. Model compounds are being used for part of the work so that reaction pathways may be traced through an analysis of intermediate and final products. In the balance of the work, asphaltenes derived by benzene extraction of coal are used to simulate the action of the catalyst on coal.

Aluminum chloride, $AlCl_3$, has been investigated as a prototype strong Lewis acid. A summary of the reactions observed with this catalyst is presented in Table 4. It is of interest to observe that $AlCl_3$ promotes the cracking of benzene but does not crack naphthalene, cyclohexane, or the hydroaromatic ring in tetralin. This behavior is unexpected since cycloaliphatic rings are expected to crack more easily than aromatic rings. A second characteristic of $AlCl_3$ is its ability to promote hydrogenation. In the case of naphthalene the necessary hydrogen derives from the solvent, benzene. A similar hydrogen donor facility does not exist when hexane is used as the solvent. The ability of benzene to donate hydrogen is also observed during the hydrogenolysis of the aliphatic bridge in bibenzyl. When gaseous hydrogen is present, $AlCl_3$ is also found capable of promoting the hydrogenation of single aromatic rings, as evidenced by the appearance of cyclohexane and cyclohexane derivatives during reaction with benzene and bibenzyl respectively. More extensive investigations of the catalytic properties of $AlCl_3$ are now in progress.

Studies of mixed metal oxides (e.g., $SiO_2 \cdot Al_2O_3$, $\cdot Cr_2O_3 \cdot Al_2O_3$, $SiO_2 \cdot ZrO_2$, etc.) have been initiated. These compounds are strong acids and possess both Lewis and Bronsted acid sites. Activity patterns for these catalysts will be examined using the same model compounds investigated with $AlCl_3$. Experiments with coal derived asphaltenes will be carried out using the same model compounds investigated with $AlCl_3$. Experiments with coal derived asphaltenes will also be conducted using these catalysts.

LOW TEMPERATURE PROCESSES FOR COAL DESULFURIZATION AND CHANGES IN PORE STRUCTURE OF COAL WITH CHEMICAL PROCESSING

(E.E. Petersen, G.S. Booras and E. Mendizabel)

A number of processes have been proposed to remove sulfur from coal. Several of these are based upon treatment with aqueous solutions at low temperatures and pressures. The effectiveness of these latter methods to remove organic and inorganic sulfur from high sulfur Illinois #6 coal was studied. The effect of leaching agent temperature, reaction time, and particle size

Table 4. Products obtained through the action of $AlCl_3$ on various model compounds

Reactant	Products	Source of hydrogen
Benzene	Toluene Ethylbenzene Diphenyl Cyclohexane derivatives	dimerization of benzene H_2
Bibenzyl	Toluene Ethylbenzene Benzene Cyclohexane derivatives	dimerization of benzene H_2
Naphthaline (in benzene solution)	Tetralin	dimerization of benzene
Naphthalene (in hexane solution)	No products	———
Cyclohexane	Methylcyclopentane	———

Reaction conditions: T = 225°C P = 1000 psi H_2.

was determined. The leaching agents studied were 10% sodium hydroxide and 0.5 M ferric sulfate.

The following major conclusions were drawn from this work:

1. Sodium hydroxide is effective in removing the major pyritic sulfur, but, even at the highest temperatures studied, it was unable to remove more than 40% of the organic sulfur from Illinois #6 coal;

2. Ferric sulfate is very effective in removal of pyritic sulfur;

3. Oxygen appears to be a promising method, but under the conditions used in this work, too much of the coal matrix was oxidized.

Carbon dioxide adsorption experiments gave the same BET surface areas at room temperature for a molecular sieve, an alumina catalyst, and a Wyoming sub-bituminous coal. These results suggest that activated diffusion was not an important factor even at 196°K. However, the adsorption of carbon dioxide on Illinois #6 coal decreased with increasing temperature.

Surface area variations of desulfurized coal, extracted coal, and reacted coal were examined by carbon dioxide adsorption at 196°K. The surface area of Illinois #6 coal, when treated with sodium hydroxide to remove sulfur, first decreased as inorganic sulfur was removed and then increased again as organic sulfur was removed.

Pyridine extractions of Roland Seam coal appeared to open new areas that were previously inaccessible to carbon dioxide. The surface areas were nearly doubled, but the average pore diameter appeared to remain essentially unchanged as evidenced by neopentane adsorptions. Large solvent molecules such as benzene were able to penetrate the coal pores, whereas a large, symmetrical molecule such as neopentane could not. These results suggest that the pores are slot shaped rather than cylindrical.

In continuing studies, pore volume changes will be followed in addition to changes in surface area in order to resolve the question of whether chemical processing creates new area within the coal or opens previously blocked parts of the original coal structure. Work in the desulfurization area will be continued by evaluating catalytic processes for removing thiophenic sulfur using model compounds, solvent refined coal, and Illinois #6 coal.

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AGGLOMERATION OF ASH IN SOLVENT-REFINED COAL

W. K. Cray and D. N. Hanson

INTRODUCTION

Filtration of ash from the hydrogenated coal stream has proved to be a highly difficult and expensive component of the process for production of solvent-refined coal. Because of the extreme fineness of the ash, filtration rates of the order of only 0.5 $m^3/hr.m^2$ can be achieved, even with a precoat of diatomaceous earth. Improvement in the filtration element of the process, through settling to concentrate the ash and through agglomeration to increase filtration rates, would substantially improve the economics of solvent-refined coal. Exploratory work to find a method of agglomeration of the ash was begun at Lawrence Berkeley Laboratory in July, 1976.

ACCOMPLISHMENTS DURING 1976

Analogies to crude oil drying through electrical coalescence of water droplets led to examination of the feasibility of electrical agglomeration. It is expected that the dielectric constant of the ash particles would be higher than that of the suspending medium, leading to induced dipoles and atractive forces between ash particles when the suspension is subjected to electric fields. The existence of the effect is demonstrated by Figs. 1 and 2. Figure 1 shows a sample of solvent-refined coal filter feed as obtained from the pilot plant of the Pittsburgh and Midway Coal Mining Company at Tacoma. Figure 2 shows the filter feed diluted with half its volume of dioxane (to lower the viscosity) and subjected to a field of the order of 5000 V/cm. Polarization of the particles has produced long chain-like agglomerates in the direction of the field. However, Fig. 2 also shows a considerable quantity of solid material which has not been agglomerated, and the agglomerates which do form are not stable. They rapidly revert to an unagglomerated state when the field is removed, reducing the effectiveness of the treatment as an aid to filtration. In addition, the fields used in Fig. 2 are higher than can be sustained in practice without an unacceptable power drain because of the high conductivity of the liquid. A series of settling experiments on filter feed, both pure and diluted with solvents, conducted at fields of 1000 V/cm confirmed the judgment that electrical agglomeration is only marginally useful.

Experiments were also conducted to find an additive or environment which would produce natural agglomeration without precipitating solvent-refined coal from the carrier solvent of the process. Dioxane at 60% volume concentration results in pronounced natural agglomeration, forming stable agglomerates which settle rapidly and completely. Figure 3 shows the agglomeration in this system. Tetrahydrofuran is effective at a concentration of 70% and hexylamine at 75%. Pyridine was ineffective.

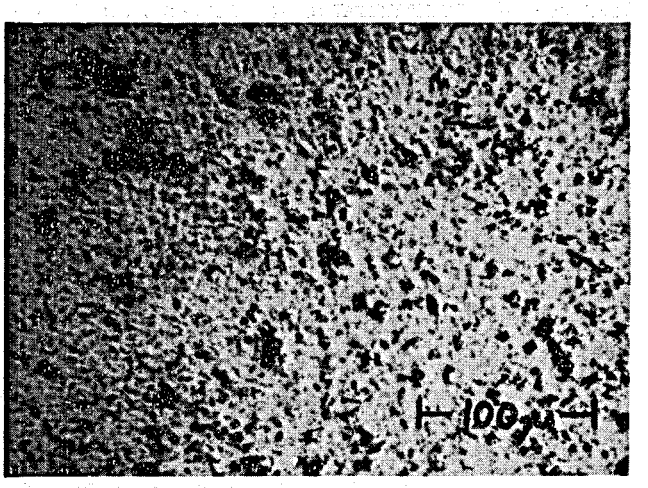

Fig. 1. Solvent-refined coal - unfiltered oil.

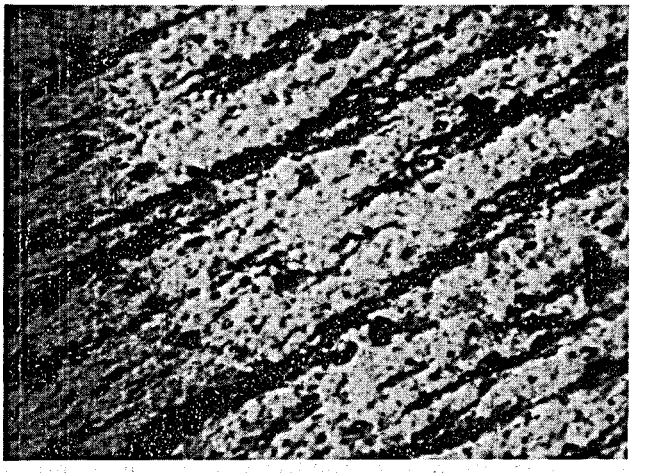

Fig. 2. Agglomeration under electrical fields.

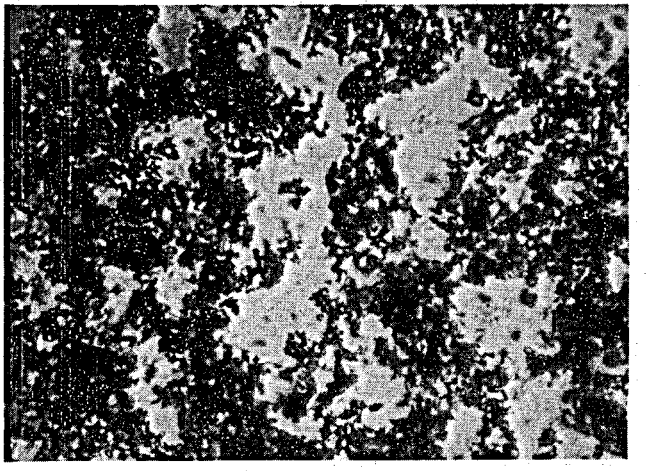

Fig. 3. Natural agglomeration in 60% dioxane.

A tentative explanation of the results can be made through hypothesizing preferential adsorption of hydronium ion on the ash particles, which causes natural stability of the suspension through electrical double layer repulsion. The presence of a considerable ion concentration is shown by the high conductivity. Since the material is not thoroughly dried in the manufacturing process, phenol, phenolic compounds, and water are all probably present in the liquid in relatively high concentrations; the presence of these components would lead to high hydrogen ion concentrations.

All of the additive solvents tested for their agglomerating ability act as based, reducing the hydrogen ion concentration. In addition, dioxane and tegrahydrofuran, because of their low dielectric constants, suppress dissociation of the phenol and compress the electrical double layer around the particles.

PLANNED ACTIVITIES FOR 1977

Experiments are planned to remove water and light phenolic compounds by inert gas stripping of the filter feed. Changes in conductivity and dielectric constant and the state of ash agglomeration will be observed. Microelectrophoretic studies will be made to determine the amount and sign of the charge on the particles under the influence of solvent addition. Saturation of the liquid with caustic or the addition of high molecular weight flocculants will be evaluated.

COAL LIQUEFACTION BY CATALYTIC HYDROGENATION IN ORGANIC-INORGANIC LIQUID MIXTURES

E. A. Grens, T. Vermeulen, F. Hershkowitz, R. R. Holten, J. L. Maienschein

INTRODUCTION

The use of inorganic metal, such as zinc chloride, as media for coal hydrogenation has been subject to considerable study and has certain advantageous features. Problems associated with this approach include control of the reaction extent of organic materials dissolving in the melt and recovery of product liquids from the melt. The utilization of two-phase reaction media composed of inorganic melts with organic solvents has the potential flexibility to resolve these problems: this investigation is intended to establish a basis for a coal liquefaction process using such mixtures. At the same time it emphasizes the conduct of hydrogenation at relatively mild temperatures and pressures, promoted by homogeneous catalysts.

In employment of the mixed reaction media, the coal would be preferentially wetted by the inorganic phase and would be hydrogenated to initial products in that phase. This hydrogenation at low (below pyrolysis) temperature can be promoted by homogeneous (liquid phase) catalysts, which have access to reaction sites in the solid coal. The inorganic media being studied are either themselves catalytic or contain dissolved catalytic materials. The initial reaction products are continuously extracted into the organic phase, reducing undesired further hydrogenation of these materials, and are recovered from this phase.

This project was initiated in January, 1976, and so is in its first year. It will draw upon information developed in another LBL project, "Selective Hydrogenation of Coal", concerning the interaction of coal with inorganic melts and the promotion of coal hydrogenation by homogeneous catalysis.

ACCOMPLISHMENTS DURING 1976

In the initial period of this project, techniques have been developed for measurement of mutual solubilities of inorganic melts and pure organic liquids and of distribution of initial reaction products (represented by SRC asphaltenes) between these phases. Preliminary coal hydrogenations in two phase mixtures have also been conducted to establish the general feasibility of the procedure.

Mixtures of zinc chloride (with small amounts of water) and tetralin have been examined at temperatures to 200°C and found to give clean phase separation when agitation is stopped. A method for measurement of the solubility of the organic material in the zinc chloride melt has been developed: it consists of hexane extraction followed by gas chromatography of the extract and provides quantitative measures of organic content to the low ppm range. The determination of zinc chloride contents of the organic phase by X-ray fluorescence is being investigated. These solubilities have been found to be extremely small, but the sensitivity of the technique holds promise for quantitative determinations.

Exploratory experiments have been undertaken involving treatment of sub-bituminuous coal (Roland Seam, Wyodak Mine) with zinc chloride/organic mixtures for 1 hour at 250°C in the presence of hydrogen at 35 atmospheres pressures. The yields of pyridine soluble materials (preasphaltenes plus asphaltenes and oils) are shown in Table 1. The high yields when zinc chloride and tetralin are used in combination suggest that these phases may serve as co-reactants: the hydrogen donor activity of the tetralin may be catalyzed by the inorganic material so that transfer occurs at this temperature, well below the threshold of about 325°C when tetralin is used alone.

The results of these initial treatment experiments will be confirmed and extended in the next year, and the influence of contacting parameters established. The interactions of the organic and inorganic phases will also be extensively examined.

Table 1. Yield of pyridine soluble material from excess organic/inorganic mixtures at 250°C for 1 hour.

Inorganic phase	Organic phase	Yield of pyridines solubles (DAF basis)
None	None	13%
None	Tetralin	20%[a]
$ZnCl_2$	None	21%
$ZnCl_2$ + HCl	Isopropylbenzene	40%[a]
$ZnCl_2$	Tetralin	77%[a]

[a]Not corrected for organic solvent incorporation in extract material.

ENHANCED RECOVERY WITH MOBILITY AND REACTIVE TENSION AGENTS

C. J. Radke and W. H. Somerton

INTRODUCTION

Significant amounts of acidic California crude oils remain trapped after waterflooding to high water/oil ratios. Because surface-active materials can be generated in-situ by the reaction of bases with acid-containing oils, the use of high pH waterflooding is economically attractive compared to conventional surfactant-polymer flooding. Actual field applications of flooding with aqueous bases, however, are limited partly because laboratory work has indicated diverse results both in terms of the ulimate recovery attainable and the governing principles. Separate laboratory studies have suggested that the mechanisms of ultralow interfacial tensions, wettability reversal (oil-wet to water-wet or water-wet to oil-wet) and spontaneous or shear emulsification with subsequent pore blockage, coalescence or entrainment may all be involved in reactive tension flooding. Flooding efficiency is sensitive to the chemistry of the oil and connate water, to the physics and chemistry of the reservoir rock, and to the specific flooding conditions such as rate, temperature, and secondary or tertiary mode. Consequently, studies done on different systems under different conditions can yield widely divergent views of the reactive tension flooding process. The lack of a coherent picture of high pH flooding impairs progress toward possible improvement and successful field applications.

The objectives of the present study are: (1) to ascertain the tertiary-mode efficiencies of flooding acidic California crude oils with dilute aqueous bases, and (2) to devise laboratory screening tests which elucidate the governing recovery mechanisms and permit development of an improved mobility-reactive tension agent flooding package. The project, which commenced in July 1976, involves studies on recovery mechanisms, displacement theory, interfacial tensions and charges, spontaneous emulsification, emulsion stability, and emulsion rheology.

PRESENT WORK AND ACCOMPLISHMENTS

A constant-rate linear displacement apparatus has been constructed which permits monitoring of pressure drop, electrical resistivity, streaming potential, and pH in addition to flowing oil and water fractions in cores up to three feet in length over a wide range of flow rates. The entire apparatus is thermostated in an air bath and provision has been made to permit testing under anaerobic conditions so that field conditions can be simulated. Initial studies have begun with model systems of mineral oils, alkyl-aryl and alkyl carboxylic acids, caustic, and Ottawa sand. When carboxylic acid-containing oils are neutralized with caustic, the liquid-liquid interface spontaneously erupts into a highly stable emulsion. However, when the carboxylic acids are neutralized by caustic in the aqueous phase, prior to contact with oil, no spontaneous emulsification occurs. Thus it is possible to establish the importance of mass transfer and spontaneous emulsification in the oil displacement process relative to capillary forces in chemical systems of identical equilibrium properties. Preliminary results with oleic acid in mineral oils displaced by dilute aqueous sodium hydroxide from one foot long 600 mD Ottawa sand cores indicate a considerable permeability reduction due to stable emulsion formation and a mobilization of residual oil in the tertiary mode. Relative permeabilities, obtained from the classical Buckley-Leverett treatment, demonstrate a water-wet core, and since flooding is performed at low capillary numbers (less than 10^{-4}), the ultralow

tension displacement mechanism is not operative. High-purity oxygen-free chemicals and careful cleaning of the core and apparatus are required to obtain reproducible quantitative displacement results.

PLANNED ACTIVITIES FOR 1977

Dynamic displacements with well characterized chemical systems will be continued including studies on the effect and scaling of the linear flooding rate and the role of the porous medium morphology and surface chemistry. Dynamic pressure drops, electrical resistivities, streaming potentials, and flow visualization will aid interpretation of the reactive tension agent flooding mechanisms. Recovery efficiencies of promising California crude-oil-- connate-water-- preserved-core systems will be examined under an anaerobic environment and at elevated reservoir temperatures. Interfacial tensions (spinning drop) and charges (microelectrophoresis) will be measured to provide correlative tools and to investigate means for establishing ultralow tensions in these systems. Rheology and stability of high pH emulsions in porous media will be studied to establish their mobility control and conformance characteristics.

FERMENTATION TECHNIQUES FOR PRODUCTION OF ETHANOL

G. Cysewski and C. R. Wilke

Ethyl alcohol is of considerable interest as a potential liquid fuel. Studies are in progress in this laboratory on the production of sugars from agricultural residues and other cellulosic wastes as a raw material for conversion to ethanol.

During the past year experimental research and a process design study of ethanol fermentation was completed.[1] The aim of the study was to develop and evaluate new fermentation technology for the production of ethanol. Using glucose as the fermentable substrate, optimal fermentation parameters of pH, temperature, oxygen tension, and sugar concentration were determined in both batch and continuous culture. The experimental results indicate that although ethanol fermentation is an anaerobic process, trace amounts of oxygen are required for maximum ethanol production. The ethanol productivity of the initial culture of Saccharomyces cerevisiae (ATCC #4126) was optimal at an oxygen tension of 0.7 mmHg and a temperature of 35 °C. However, when long term continuous culture was maintained the yeast "adapted" after 3 weeks of operation, requiring an oxygen tension of only 0.07 mmHg for optimal ethanol production. Continuous ethanol production by the "adapted" yeast was found to be 43% higher than for the "unadapted" yeast under conditions of complete substrate utilization. The pH of the broth had only a slight affect on fermentation rates between 3.5 and 5.5. However, the sugar concentration did affect ethanol productivities in continuous culture, with the optimal concentration being 10 wt% sugar, as shown in Fig. 1.

A cell recycle system employing an external settler to increase the biomass concentration in continuous fermentations was examined. The results of the recycle experiments are shown in Fig. 2. The cell mass concentration was increased fourfold in the recycle system over conventional continuous operations. This produced a corresponding fourfold increase in ethanol productivity.

In addition, a novel vacuum fermentation scheme was developed whereby ethanol was boiled away from the fermentation broth as it was produced. Vacuum operation was necessary to achieve boiling at temperatures compatible to the yeast. Since ethanol was removed from the fermenting broth as it was formed, ethanol inhibition was eliminated permitting solutions at high sugar concentration to be fermented. A sevenfold increase in ethanol productivity over conventional continuous operation was obtained in the vacuum system when a 33.4% glucose solution was fermented. As illustrated in Fig. 3, by combining the vacuum fermentation with cell recycle, yeast cell densities of 124 g dry wt/l were achieved resulting in a 14-fold increase in ethanol productivity over a simple continuous operation.

From the experimental results obtained, preliminary process designs and economic evaluations of industrial scale ethanol plants were made employing the various fermentation techniques.

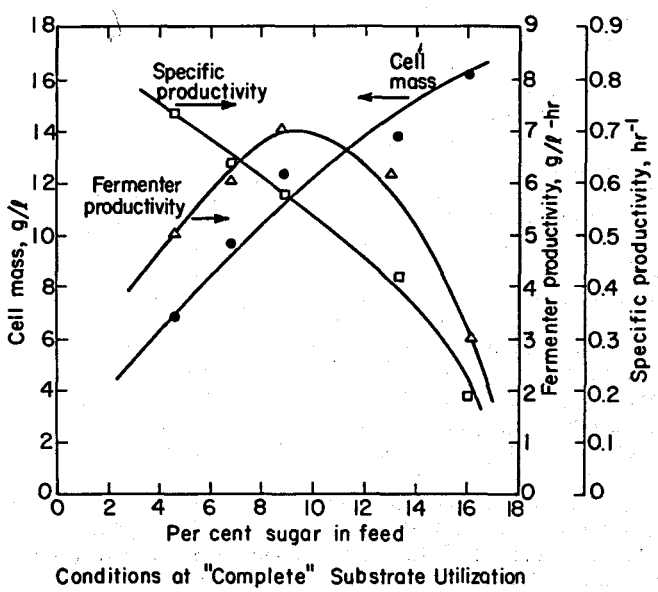

Fig. 1. Effect of feed sugar concentration on ethanol production and cell mass in continuous fermentation. (XBL 7511-9420)

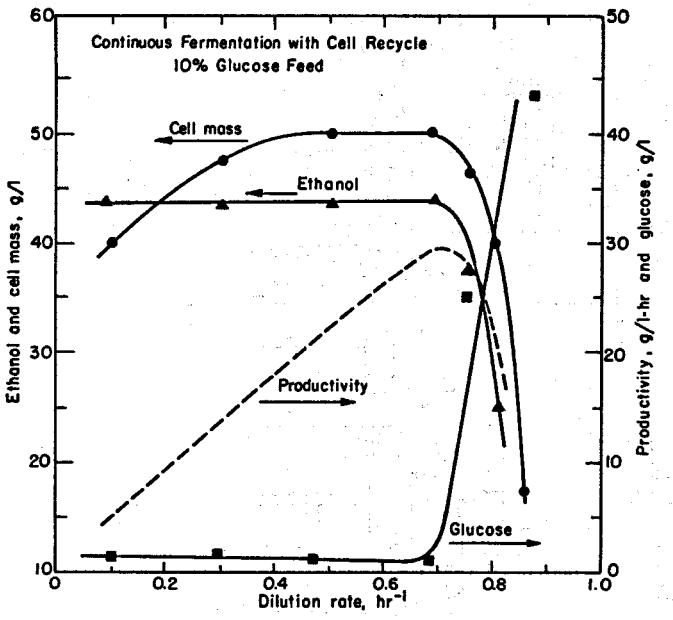

Fig. 2. Effect of increasing cell density by use of recycle in continuous fermentation. (XBL 761-6352)

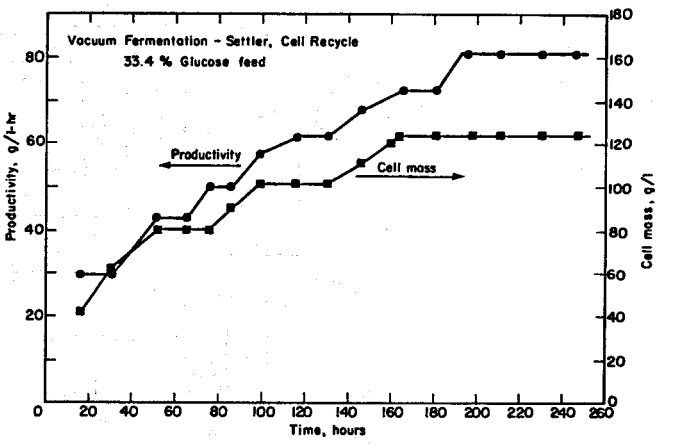

Fig. 3. Effect of increasing cell density by use of recycle in vacuum fermentation. (XBL 761-6165)

These design studies indicated that over a 50% reduction in capital expenditure may be obtained by continuous rather than batch fermentation. Further reductions in investment and operating costs were indicated for both the cell recycle and vacuum systems.

REFERENCE

1. G. R. Cysewski and C. R. Wike, Fermentation Kinetics and Process Economics for the Production of Ethanol, LBL-4480 (1976).

PRELIMINARY ASSESSMENT OF THE PRODUCTION OF ETHANOL AND SINGLE-CELL PROTEIN FROM CELLULOSE

C. R. Wilke, G. R. Cysewski, R. D. Yang, and U. von Stocker

An integrated processing scheme has been proposed based on previous studies in this laboratory of the enzymatic hydrolysis of newsprint to sugars[1] and their subsequent fermentation to ethanol and yeast cake.[2] Ethanol production from cellulose is attractive since it is currently made from petroleum based ethylene.

Figure 1 is a schematic flow diagram for the processing scheme.

Data for the sugar production section are summarized in Table 1 below.

The sugars from the hydrolysis section are concentrated to 14.3% in a seven effect evaporator and distributed to five continuous fermentors. Yeast is recovered by centrifugation and spray-dried. The 4.9% ethanol solution from the fermentor plus the aqueous stream containing the alcohol removed from the carbon dioxide are concentrated by distillation to produce 81.5 tons/day of 95% ethanol, equivalent to 25.2 gal/ton of plant feed; 16.6 tons/day of yeast are recovered from the still bottoms.

Following yeast removal, the bottoms stream from the ethanol distillation containing the hemicellulose sugars and residual glucose at 4.6% concentration and are supplied to the fermentation process to produce 32.8 tons/day of torula yeast.

A total of 132,000 lb steam/hr and 12,800 kW of electricity are produced in the combustion system of which 4,000 kW are in excess of the process requirements.

Table 1. Design specification for sugar production

Feed (-20 mesh newsprint)	885 tons/day
Cellulose content[a]	61% (dry)
Enzyme activity	3.5 FPA
Cellulose hydrolysis	50%, 40 hr, 45°C
Enzyme recovery	43%
Product (as glucose)[b]	238 tons/day
Cell recycle fraction	0.65

[a]Assumed newsprint composition: 61% α cellulose, 21% lignin, 16% hemicellulose, and 2% other.

[b]Representative sugar composition: 72% glucose, 22% cellobiose, 4.4% xylose, 1.5% mannose.

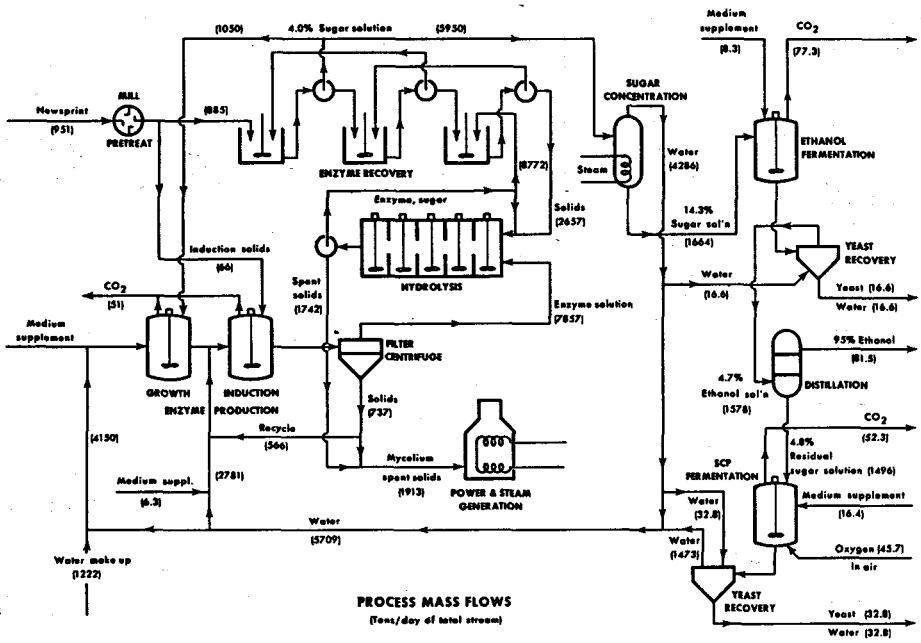

Fig. 1. Material balance flow diagram for integrated processing scheme. (XBL 762-2330)

Table 2.. Product summary and overall cost analysis

	Tons/ day	Unit	Production cost (¢/unit)	Assumed market value (¢/unit)	By-Product cost credit per gal ethanol (¢)
Ethanol (95%)	81.5	gal	105	—	—
Carbon dioxide	113.0	—	—	—	—
Yeast cake	16.6	lb	—	30	40
Torula yeast	32.8	lb	30	30	—
Electricity	—	kWhr	1	2	4

A very approximate cost analysis shown in Table 2 indicates that, exclusive of any cost for waste newsprint, it might be possible to produce 95% ethanol for 61¢ per gallon after a 44¢ credit for by-produce yeast and power. The capital investment is estimated at $33.4 million. However, it must be recognized that many uncertainties exist in the assumptions made, and that pilot plant studies will be essential to establish processing costs firmly and to assess potential operational problems.

REFERENCE

1. C. R. Wilke, Ren Der Yang, and Urs von Stockar, Biotechnol. Bioeng. Symposium No. 6, (Elmer L. Gaden, Ed., John Wiley & Sons, New York, NY 1976).

STUDIES OF LIGNIN-DEGRADING FUNGI AND ENZYMATIC DELIGNIFICATION OF CELLULOSIC MATERIALS

P. A. Carroad* and C. R. Wilke*

During the last year preliminary studies of lignin-degrading fungi and enzymatic delignification of cellulosic materials were completed. It was clearly demonstrated that delignification greatly enhances the rate of enzymatic cellulose hydrolysis by Trichoderma viride cellulase. Microbial delignification can be accomplished with any of several white-rot fungi in solid culture. Liquid culture, however, was found to be an inappropriate technique.

Groundwood was chemically delignified to various lignin contents by oxidation with sodium chlorite in acetic acid. The delignified groundwoods

were enzymatically hydrolyzed by T. viride cellulase for forty hours. Figure 1 shows the hydrolysis curves for the delignified groundwood, monitored as reducing sugar concentration in solution. It can be seen that delignification increased not only the rate of hydrolysis, but also the extent of hydrolysis by making more cellulose available for enzymatic attack. The relationship between the percent digestibility of cellulose by T. viride cellulase and the percent lignin in the groundwood sample for a forty hour hydrolysis is shown in Fig. 2. Figure 3 shows that chemical delignification results are related to those for microbial delignification. Chemical delignification followed by T. viride cellulase digestion of cellulose is similar in percent digestibility to microbial or chemical delignifications followed by bovine rumen fluid digestion. It is apparent that the method of delignification is not critical.

Microbial delignification was successfully achieved by culturing the white-rot fungi Polyporus versicolor, Sporotrichum pulverulentum, and Pleurotus ostreatus, directly on groundwood for seven weeks. Table 1 lists the results. The percentage losses of lignin ranged from three to eleven percent, Pl. ostreatus being the most active delignifying organism. Liquid culture of the fungi on groundwood substrate was not successful, presumably due to the dilution of secreted lignin-degrading enzymes. Based upon literature results of solid culture delignification, a composting scheme for large scale microbial delignification was designed. A delignified cellulosic material would be an especially advantageous substrate in a recycle system for cellulase production. An economic analysis showed, however, that the added costs of microbial delignification would not be offset by the associated decreased costs in cellulase enzyme production.

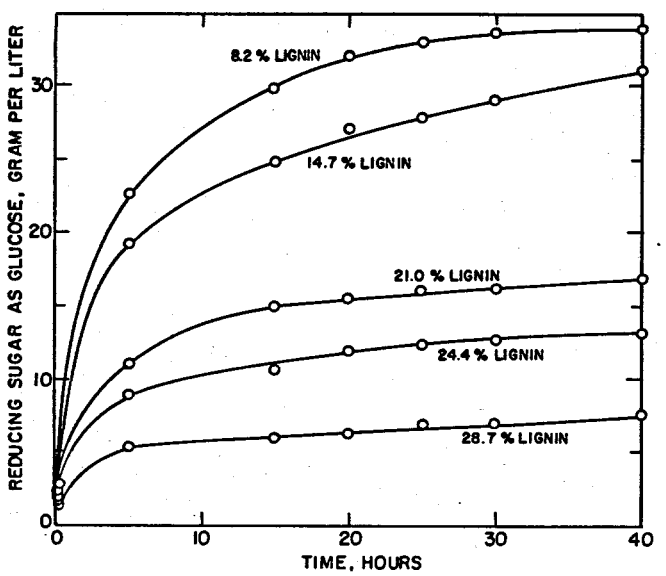

Fig. 1. Hydrolysis curves of delignified groundwood. (XBL 761-6148)

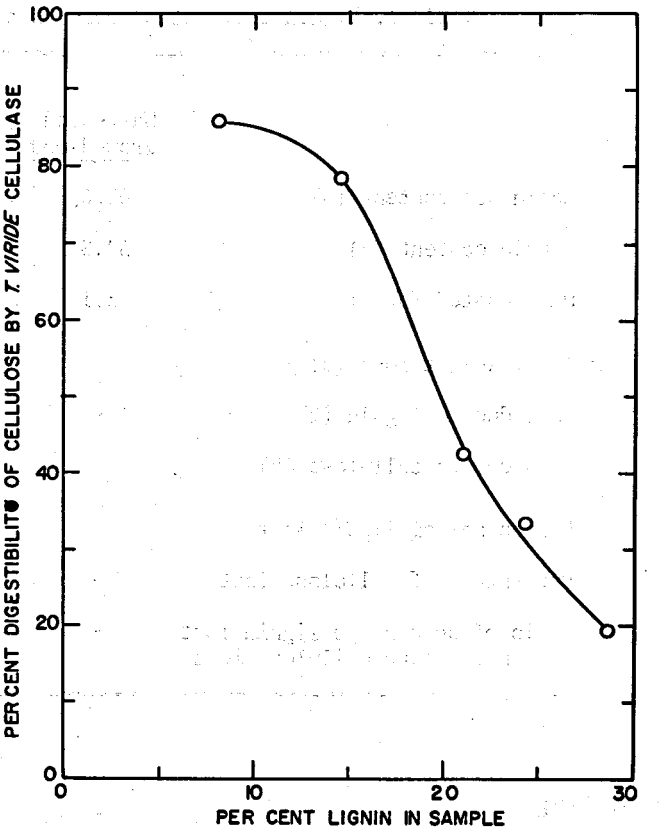

Fig. 2. Relationship between lignin content and cellulose digestibility by microbial cellulase. (XBL 761-6149)

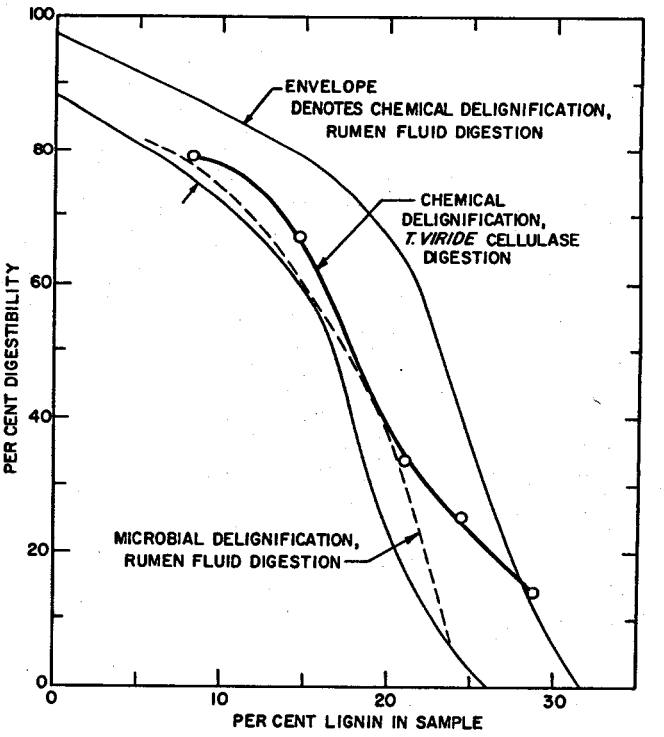

Fig. 3. Composite of relationships between lignin content and digestibility of wood. (XBL 761-6146)

Table 1. Lignin degradation results of organisms growing directly on groundwood

	Untreated groundwood	Groundwood after 7 weeks degradiation by fungi		
		P. versicolor	Sp. pulverulentum	Pl. ostreatus
Cellulose content (%)	62.6	59.5	54.8	61.2
Lignin content (%)	34.3	38.1	41.8	34.7
Unaccounted for (%)	3.1	2.4	3.4	4.1
Total weight loss (%)	-	10.2	10.0	11.1
Loss due to lignin (%)	-	2.9	1.0	3.8
Loss due to cellulose (%)	-	7.3	9.0	7.3
Percentage of lignin lost	-	8.4	2.9	11.0
Percentage of cellulose lost	-	11.7	14.3	11.9
Ratio of percentage lignin lost to percentage cellulose lost	-	0.7	0.2	0.9

FOOTNOTE

*Lawrence Berkeley Laboratory and Department of Chemical Engineering, University of California.

Engineering Sciences Program

INTRODUCTION

The Engineering Sciences program focuses specialized engineering resources from both the Lawrence Berkeley Laboratory and the University of California campus onto certain energy and environment-related problems. At present, emphasis is placed on problems in two areas – transportation and earthquake studies.

In the Transportation Studies area, two projects are under way. One of these, Mass Transit Analysis, is concerned primarily with studies of the Bay Area Rapid Transit District (BART) equipment and operations. These studies are to provide an independent appraisal of the operational capability, reliability, and safety of the transit system. Certain critical areas have been identified. Task forces have been organized to study these areas, make recommendations, and, in some cases, participate in the design of improved components and facilities.

The second transportation project is the Roadway Power System for Full-Performance Electric Cars. In this project, a method is being investigated to safely, efficiently, and economically transfer power to personal automobiles while they are traveling on highways. The purpose is to make the use of electric vehicles a practical reality, and to aid in reducing reliance on gasoline powered vehicles.

The Earthquake Studies area also has two projects. The first is concerned with a long-standing problem, namely, how to predict the occurrence of earthquakes. In this project, a potential method for predicting earthquakes through electrical resistivity methods is being investigated. Field experiments in the Hollister area are being set up to study the feasibility of the method.

In the second earthquake project, the design techniques used to provide the earthquake resistance of components for nuclear power plants are being studied through theoretical analysis and through experiment using the Earthquake Simulator at the UC Earthquake Engineering Research Center. The object is to improve the state-of-the-art of these design techniques. Such improvements will facilitate the process of evaluating the seismic qualities of proposed power plant structures while they are still in the design stage.

These projects are individually described in more detail in the following articles: (1) Mass Transit Analysis, (2) Roadway Power System for Dual Mode Electric Transportation, and (3) Earthquake Prediction.

MASS TRANSIT ANALYSIS*

D. T. Scalise, F. A. Kirsten, V. P. Elischer, K. P. Ang, A. A. Arthur, D. Bereznai, J. G. Bolger, M. Graham, R. LaPierre, R. Louis, F. Olken, R. F. Thomas, D. B. Turner, H. Vogel, K. Wiley

INTRODUCTION

The goals of the LBL Rapid Transit Study Program are to make an independent evaluation of the Automatic Train Control (ATC) systems currently in use and to engage in the investigation and design of such systems in order to improve their effectiveness, safety, and reliability.

LBL's association with the rapid transit industry began in 1974 when the California Public Utilities Commission (PUC) and the Bay Area Rapid Transit District (BART) came to an impasse over certification to begin full operation. The chairman of the State Senate Committee on Public Utilities, Transit and Energy asked LBL to give technical advice on BART's readiness to begin safe service and on the impact of the safety problems. The BART District also asked LBL for technical help in the process of improving the reliability of BART's ATC system.

As a result, work in this area is now funded through agreements with both the State Senate Committee and BART. The work with the Senate Committee is intended to help provide them with the technical information and opinions necessary in the process of formulating legislation concerned with BART. The work with BART is directed toward technical study and design problems which directly concern the operational integrity and the ultimate completion of the system.

ACCOMPLISHMENTS DURING 1976

State Senate Committee

The work under the LBL/Senate agreement has continued to be concerned mainly with monitoring, evaluating, and reporting the progress of the BART system. A report on this activity was prepared[1] for discussion at the April 6, 1976, hearings on BART by the Senate Committee. Two of the recent LBL activities covered in this report were:

(a) Safety, including continuing work on the Sequential-Occupancy-Release (SOR) system for achieving close-headways operation;

(b) Follow-up on certain "Unusual Occurrences,"

including the determination of whether the proper methodology was used in analyzing the applicable operating rules and procedures.

A study of a method of measuring the System performance of BART was also made. This method is unique in that it considers performance from the point of view of passengers – i.e., occupancy factor of the trains, deviations from expected trip times, etc. – rather than in terms of equipment utilization.

The Laboratory and the group that has been involved in this work was honored on January 14, 1976, when the Rules Committee of the California State Senate passed a resolution[2] commending the work that has been accomplished.

BART

The work under the LBL/BART agreement has been directed toward a number of technical areas. Five of these areas are briefly discussed below.

Computer Systems. In the BART system, 13 separate computer systems are used in a variety of applications, ranging from Central Train Control to cash handling. Since the operations of BART critically depend on these computer systems, the costs and resource requirements to support them and their operating effectiveness over the long term are of utmost concern. In order to identify problems associated with the existing systems and to formulate recommendations for computer system planning, a study was undertaken jointly by LBL and BART. The results of the study are reported in reference 3.

Some important conclusions were derived, which have very strong implications regarding the future plans of the system. It was concluded that serious problems exist with respect to the Central Train Control Computer system. For example, it was determined that, even with substantial modifications, it will still not be adequate to support the level of operations which the system was intended to achieve. It was also determined that the 13 computer systems lack adequate flexibility to accommodate changes in system operation. They were designed as isolated entities; program design and information transfer between systems are hampered by lack of a common data base, and by the use of non-standard communication protocol and data recording media.

The study resulted in a number of recommendations, the most far-reaching of which are: (a) to commence design of a replacement for the Central Train Control Computer system; and (b) to begin planning to provide systematic integrated control over the real-time computer systems used by the transit district.

Toward the end of 1976, a program to implement the report's recommendations was begun.

Performance Measurement Study. The automated nature of the BART system provides for the collection of a large amount of data, which presents a unique opportunity to develop a model for evaluating performance of the system. Such a model was developed by using train logger and Fare Data Acquisition System (DAS) data. The train logger data provide a history of all train movements on the BART system. The DAS data provide a history of passenger movements, specifically the points at which each passenger enters and exits the system, and the time of arrival at destination. An algorithm was developed to merge the two data sets to calculate a number of passenger-related parameters, such as, for example, the load factor of every segment of every train trip.

Maintenance Vehicle Detection System. As a standard operational procedure, maintenance vehicles of various types must have access to the tracks and right-of-way of the transit system. Many of these vehicles are normal highway-type vehicles, which are adapted to travel on the rails. Such vehicles, however, do not interact with the normal train detection and control system. Therefore, special procedures are necessary to permit them to be used safely.

This year, work on the Maintenance Vehicle Detection System (MVDS) was nearly completed. This system, designed at LBL, provides a high measure of safety in the use of maintenance vehicles. The system includes procedures and protocol for the movement of the vehicles. Most important, it provides a special set of electronics on each vehicle to interact with the train control system. As a result, each maintenance vehicle is protected by a barrier of "zero-speed commands," which will stop any train long before collisions with maintenance vehicles are imminent.

Close Headways. One of the near-term goals for BART is to increase the frequency of train service. This requires operating trains with closer headways (i.e., less distance between successive trains). During 1976, LBL has assisted in the planning and carrying out of test programs to determine the worst-case stopping distance of trains. This distance is a function of a number of parameters, including the reaction time of control systems, speed of the train, and track adhesion. The programs included a review of the original design criteria, a review of existing data on deceleration of trains in revenue service, a review of existing literature on wheel-to-rail adhesion, and additional monitoring of actual braking performance of vehicles in revenue service.

Propulsion Equipment. The propulsion equipment (motors and motor controllers) has been a major source of failures in the system. Many failures are precipitated by flashovers (arcs) in the commutator region of the motor. This year LBL has participated in the work to analyze the conditions under which flashovers occur and to design means of alleviating the problem. These have included: modifications of the motor control circuitry; improved insulation; and the design of air flow diverters to purge the air in the region of the commutator. As a result of these modifications, the incidence of motor flashovers has been reduced. They have also contributed to a significant increase in car availability.

PLANNED ACTIVITIES FOR 1977

A major effort will be expended on the computer system redesign effort. The first step will be an exhaustive analysis of the various computer systems and communication pathways in the existing system.

An emphasis will also be placed on the design of test procedures and equipment for the train control system and the propulsion equipment. The purpose is to improve the capability to detect incipient failures and marginal operation of components which could affect the reliability of system operation.

FOOTNOTE AND REFERENCES

*This work was supported by the State of California Senate Committee on Public Utilities, Transit and Energy and by the San Francisco Bay Area Rapid Transit District.

1. A Technical Overview of BART Operations and Programs, LBL Report UCID-3838 prepared for the State of California Senate Committee on Public Utilities, Transit and Energy, April 5, 1976.

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3. Long Range Report on BART Computer Systems, Joint Study Group of Lawrence Berkeley Laboratory and Bay Area Rapid Transit District, August 1976, UCID-3856.

ROADWAY POWER SYSTEM FOR DUAL MODE ELECTRIC TRANSPORTATION (DMET)

J. G. Bolger, D. T. Scalise, F. Kirsten, F. Voelker, J. Cox

INTRODUCTION

For many years, the battery-powered electric vehicle has been studied as a potential means of alleviating the well-known problems of petroleum-fuel scarcity, pollution, etc., which are associated with gasoline powered vehicles. However, the practicality of the electric vehicle as a general solution to these problems is still hampered by its restricted range and performance.

The Roadway Power System for Dual Mode Electric Transportation (DMET) is a concept aimed at solving this problem by removing those limitations. In this concept, a skeletal network of electrically powered highways permits a continuous flow of power to vehicles which are designed for two modes of operation: In one mode, they acquire operating power from the roadway and thus have unlimited range at freeway speeds; in the other mode, they use power from an on-board energy storage pack (e.g., batteries), and thus have complete freedom to operate locally on conventional roadways at lower speeds.

The central feature of the DMET system is a continuous electromagnetic power "source" installed in the center of arterial roadway lanes. The source conductor, shown in Fig. 1, carries an alternating current. The magnetic flux generated by this current is coupled via a magnetic circuit to the moving vehicle. This structure can provide not only sufficient power to propel vehicles at highway speeds, but also additional power for replenishing the stored energy in the batteries (or flywheel) which the vehicles will carry. Roadside power supplies spaced at intervals of one or two miles will receive electric power from electric utilities and supply a constant amplitude alternating current to the roadway sources.

Vehicles will carry a suspended power "pickup" whose magnetic core has poles aligned with that of the power source, also as shown in Fig. 1. The magnetic flux induced by the source current links the pickup winding and the source conductor; by the resulting transformer action, power is transferred from highway to vehicle.

The support of this program by the Division of Transportation Energy Conservation of the Energy Research and Development Administration commenced in 1976.

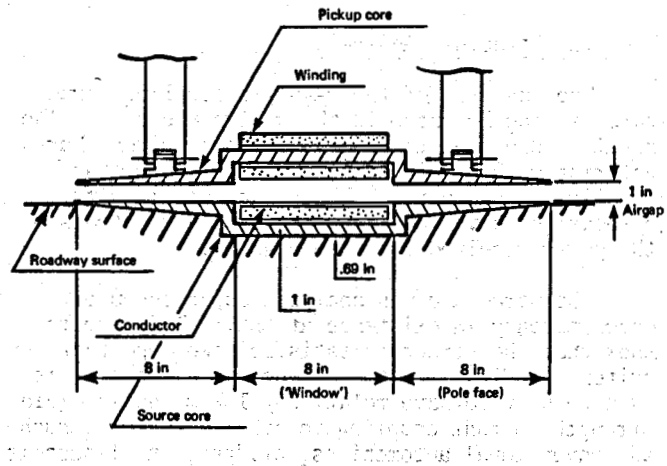

Fig. 1. Cross section of magnetic coupling chosen for preliminary design study. The "source" is imbedded in the roadway, flush with the surface; the "pickup" is suspended from the moving vehicle. The magnetic circuit includes the air gap. (XBL 773-655)

ACCOMPLISHMENTS IN 1976

The efforts during 1976 included a preliminary engineering design study and technical analysis of a complete system.[1] The specifications for the study system were formulated by making engineering estimates of the fundamental parameters of the system. Using these parameters, a rough design of each of the major components was derived. The broad purpose of the study was to:

(a) Provide documentation to show that the concept is fundamentally sound;

(b) Show that it does not depend on engineering breakthroughs; i.e., it can be constructed using current technology;

(c) Obtain rough cost estimates.

The values assumed for the study are listed in Table 1. During subsequent phases of the work, the individual parameters will be optimized, and the designs refined. Results in five areas of this study are first summarized below; then the conclusions are given.

TABLE 1. Assumed values of parameters used in preliminary design study.

Parameters	Assumed values
Geometry of magnetic coupling	As shown in Fig. 1
Maximum power to be transferred to vehicle (passenger car)	20 kilowatts
Current in source conductor	1000 amperes
Frequency of source current	180 hertz
Maximum highway loading	100 cars/mile

Magnetic Structure Analysis

The analysis of the magnetic coupling structure was the key step in the design exercise. The results were used to determine the required characteristics both of the power conditioner that supplies power to the highway, and of circuitry on-board each vehicle that accepts and controls the power received from the highway.

The structure was analyzed using computer codes already in existence at LBL.[2] The results show that the structure satisfies two important criteria. First, in the absence of a vehicle, it is necessary to have relatively low magnetic field strength so that coupling to other structures such as conventional automobiles, bridges, and fences is minimal. This "unloaded" field strength was found to be only about 10 gauss. Second, the coupled field strength, when source and pickup are meshed, must be high enough to achieve the required level of power transfer.

The magnetic analysis also provides data which permit calculation of the equivalent circuit of a segment of highway, with and without vehicle loading. A simplified form of the circuit consists of a series combination of resistance and inductance, the values of which vary with the vehicle loading. Table 2 tabulates some of these values for a one-mile section of powered highway, together with derived values of power input, efficiency, and power conditioner output voltage.

Power Conditioner

The power conditioner receives power from the electric utility at the usual 60-Hz frequency, and converts this to 180-Hz power for the highway. As shown in Table 2, a conditioner for one lane-mile of highway would have a capacity of 2 MW, and would supply 1000 A of 180-Hz current at 2000-3000 V. Since the power factor of the highway changes with loading, the voltage that the power conditioner must supply stays relatively constant.

It was determined that the cycloconverter concept could be applied to design a power conditioner to meet these requirements. The use of this concept is practical, not only in terms of its reasonable cost, but also because it can be built with currently available components. A low-power prototype of the cycloconverter was built and behaved according to expectations.

Vehicle Controls

The circuitry that will be used on board the vehicle was investigated sufficiently to demonstrate that enough power (at least 20 kW) can be transferred to the moving vehicle, and that the level of power can be controlled at the vehicle with relative ease.

Power Interfacing

Discussions with Pacific Gas & Electric Company representatives established that sufficient utility capacity to power a freeway system in the San Francisco Bay Area is available. This power is available at convenient points along the existing system.

Roadway Roughness

The practicality of an air gap of the order of one inch between source and pickup was verified in two ways. First, the California Department of Transportation provided data resulting from roughness measurements on a typical California freeway. Second, a test fixture was constructed and mounted below a passenger car. With this fixture, the maximum values of highway roughness encountered during several runs on local highways were measured. Both sets of data indicate that a gap of about one inch is feasible. Furthermore, temporary variations in air gaps are acceptable since only the time-average value of the gap determines the energy transfer efficiency.

Conclusions

The results of this preliminary study confirmed

TABLE 2. Characteristics of powered-highway source derived from magnetic circuit analysis, and based on assumed parameters of Table 1. All figures are for one lane-mile of highway.

Number of vehicles, each drawing 20 kw of power	0	5	50	100
Equivalent circuit values of loaded source:				
Resistance, R (ohms)	0.019	0.12	1.07	2.1
Inductive reactance, X (ohms)	2.3	2.3	2.2	2.1
Impedance, $(R^2 + X^2)^{\frac{1}{2}}$ (ohms)	2.3	2.3	2.44	2.97
Current in source conductor (amps)	1000	1000	1000	1000
Voltage necessary to drive source current (volts)	2310	2300	2440	2970
Input power to source (kilowatts)	19	124	1065	2112
Power absorbed by vehicles (kilowatts)	0	100	1000	2000
Efficiency (%)	0	80.8	93.9	94.7

that the concept can be implemented using known engineering techniques and available components. On the basis of the study, it is estimated that the construction cost of the roadway power system would be approximately $300,000 per lane mile; that the amortized installation cost per vehicle mile for an expected 20-year life span is less than a half cent; and that the cost of operating roadway-powered vehicles is less than the cost of operating either battery-powered vehicles or conventional gasoline-powered vehicles.

PLANNED ACTIVITIES FOR 1977

During 1976, the design and analysis efforts were based on certain engineering estimates for various parameters. These estimates were necessary to provide a basis for the preliminary round of investigation.

During 1977, efforts will concentrate on refining and optimizing these parameters. This will include:

(a) Frequency optimization – to assess the effects of operating frequency (originally chosen as 180 Hz) on the cost and efficiency of the system. Other effects such as induced interferences and parasitic losses in nearby structures will be investigated.

(b) Magnetic coupling configuration – to investigate the effects of coupling geometry on costs, fabrication considerations, and tolerance for misalignment of source and pickup.

(c) Construction techniques for magnetic coupling – to investigate the various available options for fabrication of low cost, low loss coupling components. Items to be considered include core and conductor materials, electrical insulation, and mechanical protection.

(d) Power conditioner design – to assess the design trade-offs in the design of power conditioners.

(e) Loading effects – to study the effects of rapidly changing vehicle loading due to speed changes or traffic interruptions.

In addition, communications with various local, state, and federal agencies, utilities, and other organizations that might be involved in the implementation of a DMET system will be continued.

When these studies have reached an appropriate point, work will begin on the design and construction of an engineering prototype of the system. This will include construction of a short section of source with power conditioner, a skeletal vehicle chassis with a suspended power pickup, and provisions for the necessary instrumentation. This prototype will be primarily used to verify the design work up to this point.

REFERENCES

1. Roadway Power System for Full Performance Electric Vehicles, preliminary draft reports ELN-53 (Volume I, General) and ELN-54 (Volume II, Technical), September 30, 1976.

2. The computer code POISSON was used. This is described in: K. Halbach, A Program for Inversion of System Analysis and Its Application to the Design of Magnets, UCRL-17436, July 1967.

EARTHQUAKE PREDICTION: IN-SITU STRESS MONITORING – RESISTIVITY*

W. E. Farrell, H. F. Morrison, R. Fernandez

INTRODUCTION

This project is a continuing experimental study of high accuracy measurement of the electrical resistivity of the earth. Its object is to develop measuring apparatus and techniques which are sensitive to changes in resistivity as small as 1 part in 10^5. If such measurements prove feasible, then future work will be the geophysical interpretation of data collected from a variety of field areas.

Our primary goal is the use of resistivity as a way of remotely sensing changes in stress within the shallow parts of the earth's crust. This has been an active field of research in the USSR for many years, but it is only now receiving attention in this country. Several models have been proposed to explain the coupling between stress and resistivity, but the emphasis has been to explain well-controlled laboratory experiments, rather than field observations. This is because noise signals in the field situation have up to now limited field measurements to about 1% accuracy.

The major goal of this research on the measurement and interpretation of small variations in resistivity is the search for earthquake precursors. If the goal is attained we visualize this method as one tool for detecting possibly hazardous stress buildup near major engineering structures (power plants, dams, urban areas, etc.).

ACCOMPLISHMENTS DURING 1976

Entering this second year of the project we primarily conducted feasibility studies, apparatus design, and laboratory testing.

The proposed goal of building and deploying a resistivity variometer has been attained. A complete description of the apparatus, and of the laboratory test and field experiments, is contained in the summary report[1] issued in December 1976. The variometer has continued to provide data since it was installed at the UC Berkeley Richmond Field Station in November 1976. Our preliminary field observations from 2½ months of operation are the following:

(a) During the daytime, man-made noise signals limit the sensitivity to variations in resistivity of 1 part in 10^3 rms in the frequency band 0 to 0.01 Hz. The noise seems to have a wide spectrum.

(b) During the early morning hours and weekends, the noise is an order of magnitude less.

(c) We have observed on several occasions diurnal fluctuations in resistivity of about 2×10^{-4} peak-to-peak. This is possibly related to temperature changes in the ground, but we cannot absolutely rule out instrumental effects.

(d) During several rainstorms, there were changes in resistivity of about 1 part in 10^3. The resistivity increases slightly at the beginning of the rainfall, decreases as the ground becomes wet, and then rises again as it dries out.

Our conclusions are as follows:

(a) The electrode geometry presently used limits our depth of investigation to about 30 m. This is enough to sense resistivity in the superficial alluvium only, not in the bedrock below.

(b) We have not interpreted the geophysical signals observed, but we believe they represent consequences of thermal and moisture effects, and are not stress-induced effects.

(c) Even if we employ sophisticated signal detecting techniques, the measurement of resistivity variations of 10^{-5} in an urban area will be difficult. We do not yet know the possible limitations due to naturally occurring telluric currents.

PLANNED ACTIVITIES FOR 1977

Because of the need for measurements in urban areas, we plan to attempt to reduce the noise signals by sensing them some distance away from the variometer and correcting the data for their influence. On the basis of this year's study we will include design improvements in a new system to be constructed in the summer of 1977. A digital data recording system will be installed to facilitate the collecting and processing of the observations. Finally, we will set up the present equipment near Hollister, a well-instrumented earthquake-prone region.

FOOTNOTE AND REFERENCE

*This work was supported by the U.S. Nuclear Regulatory Commission through the U.S. Energy Research and Development Administration.

1. In situ Stress Monitoring – Resistivity. Summary Report on Resistivity Variometer. EQP-38, December 1976.

Energy Use and Conservation Program

INTRODUCTION

Research in the Division's energy use and conservation program addresses a broad range of technical and institutional issues that influence the pattern of energy use. These include basic research into the physics of combustion processes, energy use in buildings, and the analysis of energy conservation strategies and measures.

Work on energy use in buildings has concentrated on two areas:

- Development of CAL-ERDA, a computer program for energy analysis of buildings, which is to be used as a tool for design, research, and the evaluation of compliance with building codes. The program emphasizes ease of input, inexpensive computation, usefulness of output, and flexibility of application.
- Initiation of a national program for energy conservation in windows and lighting. Several projects in this area are under way, including research at LBL on beam daylighting and the thermal performance of window designs, and three projects to be conducted by outside contractors.

During the past year the combustion research program has expanded greatly. Investigators at UC Davis and UC Berkeley have joined with LBL staff to form a combustion research group within the Energy and Environment Division. Among the topics now being studied by the group are combustion at boundary layers, turbulent combustion, lean combustion, the combustion of coal, and the formation of nitrogen pollutants during combustion.

Two projects provided the focus for efforts related to the analysis of energy conservation strategies and measures:

- A workshop on an energy extension service which examined a number of topics related to the development of a service that would provide information and training for energy conservation.
- An energy conservation assessment project which concentrated its efforts on work for the California Energy Resources Conservation and Development Commission. A number of specific energy conservation measures were analyzed to provide information for the Commission's "energy conservation plan."

CAL-ERDA: A NEW COMPUTER PROGRAM FOR ENERGY ANALYSIS OF BUILDINGS

A. H. Rosenfeld, F. C. Winkelmann, Z. Cumali

INTRODUCTION

Energy consumed by buildings and by the activities of the people who live and work in them is a significant portion of the energy required by our energy-intensive modern way of life. Thus energy conservation in buildings can make an important contribution to reducing energy consumption at local, national, and international levels. Saving energy in buildings involves new public policies, codes, and standards for the design of buildings and communities. It requires new design procedures and tools for engineers and architects. It also means careful operation of building energy systems, as well as their careful design.

Until the last few years, the designers of buildings have been without comprehensive tools for calculating dynamic heating and cooling loads, for simulating distribution systems for the heating and cooling of buildings, for modeling the operation of the energy-supplying equipment, and for calculating the life cycle costs of owning and operating energy systems for buildings. Calculation of the response of buildings and building systems to the dynamic variation of loads due to the weather outside and the human activity inside is practical only with the aid of an electronic computer. Those computer programs that have become available have their deficiencies: they have been difficult to use, often inflexible; they have been expensive to run; and they have been limited in scope and generality. Differences in algorithms and assumptions cause different programs to give widely differing results.

Because of this situation, there has been a growing need for an easy-to-use, fast running, completely documented, public-domain computer program for the analysis of energy usage in residential and commercial buildings. The national laboratories desired such a program for use by their technical personnel; the ERDA plant and facilities managers wanted a program to assist them in their energy conservation effort; and because of its responsibility for establishing and enforcing codes and standards, the California Energy Commission wanted a program that could be used by code officials and building designers. The result of this common need is CAL-ERDA, a joint project to write a computer program for the analysis of building energy uses.*

The initial phase of the project, summer 1976 to September 1977, will produce the computer program CAL-ERDA/1.0. This program will run on the CDC 7600 computer at LBL and is intended for technical users at the collaborating laboratories. It will become the starting point of a long-range plan for building energy analysis software, providing a public-domain package with extensive documentation and user support services. Such a package, which will eventually be verified by extensive field testing, will provide a national standard analytical tool for building energy research for design studies and trade-offs and for energy budget calculation for all building classifications proposed in local, state, or national design standards.

PLANNED CAPABILITIES OF PHASE I (CAL-ERDA/1.0)

As a tool for design, research, and code compliance, CAL-ERDA/1.0 emphasizes ease of input, inexpensive calculation, usefulness of output, and flexibility of application.[1] It permits the user to control the amount and detail of input and output at many levels. The system is organized to facilitate the substitution of a variety of program packages to meet the needs of special groups of users. It is designed also to aid fast computation, to permit the addition of new capabilities in future phases of the project, and to be transportable to a variety of computers.

The CAL-ERDA user will be able to describe a building and its HVAC systems, including the plant for supplying the required energy. He will also specify schedules of occupancies, equipment, and lights, the design criteria for the HVAC systems, and the policies controlling the operation of these systems. He can specify the period of analysis and the weather conditions during that period. Then CAL-ERDA/1.0 will compute the heating and cooling loads, simulate the HVAC systems and the operation of the plant, and calculate the first cost, operating cost, and life-cycle cost of the system. Standard output (printed and plotted) will include the thermal loads and energy consumption as functions of time, as well as the above costs. In addition to the standard reports, the user will be able to print or plot the values of other variables from a predetermined list, along with sums and maxima or minima over the period of the analysis. CAL-ERDA will also facilitate parametric runs, varying the building skin, the distribution systems, and the central plant for optimization purposes.

SYSTEM ORGANIZATION

CAL-ERDA/1.0 (see Fig. 1) will provide the user with a Building Description Language (BDL) as a convenient and concise form of input for the definition of the building, the distribution systems, the plant, and other data necessary to analyze energy usage, as well as for control of parametric runs. A Pre-Processor will transform the BDL input into a Standard File containing the data required for execution of the four principal computational programs: Loads, Systems, Plant, and Economic Analysis — known collectively as LSPE.[†]

- The Loads program computes the hourly heating and cooling loads in the building due to weather, occupants, lights, and equipment, using the ASHRAE-recommended algorithms. Loads through walls use the standard response factors of the existing public-domain programs NBSLD

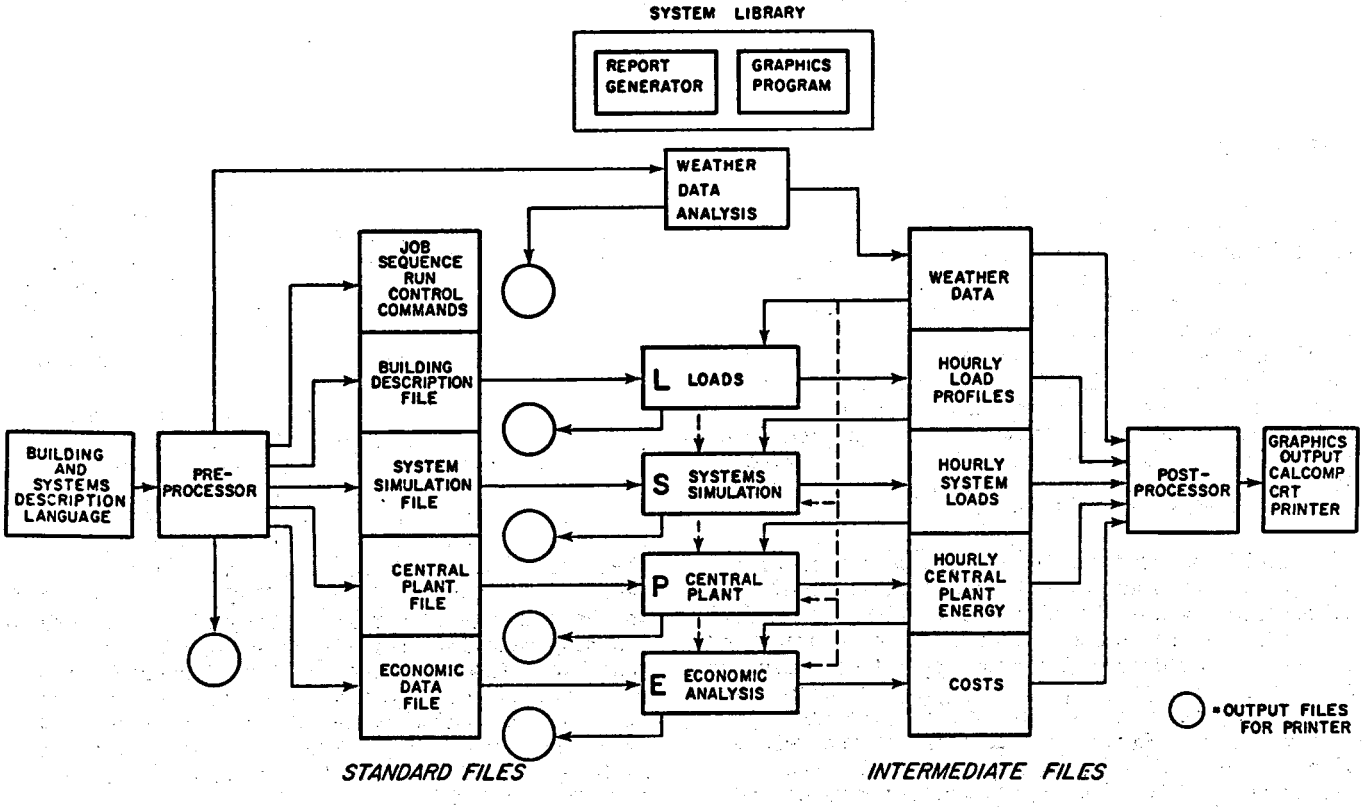

Fig. 1. CAL-ERDA system organization. (XBL 768-3273)

and NECAP. To calculate varying room temperatures, we do not use the complete NBSLD thermal balance method, but instead use the ASHRAE weighting factors which are faster and more accurate than the temperature response approximation used in NECAP.

- The Systems program simulates the operation of one of 16 energy distribution systems, also on an hourly basis.

- The Plant program takes the hourly demands of the building for heating, cooling, and hot and cold water or steam for domestic and process use and allocates the available equipment energy sources (and equipment such as boilers, chillers, and turbines, or utility electric power) so that the demand is satisfied optimally for each hour.

- The Economic Analysis program considers equipment life and frequency of overhauls to compute life-cycle costs for various discount and inflation rates.

Each of these programs writes its results into an Intermediate File, where they are available to subsequent programs. Standard reports are produced by an output module. A separate Report Generator manages output of additional user-specified variables. A Post-Processor plots data to be output graphically.

BUILDING DESCRIPTION LANGUAGE AND COMPONENT PROGRAMS

The incorporation of the Building Description Language is a major advance of CAL-ERDA over its predecessors. This language is command-structured and provides free-format combinations of commands and data. Capabilities included are:

- Forming named groups or collections of elements, such as a room defined in terms of its bounding surfaces;

- Repetition of named groups by noting changes only;

- Nesting to any depth of named groups and elements.

- Dictionary of commands for various operations such as rotation, reflection, scaling, repetition, attachment, partitioning, etc.

- Dictionary of standard items or groups of items with all associated properties built in, such as standard wall types, building types, distribution systems, weather data, etc.

With BDL, the building can be described from two points of view. At the conceptual design level the building is looked upon as a *block*, whereas at later stages of design it is considered to be made up of its *component parts*, such as rooms, wings, etc.

The main new features of component programs and their operation within the CAL-ERDA System are:

- New data structure in the programs so that only the required amount of memory is assigned;

- Separation of the Systems program from the Plant program;

- Inclusion of a component-based Plant package which permits simulation of any thermodynamically feasible combination of components specified by the user;

- Two options for plant operation: optimal assignment of components for energy minimization, or user-defined rules;

- User-defined full-load and part-load component characteristics and maintenance schedules. This is essential for retrofit studies and research;

- Self-shading of building sections automatically, without special user input;

- Inclusion of simulation of heat pumps, solar collectors, and thermal storage systems, as well as arbitrary combinations of these with other systems;

- Gas turbines, double-bundle chillers, various types of cooling towers and heat-recovery devices are included as parts of a user-defined central or total energy plant;

- Ability to make "parametric runs" without repunching input cards.

FUTURE PLANS

Plans for the future development of CAL-ERDA include several additional capabilities. The library of predefined elements invoked by BDL will be expanded. BDL itself will be extended to accommodate the new features of CAL-ERDA. Simulation of in-building energy distribution systems will be done by specifying the organization of specific components. This will allow the user to simulate essentially arbitrary systems, in the same fashion now possible in the Plant program.

Instead of simulating the operation of a specified system, systems can be operated optimally or selected based on optimization criteria. Additional investigation of energy calculation procedures is expected to lead to faster algorithms that exploit the mathematical structure of the computation process. An extension of the Loads computations will include thermal coupling between zones, and optional use of the complete thermal balance method. Implementation of CAL-ERDA on the IBM 360/370 series of hardware is also planned. Facilities for graphical input and additional graphical output in an interactive computing environment comparable with BDL are also envisioned.

Simultaneously with the current and planned development of CAL-ERDA system, there is ongoing research activity to apply its analysis capabilities to practical problems.

FOOTNOTES AND REFERENCE

*CAL-ERDA is sponsored by the California Energy Resources Conservation and Development Commission (CERCDC) and the U.S. Energy Research and Devel-

opment Administration (ERDA). Four federal laboratories are collaborating: National Bureau of Standards, Lawrence Berkeley Laboratory, Argonne National Laboratory, and Los Alamos Scientific Laboratory.

†The Loads, Systems, and Plant programs of CAL-ERDA are based on earlier programs for energy analysis developed by Consultants Computation Bureau of San Francisco, with whom LBL shares the responsibility for the design and development of this system of computer programs.

1. A. H. Rosenfeld and Z. Cumali, "CAL-ERDA, A New Computer Program for Energy Analysis of Buildings," in J. Energy and Buildings, Vol. 1, No. 1 (in press).

CONSERVATION OPTIONS IN RESIDENTIAL ENERGY USE: STUDIES USING THE COMPUTER PROGRAM TWOZONE

L. W. Wall,* T. Dey, A. J. Gadgil, A. Lilly, A. H. Rosenfeld

INTRODUCTION

The aim of this research is to quantify various methods of saving energy in the heating and cooling of houses. We have developed and used the computer program TWOZONE to study the effect on energy usage of varying the size and location of windows, adding ceiling and wall insulation and storm windows, and setting the thermostat back at night during the heating season.[1]

TWOZONE

TWOZONE was developed during the 1975 Summer Study at Berkeley on the Efficient Use of Energy in Buildings[2] to provide a simple residential model studying the effect of various changes in design. The program does an hourly heat-load calculation, driven by a NOAA weather tape. The standard ASHRAE algorithms,[3] as implemented in the subroutines of NBSLD[4] and NECAP,[5] are used to calculate solar radiation from observed cloud cover, the delayed thermal response of walls and ceilings, and the prompt solar heat gain through windows. However, instead of using the weighting factors of NECAP, the program makes two thermal approximations: the house has a lumped heat capacity, adjusted to give a moderately insulated house a relaxation time of 4 hours; and the house has a 3-hour relaxation time for solar heat incident through windows.

The house is modeled as a two-zone space connected thermally by either a fan or by convective air flow, as shown in Fig. 1. This two-zone feature was included because we were particularly interested in capturing solar heat through large south windows, and wanted to calculate the economics of moving this heat from the warm south to the cold north side of the home.

For the case of heating, the losses are due to air infiltration and to conduction and radiation through the ceiling, walls, windows, and floor. The heat sources are the furnace, solar heat gain through the glazing, and internal heat loads (people, lights, and appliances).

Improvements made to TWOZONE during the past year make it possible to include the following: interior shading at the windows; a 3-hour weighted time delay contribution to the heating and cooling loads from sunlight incident through the glazing;

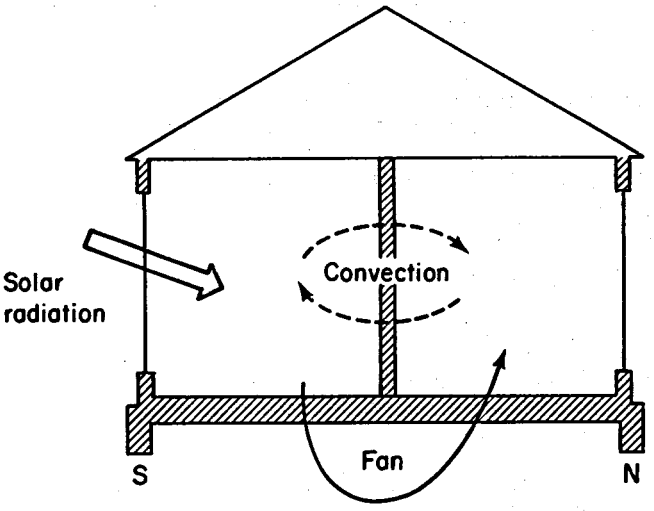

Fig. 1. Residential two-zone model, showing north and south halves of house connected only by air forced by the furnace fan (or by convection). For this work we have assumed that a 750-CFM furnace fan operates continuously. In a real house this would be accomplished by an extra thermostat, in a south room, that can turn on the fan without turning on the furnace whenever the thermostat reads more than 72°F. (XBL 7610-4299)

framing corrections for transfer function coefficients of walls and ceilings; an internal heat load schedule (people, lights, appliances); and floor losses.

There are three operating modes for the house:

(1) If the average inside air temperature (hereafter referred to as $\bar{T}$) exceeds a predefined maximum temperature (T_{HI}), the house "vents" all excess heat during winter months. In summer, depending on the outside air temperature, either the house "vents" the excess heat, or the air-conditioner turns on to keep the inside air temperature at T_{HI}.

(2) If $\bar{T}$ lies between the thermostat setting and T_{HI}, the house temperature "floats";

(3) If $\bar{T}$ is below the desired thermostat setting, the furnace is "on" until the house temperature reaches the desired setting.

In this way the hour-by-hour energy use can be calculated. The graphics printout of the program can display the hourly energy use along with the hourly inside and outside temperatures (Fig. 2).

In summary, the input to the program consists of the following: weather tape with hourly values, building description, schedules for occupancy and appliance usage, thermostat settings, exterior and interior shading. The output contains hourly heating and cooling loads, apportionment of the loads, cumulative furnace and air conditioner outputs, hourly inside temperature data, and graphical plots showing hourly loads and temperatures.

The quantitative results from TWOZONE are presently being calibrated with the NBSLD program. There has been good agreement with the field measurements that are available: Pacific Gas and Electric Company values (from household heating bills) for an uninsulated house in the Bay Area, and Southern California Edison values for electrically heated homes in Southern California.

RESULTS ON THE EFFECTIVENESS OF VARIOUS RETROFIT MEASURES

A summary of the preliminary results on the effectiveness of retrofit measures for Oakland, California (3000 degree days) is presented in Figs. 3(a) and 3(b). The typical Oakland house is taken to be a single-level, uninsulated, 1450-ft^2 house with 20% single-pane glass on the walls. In the figures, the furnace output has been apportioned to show the energy used to offset air infiltration and losses through the floor, windows, walls, and ceiling. The retrofit measures under consideration

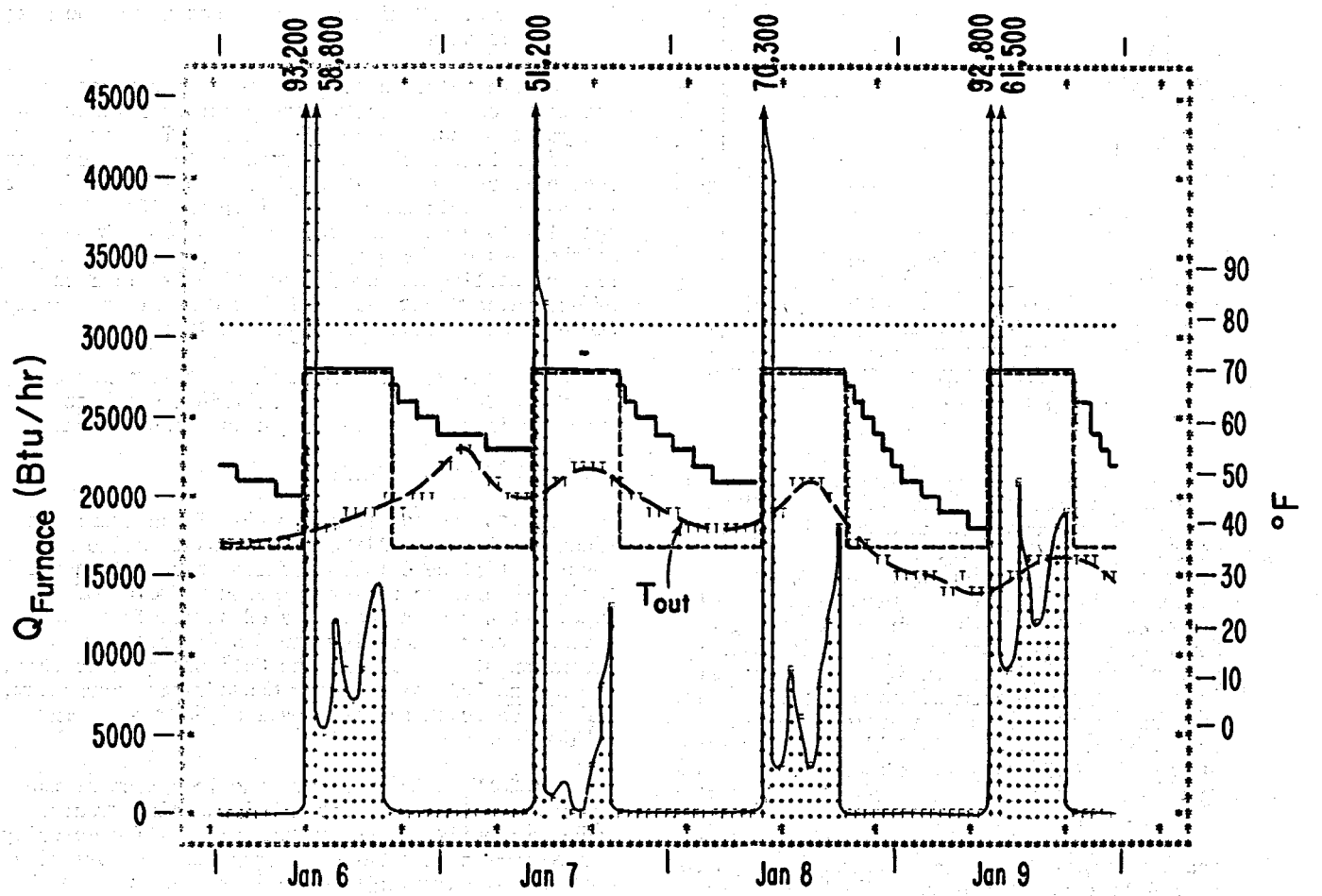

Fig. 2. Hourly temperatures and furnace output for a school of light construction with night thermostat set back to 35°F, for Washington D.C., 1962 weather. Outdoor dry bulb temperature is indicated by the heavy T_{out} line; thermostat setting by the dashed lines; inside temperature by the solid line. The hourly heat required to maintain the thermostat setting is a column of dots; thus the daily furnace output is proportional to the dotted area. When the thermostat is raised each morning, the furnace load goes off-scale, producing a daily spike on the printout. (XBL 7611-4349)

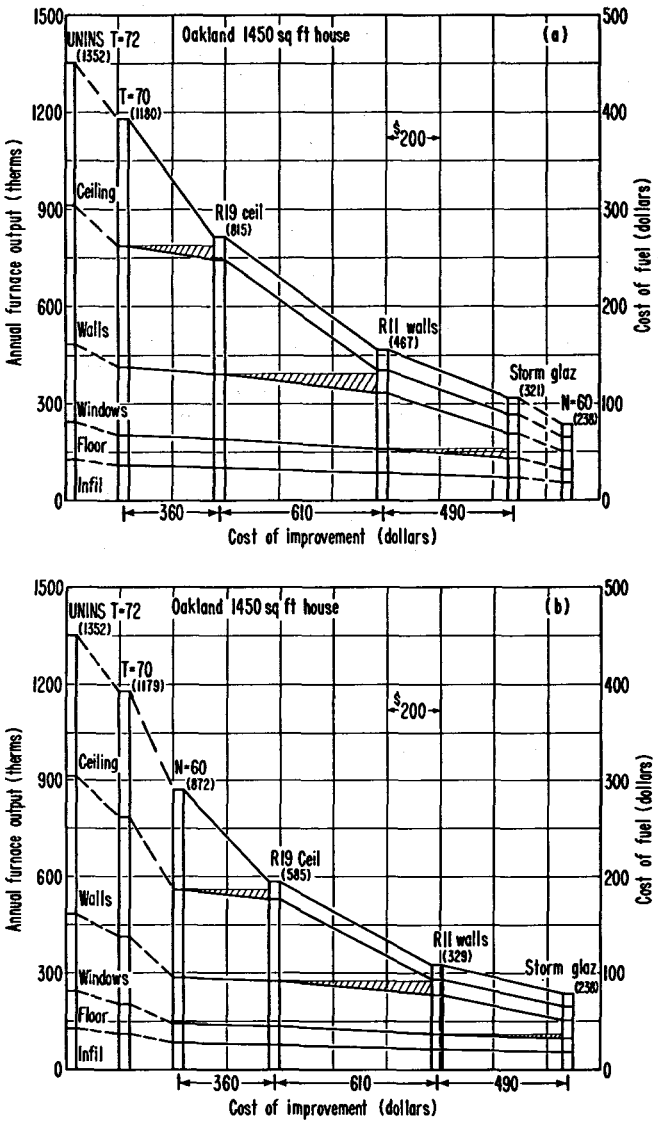

Fig. 3. Savings possible by thermostat setback or conservation retrofit measures on an uninsulated Oakland house, calculated using a 1955 weather tape. Costs for fuel and retrofit measures, and apportioning of loads, are discussed in the text. Figures 3(a) and 3(b) start at the left with a bar representing a house kept at 72°F day and night, followed by a house kept at 70°F. In 3(a), no night thermostat setback is assumed until the last bar; instead, insulation and storm windows are retrofit in sequence. In 3(b), night thermostat to 60°F (N = 60°) is assumed at the third bar. The retrofit measures come last; so they are less cost-effective. Both plots end at the same bar, representing all conservation measures, including night setback and furnace output down to 238 therms. The dollar cost scale at the right is based on a gas price of 20¢ per therm divided by a furnace efficiency of 0.6, resulting in a cost of 33¢ per therm of furnace output. (XBL 773-450A)

are the following: thermostat timers, ceiling insulation, wall insulation, and storm windows.

Retrofit costs per sq.ft. were assumed to be:

to add R-19 insulation to ceilings – 25¢/ft^2
to add R-11 insulation to walls – 50¢/ft^2
to add storm windows – \$2/ft^2.

From Fig. 3(a) we see that:

(1) Simply lowering the thermostat decreases the fuel bill by 6% per degree.

(2) Adding R-19 ceiling insulation decreases the fuel bill by \$90; if installation cost is \$360, this gives a 25% annual return or a payback time of four years.

(3) Adding R-11 wall insulation gives a 14% return or approximately a 7-year payback time.

(4) The installation of storm windows gives an annual return of 7% or a payback time of over 14 years.

(5) A further reduction in the heating bill can be attained by night temperature setbacks, say from 70°F to 60°F at bedtime until 30 minutes before waking up the next morning.

Alternately, in terms of cost effectiveness, one might choose nighttime temperature setbacks as the *first* measure to be instituted. This is illustrated in Fig. 3(b). A setback of 10°F reduces the fuel bill by approximately 25%. The installed cost for an automatic thermostat timer is \$100. The annual return on this investment is 75%. Looking at the rest of the graph, we see that the installation of ceiling and wall insulation is still cost-effective, with returns of 19% and 11%, respectively, whereas storm windows give only a 4% return.

In summary, the recommended retrofit measures for Oakland are repairs and caulking, clock thermostats, ceiling insulation, and wall insulation.

FUTURE ROLE OF TWOZONE

In its present form, TWOZONE is an excellent educational tool. Although its quantitative results still need further calibration, its qualitative results agree with previous studies of this type. It has been demonstrated successfully at several events including the San Francisco Twin Bicentennial Exposition, the California State Fair, the Second ERDA-Wide Energy Conservation Symposium, and the on-going Lawrence Hall of Science Energy Exhibition.

TWOZONE, written before the inception of the CAL-ERDA project to write public-domain computer codes for building energy analysis, will eventually become part of the CAL-ERDA program. The principal work that remains to be done is to incorporate the ASHRAE weighting functions and/or the NBSLD heat balance equations. The new version of TWOZONE will retain most of its original simplicity but will be more accurate. Future residential models will consist of three zones (north and south zones plus attic zone) or four zones (north and south zones plus attic and basement zones).

FOOTNOTE AND REFERENCES

*Department of Physics, California Polytechnic State University, San Luis Obispo, CA 93407.

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3. Procedure for Determining Heating and Cooling Loads for Computerizing Energy Calculations, ASHRAE Task Group on Energy Requirements for Heating and Cooling of Buildings, February 1975.

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NATIONAL PROGRAM FOR ENERGY CONSERVATION IN WINDOWS AND LIGHTING

S. M. Berman and S. Selkowitz

INTRODUCTION

In June 1975, LBL sponsored a four-week summer study on the efficient use of energy in buildings, and soon thereafter began developing a variety of promising prototype devices to improve the thermal performance of windows and to utilize direct sunlight for interior illumination. As a result, LBL was designated by ERDA in September 1976 to be a lead National Laboratory, with the responsibility for formulating a national research, development, and demonstration plan in the area of windows and lighting systems. Thus in addition to its own in-house research efforts, LBL now has the task of implementing the national plan and of continuing technical management of projects performed by contractors.

Windows are a major element in the external architectural expression of a building and have important physiological and psychological effects on the occupants. They also account, directly and indirectly, for a disproportionate share of the energy consumed in a building because of their impact on requirements for heating and lighting. It has been estimated that 20% of our national energy production is being used for the space conditioning of residential and commercial buildings. Windows, because of their comparatively high thermal conductivity, account for perhaps 25% of the annual consumption, or 3.5 quads, which is the equivalent of 1.7 million barrels of oil per day. Architects and designers have long recognized these facts. However, the lack of strong economic incentives – due to cheap and readily available energy – and ignorance of the complex relationships among all of the relevant design parameters have resulted in buildings that are often wasteful in their use of energy.

Lighting accounts for one-third to one-half of the total energy consumed in a typical commercial building. Lighting for all buildings in the residential, commercial, industrial, and public sectors requires about 400 billion kWh each year – about 23% of the electricity sold annually in the U.S., or the equivalent of 1.9 million barrels of oil per day.

The potential for reducing energy consumption in these two areas is enormous according to preliminary analysis. However, to effect significant reductions in actual energy consumption will require considerable emphasis on implementation. Recent studies of problems concerning diffusion of innovation into the building industry suggest that in the area of windows and lighting, the development of technically usable energy-conserving products and practices will not necessarily be sufficient to guarantee their acceptance, their utilization, or their effective impact in reducing energy consumption. We have thus proposed a program that not only will develop innovative and effective conservation measures, but also will ensure that they are recognized, accepted, and utilized by design professionals and the public at large.

ACCOMPLISHMENTS DURING 1976

Several major projects have been initiated by LBL as part of the National Plan for Energy Conservation in Windows and Lighting. Because this activity began in October 1976, many of the projects were just getting under way at the end of the year.

National Plan

A research, development, and demonstration plan has been formulated for the areas of windows and lighting. Broad goals were developed and a specific research agenda was identified, with a national advisory input from manufacturers, consulting engineers, and other research organizations. An array of strategies was generated to achieve these research goals as part of an integrated program to translate promising products or policies into effective and widely utilized conservation techniques. The specific strategies to be employed depend upon the nature of the proposed conservation

opportunity, its degree of prior development, and its energy saving potential.

LBL In-House Research Activities

Beam-sunlighting prototypes are being designed, developed, and tested in cooperation with a faculty/student team in the Department of Architecture at the University of California, Berkeley. These devices are intended to reflect incident sunlight from the upper portion of a window onto the ceiling, and then scatter it diffusely to illuminate the room. Analytical techniques have been worked out to predict illumination levels resulting from use of these devices, and initial scale-model testing has been completed. The prototype design and various activation and control mechanisms are under development.

Thermal performance of a variety of existing as well as novel window designs will be studied with the aid of new computer programs that are being developed. Testing facilities are being designed to enable us to measure relevant optical and thermal properties of glazing materials as well as of novel window prototypes. This analytical and experimental capability will then be used to assist in the development of prototype "dual-mode" shades and blinds. These devices, similar in appearance to their conventional counterparts, have a heat-absorbing mode for winter operation and then are reconfigured to a heat-rejecting mode in summer. In addition, they allow visual contact with the outdoors and reduce conduction/convection gains and losses in all seasons. Since they are based on refinements of existing materials and components, these prototypes should lend themselves to immediate application and use. We have initiated a feasibility study to assess the applicability of such devices for a retrofit application in Building 50 at LBL.

Research and Development Contracts

Suntek Research Associates have previously developed two materials of interest to our windows research program:

- The "heat mirror," which is a long-wave infrared-reflecting coating deposited on plastic film. It can significantly reduce winter heat loss when applied as part of an insulating glass assembly.

- The "optical shutter," which is a light and heat sensitive sandwich film that is normally transparent but turns translucent white in the presence of high temperature and sunlight. The white, reflecting state will significantly reduce solar gain and thus reduce air-conditioning loads.

Under subcontract to LBL, Suntek has developed manufacturing processes for these products and has conducted marketing studies as part of a larger commercialization effort to speed these products to the marketplace.

High-frequency ballasts for fluorescent lighting systems were identified in our planning activities as an area that promised significant energy savings and a high probability for successful market introduction. When compared with conventional ballasts, these electronic ballasts have been shown to require 35% less input energy with equal light output. Additional substantial savings may be realized if the dimming capabilities of these ballasts are effectively utilized. At the end of 1976, we initiated a Request for Proposals to fund a two-phase program to demonstrate and validate the performance of these ballasts, and to assist in the introduction of these energy-conserving devices into the lighting market.

Preliminary negotiations were completed with a firm to test and evaluate a novel glass coating process by which weather-resistant thin films can be applied to the exterior surface of single-glazed windows. The coatings would be tuned to reflect the infrared portion of incident solar energy, thus reducing heat gain without reducing the daylighting potential. Such coated glasses would find their primary application in commercial buildings having substantial cooling loads.

PLANNED ACTIVITIES FOR 1977

All the research, development, and demonstration activities described in the previous section were initiated in the last half of 1976; all will continue into 1977 and most will be expanded. In addition to funding additional work outside the Laboratory, we anticipate extending our in-house research activity. At LBL, the beam-sunlighting activity will move into a demonstration phase; and interactions with the artificial lighting and control systems will be studied. The windows effort will add an assessment of the daylighting potential to the thermal analysis results and attempt to generate guidelines for optimal window design and size as a function of a large array of relevant variables. Our program planning and management activities will continue to grow as the number and size of our subcontracted projects increase.

COMBUSTION RESEARCH

F. Robben, Y. Agrawal, B. Angeli, P. Bernard, M. C. Branch, N. J. Brown, C. Chan, R. Cheng, W. K. Chin, A. J. Chorin, P. Concus, J. W. Daily, H. A. Dwyer, C. Fenimore, A. Ganji, H. Glaz, R. Greif, W. L. Grosshandler, T. Hadeishi, K. Hayashi, J. Kurylo, B. Launder, R. D. Matthews, I. Namer, A. K. Oppenheim, P. J. Pagni, R. Pitz, R. F. Sawyer, R. W. Schefer, D. M. Silver*

INTRODUCTION

Research on combustion processes is an important part of our national program on energy conservation and environmental protection. These two subjects are closely linked in many areas, particularly in regard to the generation of energy by the combustion of fossil fuels. It is this coupling which makes necessary a deeper, more fundamental understanding of the process of combustion, in order to design optimized combustion systems.

A very large fraction of our national energy needs are met by the combustion of fossil fuels, and most projections indicate that fossil fuels will continue to be the major energy source for the next 50 to 100 years. Thus improvements in combustion made in the next 10 to 20 years will have a large effect on the rate at which fossil fuels are consumed, and on the atmospheric pollution produced thereby.

Because combustion is a highly complex process, combining fluid mechanics and chemistry, it requires high-level scientific expertise and techniques to make significant advances in our understanding. Thus a combustion research group, operating in the LBL Energy and Environment Division, was formed this year by investigators doing combustion research at LBL and at the University of California at Davis and at Berkeley. It is felt that the interaction among members of this group, combined with the scientific, technical, and management capabilities of LBL, will produce a significant impact in the field of combustion science.

COMBUSTION IN BOUNDARY LAYERS: SURFACE CATALYZED COMBUSTION AND TURBULENT COMBUSTION (Agrawal, Schefer, Namer, Robben)

Introduction

This report presents the status and future plans of two current studies: the surface catalyzed combustion of lean premixed mixtures in the laminar boundary layer over a strongly heated flat plate; and the study of turbulence under these conditions – as contrasted with the well researched, although not completely characterized, turbulence without chemical reaction.

Interest in surface catalyzed combustion stems from the well known fact[1] that clean and efficient systems (e.g., gas turbine combustors and industrial and domestic furnaces) can be developed by use of lean premixed combustion systems. In addition to eliminating unburned hydrocarbon soot and thermal NO_x emissions, such combustion systems make new sources of energy available, such as vent gases from mines. The structure of the turbulence that accompanies combustion is a problem of fundamental interest.

Our studies are conducted in the boundary layer formed over a flat plate, a geometry specifically chosen for its well understood aerodynamics. In the catalytic work, we hope to develop a fundamental numerical model of the surface activity of the catalyst, to study catalytic activity and performance over a wide range of parameters, and later to evaluate practical systems.

A schematic of the experimental facility is shown in Fig. 1. A flat plate with a sharp leading edge, made of 0.3 μm platinum coated quartz (1.5 mm thick), is placed in a jet of uniform velocity air-fuel mixture. Electrical heating of the platinum is used to heat the flat plate. The plate may be used to study platinum catalysis; it may be coated with SiO for noncatalytic studies; or it may be coated with other catalytic materials. The main jet of air-fuel mixture is derived from a carefully designed stagnation chamber (20 cm diam) where flow is smoothed and straightened before passing through a strong contraction into a streamlined nozzle (2.5 cm diam). The range of available flow speeds is broad enough to cover laminar flows and the transition to turbulence in the viscous boundary layer over the flat plate.

Diagnostics involve measurements of flow velocity by laser doppler velocimetry (LDV), density by Rayleigh and Raman scattering of laser light, and plate surface temperature by optical pyrometry. Since the overall gas density is known from the Rayleigh scattering, the temperature of the gases may be obtained. The density of the major species, N_2 and O_2 are relatively easy to determine. If the density of H_2O is known with sufficient accuracy, the degree of reaction may be determined. Trace species and radicals will be measured in the future using gas chromatograph-mass spectrometer systems, as well as other optical techniques now being developed.

The computer codes used to model the combustion process under study are expected to compute the boundary layer flows, both laminar and turbulent (using available closure models) with and without chemical reaction. Two codes, developed by Blottner[2] and Pratt,[3] have been combined so that we can model several flow geometries and incorporate realistic finite-rate chemistry.

Accomplishments During 1976

The experimental facility has been completed. The open-jet wind-tunnel facility and several flat plates have been constructed. The laser doppler velocimeter is operating, and refinements have been made to improve measurement accuracy. A 0.3-m McPherson spectrometer and associated optics are in place for Rayleigh and Raman measurements.

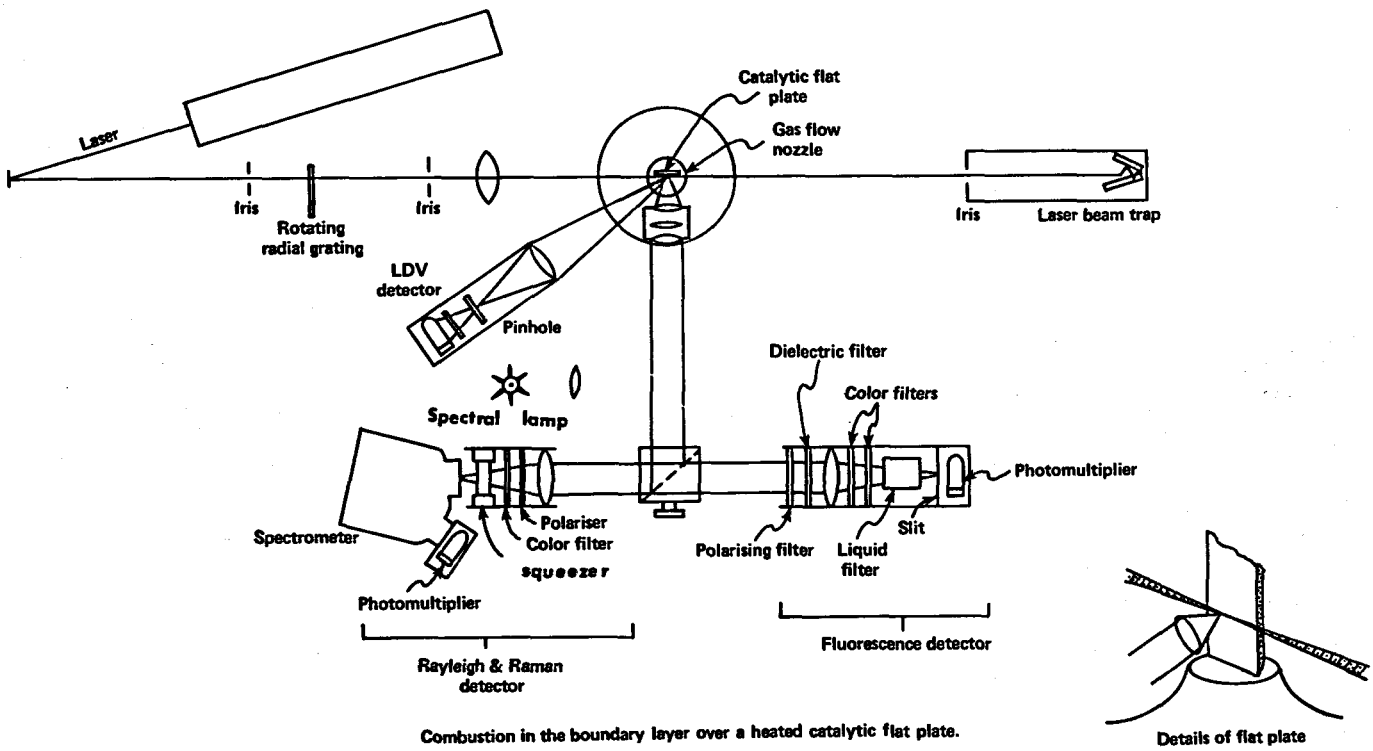

Fig. 1. Schematic of equipment for combustion in the boundary layer over a heated catalytic flat plate. (XBL 764-2757)

The laser velocimeter has been used to map the flow field of the mainjet (the model wind-tunnel). Measurements in the boundary layer of a cold plate have been made. Typical data (Fig. 2) are compared with the exact solution of Blasius. Successful measurements of velocity in the heated boundary layer have also been made. One of the most difficult problems so far has been to obtain a uniform temperature (of the order of 600-1200°K) on the plate surface. This is expected to be achieved with the quartz plate. In the meantime, stainless plates heated with embedded SiC rods have been employed. The phenomenon of thermophoresis was rediscovered in the context of laser velocimetry, and it appears that LDV measurements in a subregion of the heated boundary layer, close to the plate wall, will not be possible due to thermophoresis.

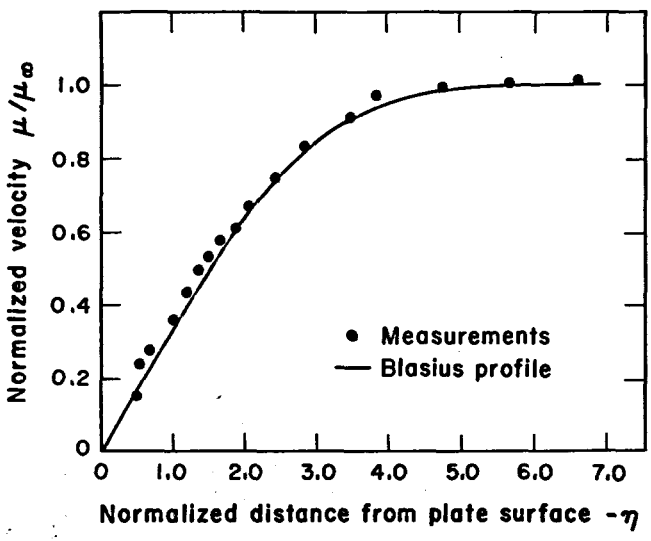

Fig. 2. Comparison of measurements in the boundary layer of a cold plate with theory. (XBL 773-639)

Rayleigh and Raman signals have been observed. At present, it appears that accurate measurements of overall gas density (and hence temperature) by Rayleigh scattering will be possible. N_2 and O_2 measurements by Raman scattering were possible in the absence of background thermal emission from the plate surface. More careful measurements have not been attempted.

We have been able to measure turbulence velocities and construct statistical correlations and probability distributions. Measurements of time-resolved density have not been attempted.

The computer codes by Pratt and Blottner have been combined successfully, and numerical solutions are routinely available for comparisons with experiments. Improved gas kinetic data and transport properties are being incorporated.

Planned Activities for 1977

Detailed and complete velocity and temperature data will be obtained in the laminar boundary layers over cold, heated without combustion, and heated with combustion, quartz plates. These will be checked for similarity in well-known dimensionless variables – an essential step if data are to be of a fundamental nature. Combustion will be studied

with both catalytic and noncatalytic surfaces, and various catalysts will be tested. It is expected that considerable effort will be involved in the study of catalytic activity over extended periods of time.

Simultaneously, numerical solutions will be generated for the experimental conditions; and a search for a model that describes catalytic surface activity will be attempted.

A study of turbulence under all of the above conditions will be carried out, although data processing will be limited to single-point measurements, and to routine statistical analysis and spectral decomposition in the time domain. A continued liaison with industry will make commercially-used catalysts available for evaluation. At present, such contacts exist with Aerotherm, Inc., Matthey-Bishop, and Oxy-Catalyst.

Acquisition of a mass spectrometer for trace species analysis and measurement is planned. The results of these measurements will also be compared with numerically generated solutions.

NUMERICAL STUDY OF TURBULENT COMBUSTION, WITH APPLICATION TO THE INTERNAL COMBUSTION ENGINE
(Chorin, Concus, Oppenheim, Bernard, Fenimore, Glaz)

The goal of this project is to construct a reliable numerical model of turbulent combustion for use in the design and development of combustion systems. The methods we develop should have wide applicability, but we plan to concentrate on applications to internal combustion engine problems.

The first step in developing the model involved the design of numerical methods capable of handling combustion problems. In particular, such methods must be able to describe complex patterns of discontinuities, several scales in both time and space, and the dynamical effects of exothermic reactors. We have been successful in developing novel methods that satisfy these requirements.

We are now working on the appropriate description of turbulence. The most important fact about turbulent combustion is that the chemical processes in a mean flow differ from those in a real flow; i.e., the fluctuations in the pressure and temperature fields have a substantial impact on the chemistry. We are testing a new procedure for describing the interaction of chemistry with a random flow field, using ideas drawn from parametric inference theory.

NUMERICAL MODELING OF TURBULENT COMBUSTION
(Dwyer, Robben, Launder)

Introduction

At the present time there does not exist a proven fundamental method of approach to describe the combustion of a fossil fuel in a turbulent environment. Since the majority of real environments for which combustion occurs are turbulent, this implies that all energy devices using fossil fuels are basically designed by a "cut-and-try, trial-and-error" approach. The present project is a theoretical study aimed at developing methods of modeling turbulent combustion flows, and solving these problems through the use of numerical methods. The starting point for the project will be the simplest turbulent shear flow, that over a flat plate. This geometry generates one of the few experimentally documented flows for which theoretical methods have been successful in predicting time-average flow behavior. However, for flat plate flow with combustion, neither experimental results nor theoretical models are available. Moreover, new numerical methods for solving the complex equations with chemistry must be developed. It will be the immediate object of this particular study to provide theoretical calculations for comparison with the parallel experimental program, "Combustion in Boundary Layers," previously described.

The physical problem consists of a pre-mixed combustible gas flow over a sharp-edged flat plate. The wall of the plate is heated and may also be catalytic; a large variation in the mixture of fuel to air can be studied. This situation is of fundamental importance to the performance and understanding of catalytic converters used as pollution control devices, as well as being the most basic wall turbulent shear flow. Successful development of a theoretical model along with a numerical solution method will be an important basic step in understanding and designing energy devices based on combustion.

The project described herein began October 1976, and we are now in the process of developing the tools necessary to complete the study. However, the method of approach has been worked out for the initial phases of the project.

Accomplishments Expected During 1977

The basic approach taken is to solve the time-average equations of motion that describe the flow of a combustible mixture of gases. The problems are:

(1) physical modeling of the fluctuating turbulence terms caused by time averaging;

(2) numerical modeling of a flow with multiple space scales caused by chemical reactions;

(3) physical modeling of the reactions and kinetics that exist in a combustion flame.

In the present research task, only the first two problems will be addressed directly. The reaction mechanisms and kinetics will be obtained from other sources.

The starting point for physical modeling of turbulence will be the existing closure schemes that have been developed for nonreacting flows.[4-7] We plan to model the flat-plate flow with three levels of closure – eddy viscosity, turbulent kinetic energy, and full Reynolds stress closure – and compare the predictions with experiments. From these comparisons, new closure models will be hypothesized and their universality tested.

The numerical procedures that are being developed to solve the complex equations with chemistry will center around the relatively new techniques of

operator splitting and adaptive grids.[8,9] With these techniques the multiple scales and stiffness associated with chemically reacting flows can be properly treated, and converged numerical solutions obtained with good efficiency. These techniques also show promise of being very useful on more general problems than the flat-plate system being used for the initial stages of the project.

The end result of this research will be that the successes and failures of the existing turbulence closure schemes will be exposed. With this knowledge, and with the development of new numerical methods, a comprehensive program of research can be pursued to develop a rational and complete model of turbulent flow with combustion.

Planned Activities

Besides developing new physical models for turbulent shear flows with combustion, we hope eventually to expand our research to the very important cases of combustion in a straining flow and to turbulent diffusion flames, rather than just to the pre-mixed flows of the initial study. All of the methods developed for the simple flat plate study can be extended directly to these other combustion flow research areas.

AUTOMOTIVE ENGINE COMBUSTION WITH EXCESS AIR
(Sawyer, Branch, Daily, Greiff, Oppenheim, Pagni)

Introduction

Lean burn, stratified charge, and diesel engines all involve combustion in the presence of excess air. All have a potential for improved efficiency and reduced emissions compared with the conventional spark-ignition engine. The full realization of this potential has been hampered by difficulties in initiating and sustaining the combustion process in very lean mixtures. As the lean flammability limit is approached, engine performance drops and hydrocarbon emissions increase.

Accomplishments During 1976

Under NSF/RANN sponsorship, a single-pulse, compression-expansion machine simulating a reciprocating engine has been constructed for the study of the fundamentals of engine combustion processes. This facility, located in the Combustion Dynamics Laboratory of the Department of Mechanical Engineering at the University of California at Berkeley, provides for full optical access for observations of both the ignition and propagation of combustion (Fig. 3). The machine consists of three main elements: a square test section, the driver section, and the snubber section. The end block of the test chamber is interchangeable to allow for a variety of configurations, such as spark ignition, torch ignition, stratified charge operation, or fuel injection. Compression ratios from about 5:1

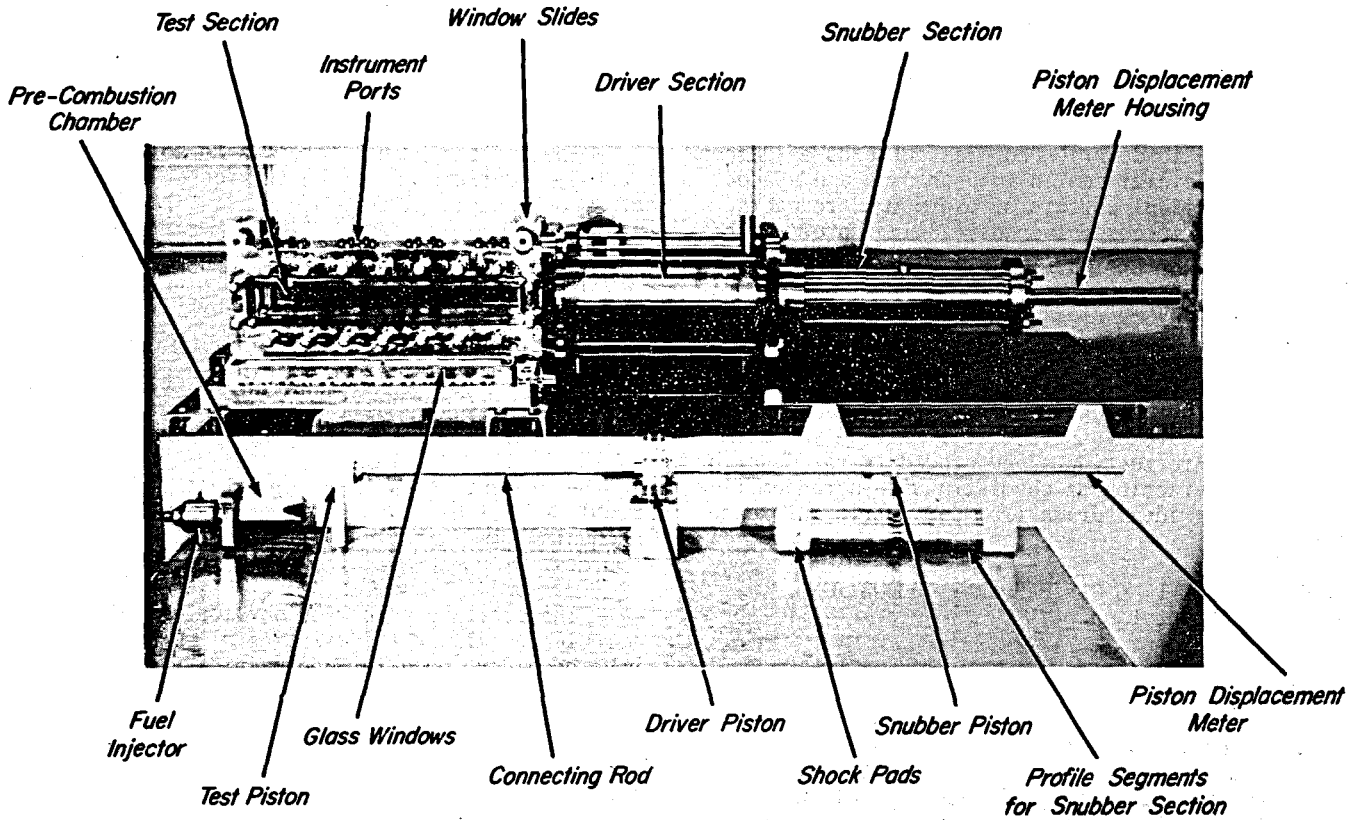

Fig. 3. Exploded view of the single-pulse machine. (XBL 773-2348)

to 20:1 can be obtained, with a stroke up to 133 mm, and an equivalent speed of up to 1800 revolutions per minute.

High speed, color, schlieren motion picture records have been obtained which provide detailed flow visualization of processes occurring within the combustion chamber. Such phenomena as the growth of the piston generated vortex (Fig. 4), ignition, flame propagation, and quenching of the combustion process at the walls have been observed. The advantages of torch ignition for very lean mixtures, including the lowering of pollutant emission levels, have been observed.

Studies to date have been upon premixed methane and air. Methane was selected as a fuel to simplify understanding of the chemical kinetic mechanisms that are likely to control combustion near the lean flammability limit. Modeling of the combustion process is being pursued to provide a fundamental understanding and interpretation of the experiments. The apparatus also has provided a test facility for the time-resolved measurement of wall heat fluxes and heat transfer coefficients.

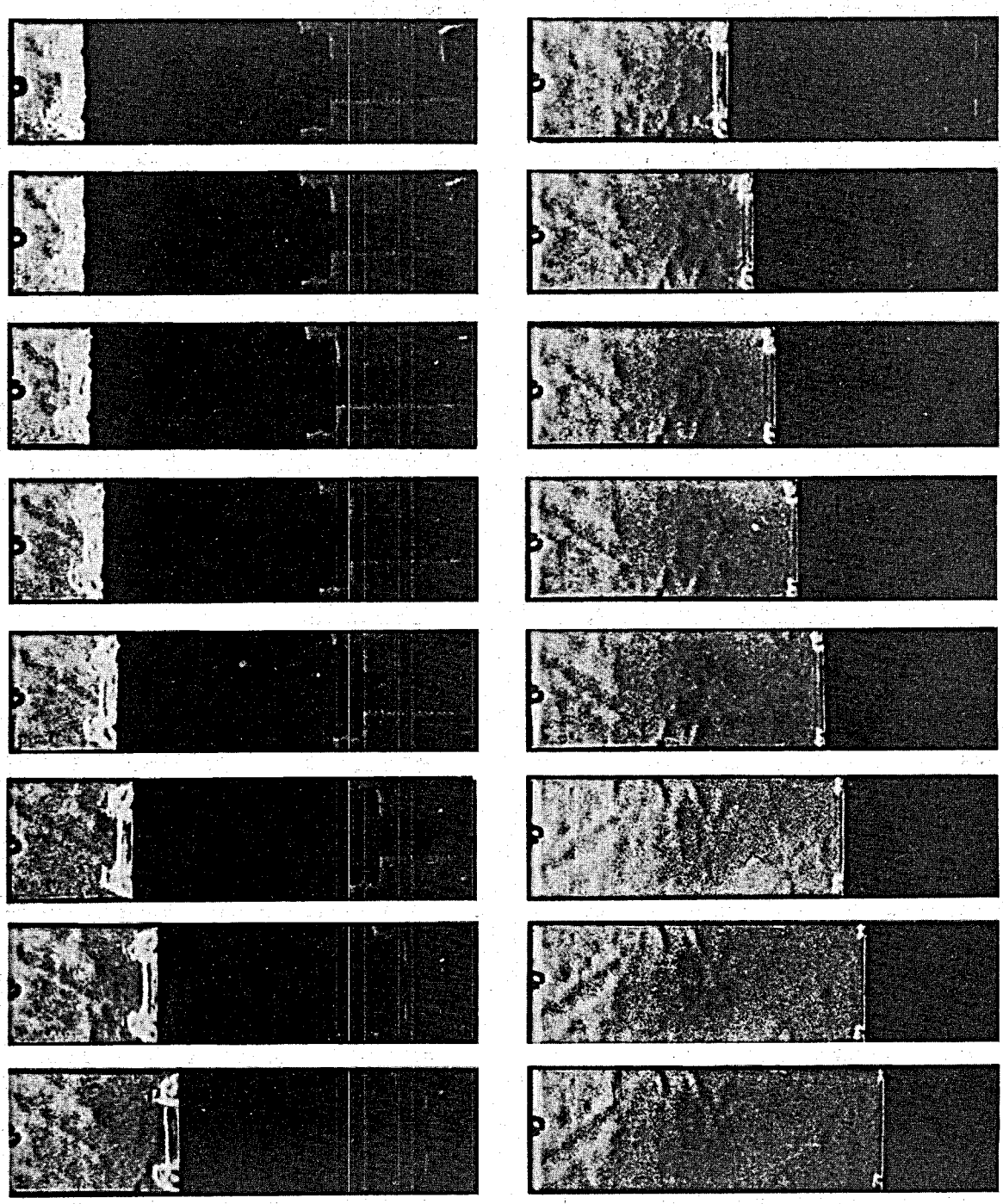

Fig. 4. Cinematographic sequence of schlieren photographs of rolling vortex. Compression ratio 8.5:1; stroke 13.3 cm; cross section 3.81 cm × 3.81 cm.

Planned Activities for 1977

The unique capabilities of this experimental facility provide the opportunity for detailed observations of engine combustion processes in a manner previously not possible. In the coming year, quantitative data on required ignition energies, flame propagation velocities, wall temperature gradients, wall heat transfer coefficients, and the formation of pollutant emissions are to be obtained. In many of these studies a line igniter will be employed to promote a two-dimensional flame and resultant simplifications in data analysis. Hydrocarbon/air reactants will be continued.

TECHNIQUES FOR STABILIZATION OF LEAN COMBUSTION
(Daily, Sawyer, Oppenheim, Ganji, Angeli, Pitz)

As part of its continuing program to improve ambient air quality, the U.S. Environmental Protection Agency has published maximum aircraft emission standards, scheduled to go into effect in 1979, for carbon monoxide, oxides of nitrogen and unburned hydrocarbons. In an effort to generate technology and demonstrate hardware required to meet these emission standards, the NASA Lewis Research Center is administrating the Experimental Clean Combustor Program. The research described herein is oriented toward the fundamental study of stabilization of lean mixtures in gas turbine combustors and is undertaken to supplement the NASA program.

Pollutant emissions from gas turbine engines are greatest under two extremes of operation: idle or low power, and takeoff or high power. High-power operation is usually characterized by high combustion efficiency, high combustor temperature, and hence increased NO emissions. When richness of the primary zone of the combustor is increased at high power, smoke emissions also increase. Emissions at low power to taxi/idle operation result from low combustor efficiency at the low combustor inlet pressure and temperature; in this case, carbon monoxide and hydrocarbon emissions are high while nitric oxide is reduced. Aldehyde emissions reflect a dependence on engine power similar to that of hydrocarbons.

The condition most consistent with simultaneous reduction of *all* emissions is lean burning with high-intensity, stable combustion. In conventional gas turbine combustors, nitric oxide is produced predominately in the primary zone in which near stoichiometric mixtures are burned in order to maintain a high, final flame temperature and a stable combustion throughout the system. So long as these high temperatures are the principal variable controlling combustion intensity, the production of NO remains tied to combustion stability.

The activities of our research program have concentrated in three areas:

- The major effort has been the development and use of a two-dimensional combustion tunnel. This tunnel, with quartz windows for optical access, allows detailed examination of the combustion process with advanced optical diagnostic tools.
- Studies concerned with a fundamental understanding of aerodynamic means of stabilizing lean combustion have been undertaken in an opposed reacting jet.
- Theoretical and experimental studies of the use of heat recirculation for stabilizing flames at very lean mixture rates are being performed.

STUDIES OF EXOTHERMIC PROCESSES IN COMBUSTION
(Oppenheim, Cheng, Kurylo, Hayashi)

Introduction

The purpose of this program is to study the dynamic effects of exothermic processes in chemically reacting gas mixtures in order to provide basic data for analyzing the initiation and propagation of the combustion process, especially under the relatively low-temperature conditions that exist in the case of lean combustion or low-Btu fuel.

In practically all combustion systems used today, burning is controlled principally by the rate at which fuel is mixed with air, while chemistry plays a lesser role. Modern trends, in response to environmental constraints, are directed towards the use of ultra-lean premixed fuel-air mixtures, as well as low-Btu fuels, which for control rely more on the dynamic effects of chemical reactions of combustion. Such effects are due entirely to exothermic processes, the major source of feedback on the flow system in a combustion chamber. It is the experimental observation of such effects and the establishment of their theoretical background that forms the major objective of our studies.

Previous Work

Experiment

The experimental technique we developed for the study of the initiation of exothermic processes in combustion systems has by now evolved into a well-defined procedure by which we can investigate systematically gas-dynamic properties of weak and strong ignition in progressively more complex chemical systems. Preliminary studies of the hydrogen-oxygen and the methane-oxygen systems have been completed.[10,11] At present, we are conducting experiments to reveal the effect of hydrogen used as a reaction-promoting agent in a methane-oxygen system. Diagnostics include pressure measurements using high-frequency transducers, as well as the cinematographic laser schlieren and laser shear interferometry used for the determination of density profiles and their development, at a microsecond resolution in time.[12]

The cinematographic system is capable of recording profiles of refractive index across the whole width (3.2 cm) of the test section of our shock tube at a rate of up to 1 million frames per second. It has been used for the study of strong ignition in methane combustion. The method is akin to holography in that the eventual photographic result is obtained by reconstruction of diffraction records taken in the course of the experiment.

These are, for this purpose, superimposed on similar records made previously of the test section, to provide information on the undistorted field under observation. Thus from a single experimental record one can reconstruct three cinematographic sequences: 1) schlieren photographs furnishing information on the trajectories in the time-space domain of the fronts of shocks and compression waves generated by exothermic energy from the combustion process, 2) infinite fringe interferograms providing information on density distribution across the test section, and 3) finite fringe interferograms yielding information on density profiles throughout the flow field under study.

Theory

Interpretation of experimental results is closely coupled with the concept of exothermic centers.[13,14] These combustion models have been studied over representative sets of initial conditions, as well as thermodynamic and gas-dynamic constraints (constant value, constant pressure, and Chapman-Jouguet deflatrations along appropriate Rayleigh lines), in one-dimensional, point-, line-, or plane-symmetrical geometry, for a variety of reacting mixtures. In the course of our analytical studies we have established the concept of a phase diagram in the plane of exothermic energy and its rate of evolution (the exothermic power) as the most convenient means of expressing the driving term for the analysis of the dynamic effects of combustion. Flow fields associated with strong ignition are modeled as a coherent array of exothermic centers whose dynamic properties are represented by energy source terms specified in terms of integral curves in such a phase diagram. For the chemical systems under study we have found a satisfactory agreement between analytical prediction based on this modeling technique and the experimental results pertaining to wave trajectories and density profiles.

At the same time, as an integral part of our research program, we are evaluating concentration histories for all the reacting species,[15] following, in effect, the methods of Kondratiev,[16] Brokaw,[17] and Schott and Getzinger.[18] In this connection we have developed an approximate analytical technique applicable to diluted combustible mixtures whereby the chemical kinetic rates are expressed in terms of a simple set of algebraic and ordinary differential equations. These lend themselves readily to integration without any difficulties due to stiffness, the characteristic feature of the exact set of kinetic rate equations.

Concomitantly, we have studied a variety of blast wave problems, including such effects as the influence of transport properties,[19] atmospheric density distribution,[20] and unusual thermodynamic properties of the medium.[21] Currently under study is the development of a novel method of phase space for the analysis of non-self-similar blast waves,[22] and of point explosions with variable energy.[23]

The results of these studies can be summarized as follows:

(1) Reduction in size of kernels of exothermic centers cause their dynamic behavior, as expressed by the power pulse on the phase diagram, to approach that of an adiabatic process at constant pressure, while increase in their size leads to the opposite limit of an adiabatic process at constant volume. The shape of the exothermic power pulse on the phase diagram is practically independent of the concentration of reactants. The dilution by an inert gas has a significant influence on the value of the maximum of the specific power, while its effects on the abscissa of the point of maximum power and on the half-width of the pulse are relatively minor.

(2) The boundary layer in a blast wave is due to the fact that the temperature gradient at the center must be zero. This gives rise to a layer in the central region of blast waves where the effects of transport properties cannot be neglected. Our analysis provides means for the evaluation of the size of this central region. The solution indicates to what extent the results of inviscid analyses can be trusted, in spite of the well-known anomaly they exhibit in maintaining zero density and infinite temperature at the center for all times, even when the blast wave has decayed to a mere sound wave. This is of particular importance, since the preponderance of publications one finds on blast waves are concerned exclusively with inviscid media.

(3) A comprehensive analysis of gas motion created by strong explosion in an atmosphere whose density is an exponential function of altitude has been worked out. In particular, it provided a link between the results of a number of seemingly unrelated studies which have been performed in the past by many investigators, including such outstanding authorities as Zel'dovich, Raizer, Hayes, and Probstein.

(4) An analytical method of phase space has been developed for the treatment of non-self-similar blast waves. The method has been applied to the classical problem of point explosion with non-zero counter-pressure, yielding a smoother approach to sonic bound than that obtainable by strictly numerical solutions.

(5) Self-similar solutions for blast waves of variable energy have been derived for a full range of rates at which energy can be deposited or removed from the flow field. Results for a number of representative cases, obtained as integral curves on the phase plane of reduced wave variables, are expressed in terms of the particle velocity, density, pressure, and temperature profiles throughout the flow field. In particular, they emphasize the importance of differentiating among three fundamentally different modes by which energy can be deposited: at the front of the wave, at its center, or in the middle of the flow field. It is the third case that is most difficult to analyze and the least understood, forming therefore a prominent objective for future studies.

Future Work

The concept upon which we propose to base our studies is as follows. Both the initiation and the propagation of the combustion process in a gaseous medium are crucially dependent upon the amount and

rate at which energy is deposited in the substance. For initiation this energy is supplied from outside, while for propagation it is derived from the exothermic process of combustion. Non-steady gas-dynamic features play a predominant role in both cases. We propose to observe and study these features with particular care in a well coordinated manner.

To ignite lean gaseous mixtures, more energy is required than in the stoichiometric case. However, the amount of energy generated by combustion per unit mass of the substance is then smaller. The practical way of dealing with this problem is to distribute the ignition energy over a sufficiently large volume so that the combustion process is properly enhanced throughout the whole extent of the charge without a destructive explosion. In order to accomplish this successfully, fundamental data are required on the effect of the rate of energy deposition on the initial non-steady stages of the combustion process. We propose to acquire such data by an experimental and theoretical program of studies.

Experiments will be performed using hydrocarbon fuels mixed in the gaseous phase with air, nitrogen, or argon, depending upon the particular requirements for the interpretation of the results. The test gas will be contained initially at room temperature and atmospheric or subatmospheric pressure in an explosion vessel fitted with optical windows and instrument plugs, or in a properly instrumented shock tube. Both types of apparatus are available in our laboratory. Combustion will be initiated by various means, ranging from shock heating, with observations made behind the reflected shock wave as in our previous studies, to an assortment of flame torch igniters, spark plugs, and plasma jets, with or without electromagnetic enhancement.

Experimental records will be primarily photographic in nature, being obtained by the use of techniques developed in our laboratory for the observation of refractive index fields with a high time resolution. Prominent among them is the cinematographic schlieren and interferometer system associated with a stroboscopic laser used as the light source. Whereas the cinematographic schlieren technique was developed and has been used by us before, the capability for cinematographic interferometry has been just attained. The first is capable of yielding up to 10^6 frames per second, while the second can provide records from which time-frozen density profiles across the full extent of the test section can be deduced at time intervals of 2-5 microseconds. These data will be supplemented with pressure records obtained by the use of ultra-high-frequency response transducers developed in our laboratory, as well as pulse laser spectroscopy for time resolved measurements of temperature and species concentration.

Experimental results will be interpreted by the use of numerical and analytical techniques described in the previous section. As far as the properties of the reacting medium are concerned, the information obtained thereby will be expressed in terms of power pulses relating the rate of the evolution of exothermic energy with its relative amount.

The analytical studies will elucidate the gas-dynamic features of the non-steady flow fields generated by the deposition of energy in the medium. In this respect our studies should also bear upon the gas-dynamic phenomena associated with laser fusion.

THE COMBUSTION OF COAL AND COAL-DERIVED FUELS
(Sawyer, Grosshandler, Brown, Chin)

Introduction

The utilization of coal in energy-producing devices requires either the direct combustion of the coal or the combustion of a fuel derived from coal. Major problems in the successful use of both coal and coal-derived fuels concern their adaptation to existing and planned combustion devices, and their likely production of increased pollutant emissions compared with petroleum fuels and natural gas.

Fundamental and exploratory studies have been initiated on the *mechanisms of coal burning* with emphasis on adaptation of the opposed-flow diffusion flame apparatus (Fig. 5) to the burning of coal fuels. This technique and apparatus, originally developed under NSF sponsorship for studying the

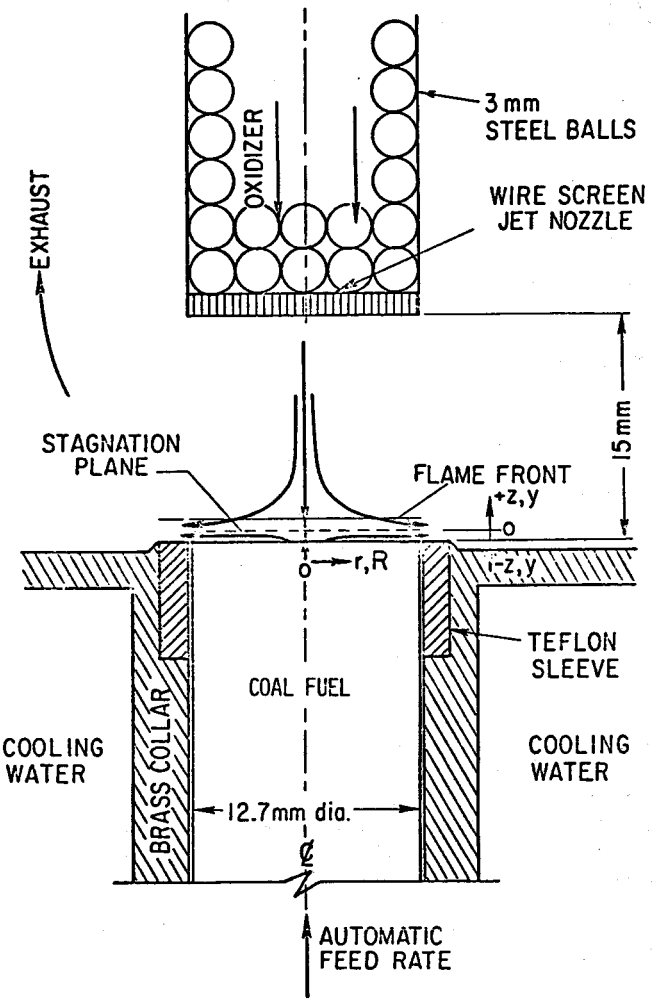

Fig. 5. Schematic of opposed-flow diffusion flame.

burning of polymers (thermoplastics, charring plastics, and wood), provides a laboratory tool for the steady-state combustion and detailed observation of solid fuels. It is particularly suited to determining the gas phase flame structure, temperature profiles in both the gas and solid (pyrolysis region) phases, and the formation of pollutants from fuel-contained compounds (particularly those containing nitrogen and sulfur). Standard probe sampling techniques can be complemented by optical measurements to analyze gas phase compositions.

A study of the *combustion characteristics of a coal/methanol slurry* was undertaken to determine the radiation heat transfer characteristics of the combustion gases. The use of methanol in conventional furnaces or boilers is hampered by the low emissivity of the methanol combustion products, especially in comparison with residual and distillate oil fuels. The augmentation of emissivity through the addition of pulverized coal to the methanol was sought. Coal/methanol slurries are of additional interest because of their advantage in the pipeline transportation of coal and because of their potential use as a direct substitute for petroleum fuels.

Both these projects relate directly to the formation of odd-nitrogen pollutants in combustion processes. Coal fuels contain high concentrations, up to 3% by weight, of bound nitrogen which results in high emission levels of the oxides of nitrogen and possibly other nitrogen-containing products.

Accomplishments During 1976

The suitability of the opposed-flow diffusion flame apparatus to burning rods of graphite and pressed pulverized coal has been demonstrated. Techniques for pressing pulverized coal into rods have been developed, and the use of more sophisticated sample preparation procedures is currently being explored.

Our study of the combustion of coal/methanol slurries has been completed and reported. An experimental facility was built to examine the combustion of methanol and a slurry of methanol plus 5% coal in an environment similar to that of industrial and utility boilers. The furnace used (Fig. 6) was a horizontal water-cooled cylinder, 20 cm diam × 100 cm long, with a firing rate of 60 kW. Measurements taken throughout the furnace included temperature and concentration of carbon monoxide, carbon dioxide, water, oxides of nitrogen, methanol, and particulates; spectral radiation intensity measurements were taken along the axis of the furnace.

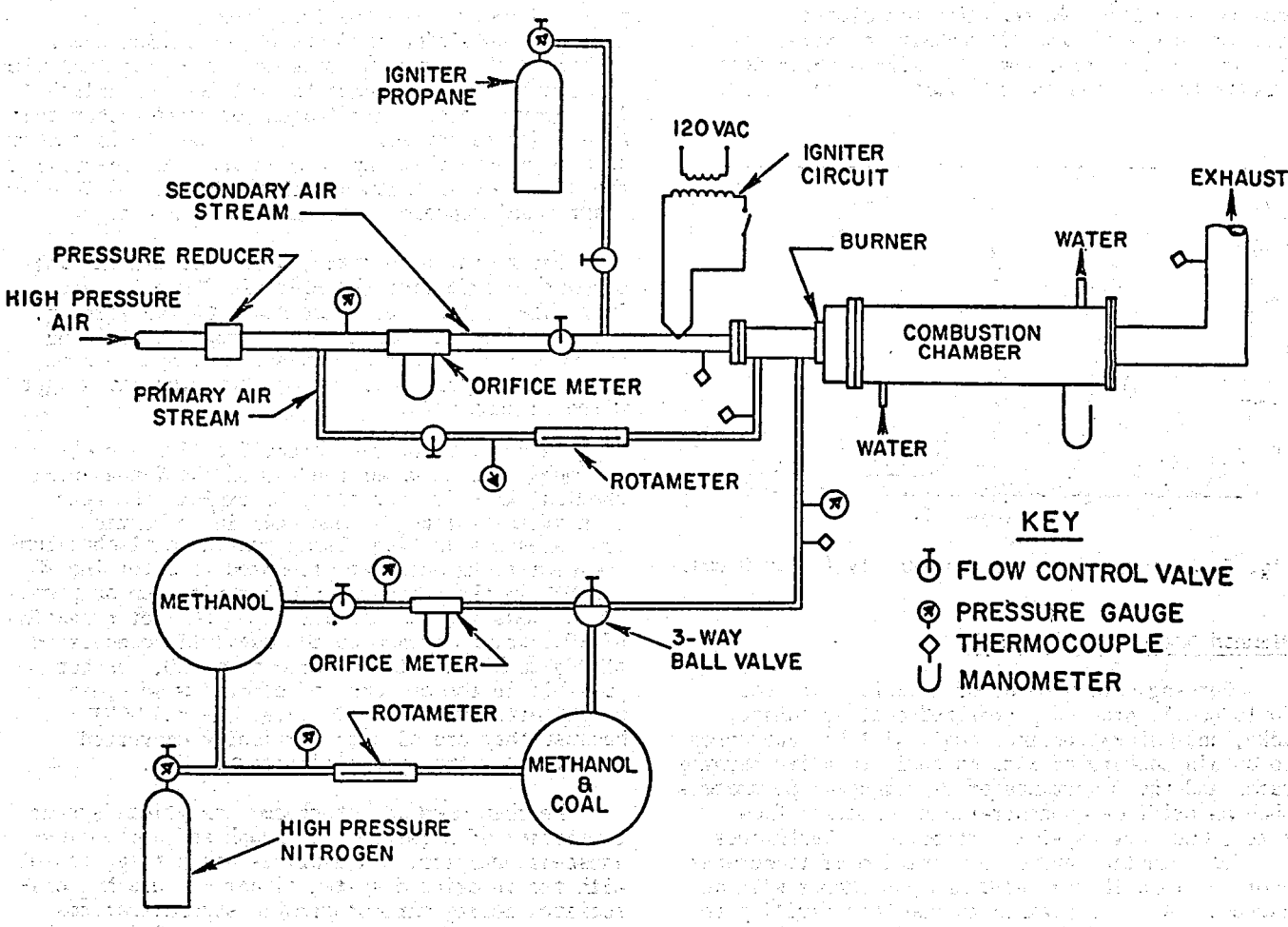

Fig. 6. Flow diagram of methanol furnace.

We found that, in general, temperatures in the pure methanol flame were higher than in the methanol/coal flame. Levels of nitrogen oxides were low in the pure methanol flame, less than 20 ppm NO; but addition of 5% coal to the methanol caused the NO concentration to increase to 100 ppm. This represented a conversion of 40% of the coal bound nitrogen to NO. Particulate levels increased from less than 0.001 g/m^3 for the pure methanol to over 0.25 g/m^3 when pulverized coal was added.

The low levels of soot and particulates in the methanol flame were found to have an effect on the spectral intensity. No continuous radiation was measured in the methanol flame, but a small amount of particulate radiation was observed in the spectra of the methanol/coal flame. The total emittance of the flame increased from about 0.10 to 0.135 with the addition of 5% pulverized coal, but the radiation intensity was reduced because of the lower flame temperatures. This effect was due, in part, to the presence of the coal particles and to the different nozzle that was used to burn the slurry.

A numerical program was written to calculate the spectral intensity from an inhomogeneous mixture of combustion products. Comparisons were made between the calculated intensity and the measured intensity for both fuel systems; Fig. 7 shows the results for the pure methanol case. The numerical results were approximately 25% lower than the measured results. Reasons for the discrepancy were investigated, and the results of other simplified models were also compared with experimental results to test the applicability of the models.

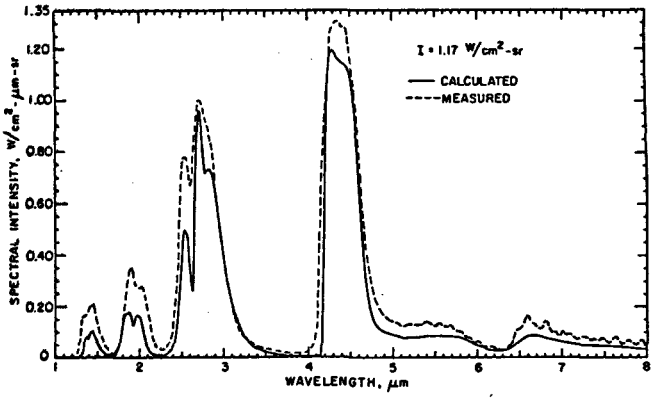

Fig. 7. Calculated spectral intensity (χ = 26.9 cm).

Planned Activities for 1977

Burning rate studies of a variety of coal fuels (coal, pressed pulverized coal, graphite, coke, and solvent refined coal) will be undertaken to obtain background data on their relative burning rates and the importance of experimental parameters such as oxidizer concentrations, oxidizer flow rates, and fuel physical properties. Techniques for determination and interpretation of temperature profiles in both the solid and gas phases will be pursued. We also planned to use this facility to study the fate of fuel nitrogen in the combustion of coal fuels.

FORMATION OF ODD-NITROGEN POLLUTANTS IN COMBUSTION PROCESSES (Brown, Sawyer, Schefer, Matthews)

Combustion processes are the primary sources of nitrogen oxides as air pollutants. In the combustion of conventional fuels, nitrogen oxides result principally from the oxidation of atmospheric molecular nitrogen (thermal NO_x) and the oxidation of nitrogen-containing compounds in the fuel (fuel nitrogen NO_x). According to Mezey et al.,[24] the amount of fuel nitrogen contained in fossil fuels can vary considerably, with negligible amounts in natural gas, significant amounts in distillate fuels, and amounts from 0.5 - 3% by weight in heavier fuels (residual oil, coal, coal-derived and shale-derived fuels). Fuel nitrogen will become a significant and even dominant source of NO_x in the future because of increased reliance on heavier fossil fuels.

Consideration of odd-nitrogen compounds (essentially all nitrogen-containing compounds other than N_2) as air pollutants has been primarily focused upon the nitrogen oxides, NO and NO_2, with occasional interest in ammonia. Although the thermal NO_x mechanism in lean and near stoichiometric mixtures is treated successfully with Zeldovich kinetics,[25] and it is now possible to qualitatively describe some features of the fuel nitrogen conversion to NO_x, no single experiment to date has quantitatively accounted for all the nitrogen in product gas analysis. Moreover, the chemical identity of the nitrogen-containing products of combustion under rich conditions and in processes involving fuel with chemically bound nitrogen has not been established. The importance of odd-nitrogen compounds other than NO and NO_2 is not well understood, but it is reasonable to assume that they are at least as reactive as the oxides of nitrogen and therefore should be of at least equal concern on an equal-mass basis.

Our research to date (which received initial support in 1975 from the Electric Power Research Institute[26]) has been concerned with the identification and quantification of nitrogen-containing products formed in the combustion of hydrocarbon fuels containing additives of low molecular weight nitrogen compounds.

In a review of the scientific literature, we found that an understanding of the fundamental chemical kinetics necessary to explain the reaction of fuel nitrogen compounds in combustion processes was lacking. Using conventional chemiluminescent techniques, we attempted to determine NO and NO_2 in the presence of other nitrogen compounds. NO was measured successfully; but the determination of NO_2, which depends on the catalytic conversion of NO_2 to NO and its measurement as NO, was not possible in the presence of other low molecular weight nitrogen compounds (e.g. NH_3 and HCN) because they are also catalytically converted to NO, under the same conditions as NO_2.

We then used an interfaced analytical system consisting of a gas chromatograph and a chemiluminescent analyzer. NO_2 analysis was not successful with the interfaced system either because NO_2 dissociated during chromatographic separation; however, NH_3 and HCN analysis appear promising with this technique.

Conversion of the low molecular weight nitrogen compounds to NO in four catalytic reactors was investigated. We found that the stainless steel reactor offered the best compromise among ease of construction, structual integrity, and quantitative conversion. Product compositions of fuel-rich $C_3H_8/O_2/Ar$ premixed, laminar flames were measured, with either ammonia or nitric oxide addition; in both cases, more than half of the nitrogen appears in the combustion products as species other than N_2, NH_x or NO. Although positive identificiation and quantitative analysis were not obtained, likely candidates include nitrogen dioxide, hydrogen cyanide, amines, and other cyano compounds.

In an additional study of NO and NO_2 measurement via chemiluminescent techniques,[27] we found two factors that affect the quantification of NO and NO_2 concentrations measured with chemiluminescent analyzers. The first is the dependence of the chemiluminescent intensity on the quenching efficiencies of various gases present in combustion gas samples. Quenching efficiencies were as a function of concentration (Fig. 8); and an expression was derived that allows calculation of the actual concentration of NO, given the measured concentration of NO and the concentrations of species in the product gas sample. The second factor investigated involves the conversion of low molecular weight nitrogen compounds to NO in commercial NO_x catalytic reactors. Conversion efficiences for six species were determined using a commercial stainless steel conversion oven at 920K.

An atmospheric pressure flame study in which low molecular weight nitrogen compounds are admixed to propane/oxygen/argon is in progress. Product gas composition will be analyzed for N_2, NO, NO_2, NH_3, and HCN to determine the fate of the fuel nitrogen. Various analytical techniques are being pursued to successfully analyze these compounds. The construction of a flat flame burner having a monolithic ceramic substrate with a γ-alumina washcoat and 10% platinum loading has been completed. Initial experiments are under way to characterize the flow downstream from the catalyst; preliminary results indicate flame stability.

Because the research facilities and possible collaboration with other investigators at Lawrence Berkeley Laboratory present an opportunity for definitive research in this area, two-year experimental and theoretical program consisting of four following primary tasks is proposed:

1) Identification and classification of odd-nitrogen compounds and preliminary estimation of source concentrations based on existing data;
2) Exploration and evaluation of the adequacy of analytical measurement techniques;
3) Identification of odd-nitrogen compound formation mechanisms and product levels in combustion processes;
4) Identification of odd-nitrogen compound formation mechanisms and product levels in pollutant control processes.

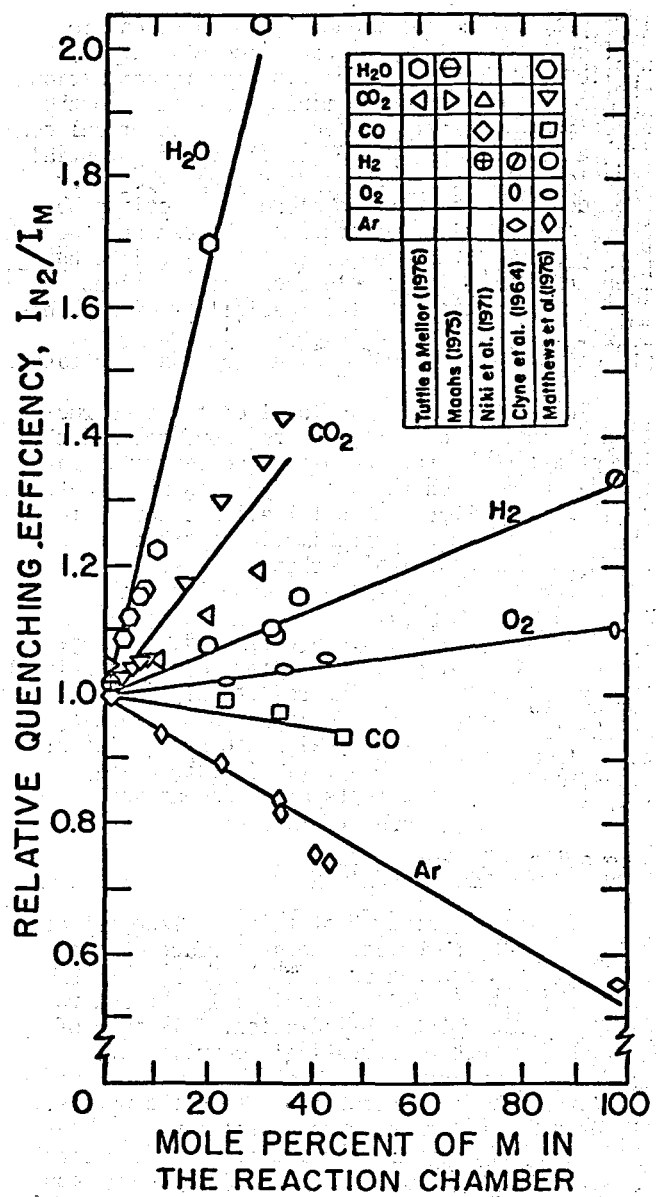

Fig. 8. Relative chemiluminescent intensity as a function of the third body concentration in the reaction chamber.[28-31]

The new gas chromatograph-mass spectrometer analytical system at Lawrence Berkeley Laboratory will improve the sensitivity of nitrogen compound analysis. The spectroscopic measurement of NO, NO_2, NH_3, and HCN as an independent check on the gas analysis procedures using aerodynamically quenching microprobes will be an important part of this work.

REACTIVE AND INELASTIC SCATTERING OF H_2+D_2 (Brown, Silver*)

Introduction

Combustion science is concerned with chemistry and fluid mechanics and the coupling between them. A detailed knowledge of combustion chemistry remains elusive since multistep mechan-

isms prevail and individual reaction steps are difficult to isolate for experimental study. The application of theoretical kinetics to combustion chemistry has been quite minimal relative to the experimental effort; however, some theoretical considerations are often used to eliminate potential reaction steps in a proposed chemical mechanism. One such idea is that biomolecular reactions between stable molecules generally have high reaction barriers and low frequency factors. The idea has been challenged for simple exchange reactions.[32-38] To further investigate the feasibility of such bimolecular reactions, a theoretical study of a prototype reaction, H_2+D_2 exchange, was undertaken.

This four-part study involved the construction of four H_4 potential energy surfaces and the investigation of the inelastic and reactive scattering of H_2+D_2 on them. The dynamics are treated quasi-classically; this formalism incorporates the following three approximations: treating the dynamics with classical mechanics, restricting initial molecular energies to experimentally determined eigenenergies, and using Monte Carlo techniques to compute average final state properties of several collisions with identical initial energy configurations. The results of the scattering study are presented in terms of reaction probabilities, average final state properties of the molecules, and average final state energy distributions. The effects of alignment and surface properties are examined.

Accomplishments During 1976

The initial study[39] of this set made use of a simple model potential energy surface of the London type which had an anomalously low barrier (compared with *ab initio* results) in the square planar saddle point configuration. This type of surface has become increasingly popular for molecular scattering calculations because of its relative ease of construction. Hence the purpose of our study was to provide a prototype calculation of a bimolecular reaction process occurring on a London surface. The total system energy considered in the study was less than the H_2 dissociation energy. The only reaction observed was the four center exchange reaction forming two HD molecules; its probability decreased with increasing initial vibrational energy, since vibrational energy decreased the probability for the favored reaction geometry. The product molecules exhibited a greater degree of vibrational excitation than rotational. Examination of the nonreactive inelastic collisions revealed comparable amounts of T → V and T → R energy transfer. Evidence for intermolecular (Figs. 9 and 10) and intramolecular energy transfer was presented.

A second study employing a semiempirical valence bond type surface was conducted at total energies of 150 kcal/mole. Four reaction paths were found:

H_2+D_2 → 2H+D_2 (hydrogen dissociation)

H_2+D_2 → H_2+2D(deuterium dissociation)

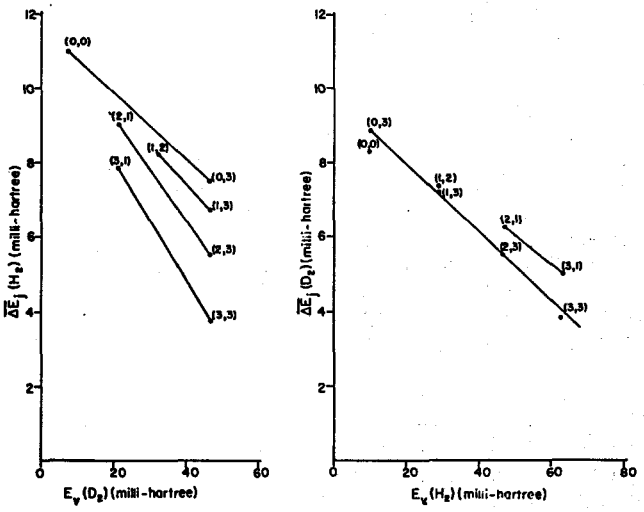

Fig. 9. Evidence for intermolecular energy transfer.

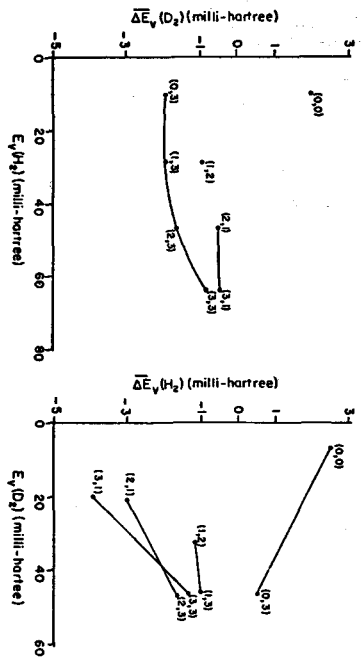

Fig. 10. Evidence for intermolecular energy transfer.

H_2+D_2 → HD+H+D(single exchange)

H_2+D_2 → 2HD(double exchange).

The particular path followed by the reactants was found to be extremely sensitive to the system's initial energy configuraiton. In general, total reactivity was directly related to the amount of initial vibrational energy in the system; and specific reactivity along the four paths was related to the distribution of initial vibrational energy between the reactant molecules. The results for the various sets considered are summarized in Table 1; a set is designated by values of the four initial quantum numbers (j_{H_2}, v_{H_2}, j_{D_2}, v_{D_2}). The

Table 1. Reactivity of the H_2+D_2 system on the repulsive valence bond surface.

Set	Total energy (milli-hartrees)	E_k	$E_j(H_2)$	$E_j(D_2)$	$E_v(H_2)$	$E_v(D_2)$	% Un-reactive	% H_2 dis-sociation	% D_2 dis-sociation	% single exchange	% double exchange
(0000)	240	223	0	0	9.89	7.02	100				
(3030)	240	218	3.2	1.6	9.89	7.02	100				
(0101)	240	189	0	0	28.8	20.7	99.3	0.7			
(0300)	240	172	0	0	63.6	7.02	78.0	22.0			
(0202)	240	160	0	0	46.7	33.8	93.3	4.7		2.0	
(0500)	240	138	0	0	94.2	7.02	68.7	31.3			
(0204)	240	133	0	0	46.7	58.4	93.0	0.3	0.3	5.3	1.0
(3234)	240	130	2.9	1.3	46.7	58.4	94.7		0.3	4.0	1.0
(0008)	240	128	0	0	9.89	101.4	75.0		24.0	1.0	
(0303)	240	128	0	0	63.6	46.3	86.0	5.0		7.0	1.7
(3333)	240	125	2.7	1.5	63.6	46.3	87.0	5.7		4.3	2.3
(0000)	330	313	0	0	9.89	7.02	88.0	12.0			
(0204)	271	165	0	0	46.7	58.4	81.0	6.0	0.7	8.7	2.7
(0303)	270	160	0	0	63.6	46.3	73.3	15.0		9.3	1.7
(0303)	213	102	0	0	63.6	46.3	97.3			2.3	0.3

energy transfer for both non-reactive and reactive collisions was examined and related to initial conditions.

Planned Activities for 1977

Two additional potential energy surfaces have been constructed using the valence bond theory to generate a simple model wavefunction, and are presently being analyzed and described. These surfaces are constructed using the semiempirical treatment of the London-Eyring-Polanyi-Sato type, but modified to include all overlap and multiple exchange integrals. Comparative scattering studies have been performed on the four potential energy surfaces to relate reactivity and energy transfer to surface properties; analysis and description will follow.

MEASUREMENT OF NO DENSITY BY RESONANCE ABSORPTION OF ZEEMAN TUNED Cd^+ LINE (Hadeishi, Agrawal, Robben)

Introduction

In situ measurements of chemical species in combustion are essential to the development and evaluation of fundamental theories concerning pollutant formation. Of particular interest from the environmental viewpoint have been the oxides of nitrogen, NO and NO_2. The prevalent technique of species measurement by probe sampling and subsequent analysis is not entirely reliable because of the chemical reactions in the probes themselves; these reactions form the subject of several current investigations, some within our own effort. Moreover, the extractive process does not permit rapid measurements which are required for studying turbulent combustion.

Optical techniques offer the promise of non-extractive measurement with good space and time resolution. Our current effort is directed toward measuring NO_2 by laser excited fluorescence and NO by resonance absorption. Several other researchers have also attempted species specific absorption measurements of NO; however, in all these cases the problem of calibration (also *in situ*) has not been resolved. The technique described below, in principle, circumvents the problem. In addition, it can be further developed for extremely good space and time resolution by use of frequency-doubled uv lasers.

Description of Project

In essence, resonance excitation of a single rotational level of NO is achieved by the Zeeman tuning of an atomic line. Several such atomic lines are available; however, from the standpoint of obtaining large oscillator strengths to achieve high sensitivity, the 2144.38Å Cd II line was used to excite the $A^2\Sigma$ K = 13 transition of the 0-1 vibrational band of NO. The cadmium lamp is placed in a magnetic field leading to splitting of the above line into its σ^+ and σ^- components. The σ^+ and σ^- lines each have two components whose separation is proportional to the magnetic field. The total intensity in the right circularly polarised light (σ^+) and the left circularly polarised light (σ^-) is exactly equal. By adjusting the magnetic field, the σ^- lines are brought into resonance with the NO line. The other components, σ^- , are used as reference and their absorption is attributed to particulate matter or other species. The differential absorption is due to NO. The absorption line-shape is mapped by scanning the magnetic field, and then is deconvoluted on computer to obtain the NO line shape. The measurement of the differential absorption in this manner makes the technique insensitive to the presence of other absorbing species unless such a species also has a line coincident with the NO line and of a comparable width. By measuring the absolute absorption, we obtain absorption cross-sections under low pressure conditions.

The problem of calibration is circumvented in the following way. When measuring in combustion, by scanning the magnetic field, we obtain the *in situ* line-shape of NO. Knowing the *in situ* absorption line shape, we apply a correction to the measured absorption which yields the absolute concentration of nitric oxide. From independent knowledge of the temperature (e.g. from the intensity of the Rayleigh scattering of laser light and from pressure) corrections for the Boltzmann distributions can be applied. It must be emphasized that a direct calibration of NO in combustion is impossible since calibrated quantities of NO introduced into the flames are altered by the combustion processes.

Accomplishments During 1976

An experimental set up was devised to test the proof of concept. The basic equipment is the same as used for IZAA and is described elsewhere,[40] except that the lamp was placed in a variable-field electromagnet. Lineshape at low pressure, pressure broadening, and collision broadening cross-sections for NO and N_2 were measured. Absolute measurement sensitivity was determined to be 1 ppm over a 10 cm path length, although it is believed that this limit can be lowered considerably by improved signal processing. Preliminary measurements in a hydrogen-air flame were made to demonstrate feasibility. Careful calibrated measurements are under way. A computer program to process the obtained data was also developed. Further details can be obtained in a preliminary report.[41]

Planned Activities During 1977

Further work will improve signal processing to increase the sensitivity of the instrument; this will primarily involve multiple-scan signal averaging to obtain the absorption lineshapes. We expect this will be followed by carefully calibrated measurements in flat flame burners where similar data on NO concentrations are available from sampling probe studies. A comparison of the two will yield important information on the reliability of the probe measurements.

A few shortcomings of the method must be acknowledged. Because it involves a line-of-sight absorption measurement, point measurements cannot be obtained. (Fluorescence measurements are made unduly complex by severe quenching due to O_2.)

Furthermore, incoherent light sources such as the one employed here do not allow high space resolution. And since the exciting source is not very bright, improved temporal resolution is at present not possible. However, as uv lasers become available in this wavelength region, it is conceivable that greatly improved sensitivities and resolutions in both time and space will become possible.

LASER-INDUCED FLUORESCENCE SPECTROSCOPY APPLIED TO TURBULENT COMBUSTION FLOWS (Daily, Chan)

Most of the energy needs of the United States are satisfied by the combustion of hydrocarbon fuels. As has been well documented, an understanding of the combustion process is essential to the development of more efficient and less polluting devices, and devices operating on newer, untested fuels. Such devices include laboratory burners, gas turbine engines, automboile engines, and combustion driven MHD generators. The major contribution to such understanding must come from the laboratory. Until recently, though, it has been virtually impossible to make *in situ* nondisturbing measurements of the parameters of most interest in a flame: velocity, temperature, and species concentration. The advent of lasers has opened the door for diagnostic techniques that can make such measurements.

One technique that shows great promise as a diagnostic tool for measuring species concentrations is that of laser-induced fluorescence spectroscopy (LIFS.) The method consists of illuminating the gas with a laser source tuned to an absorption line of the species of interest. The molecules are excited, re-radiating spontaneously, and fluorescence is observed at 90° to the laser beam. The beam diameter and the collection optics define the spatial resolution which may be as fine as 0.1 to 0.5 mm. In our laboratory we are examining the use of LIFS to measure radical species concentrations.

The primary difficulty with using laser-induced fluorescence spectroscopic to make density measurements has been that collisional de-excitation in high pressure flames completely dominates radiative de-excitation, causing fluorescence quenching. In the present work, this difficulty is overcome by using a laser source of sufficient intensity to saturate the exciting transition.

FOOTNOTE AND REFERENCES

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1976 WORKSHOP ON AN ENERGY EXTENSION SERVICE

A. H. Rosenfeld, C. York, P. P. Craig

BACKGROUND OF THE WORKSHOP

A Workshop on an Energy Extension Service was held July 19-22, 1976, on the Berkeley campus of the University of California. It was organized by Lawrence Berkeley Laboratory and the U. C. Council on Energy and Resources, and sponsored by the U. S. Energy Research and Development Administration, the Office of University Programs, the Federal Energy Administration (through the California Public Utilities Commission), and the California Energy Resources Conservation and Development Commission.

The 143 workshop participants, who included staff from federal and state agencies, private industry, utility companies, colleges and universities, national laboratories, public interest groups, and labor unions, attended meetings on five topics:

- Reexamination of the analogy between Agricultural Extension and Extended Learning Programs and the concept of an Energy Extension Service;
- Review and assessment of current programs dealing with energy conservation;
- Review of the plans and programs in energy extension services in a few states;

- Estimate of the economic impacts of energy conservation in both the United States and other countries;
- Conservation programs that have been instituted by utility companies.

General agreement was reached in the following areas:

INFORMATION BASE FOR ENERGY CONSERVATION

Every program dealing with the concept of an Energy Extension Service postulated the existence of a credible body of knowledge about energy conservation. Much of the discussion, however, centered on the lack of specific credible and accurate information and data in certain areas. The organizational plan for knowledge about energy conservation was based on the major economic sectors of our society. Although this choice led to certain overlaps and redundancies, for example in the insulation of residential, commercial, industrial, and government buildings, it has provided a familiar frame work for organization. There was broad consensus that an authoritative information source or clearinghouse needs to be established to prevent wasteful duplication of effort as the Energy Extension Service spreads throughout all fifty states. Such a clearinghouse system would not be a static inventory of ideas, but would be updated continually as new concepts and devices emerge and develop from the experimental state to generally accepted practice.

NEW KNOWLEDGE ABOUT ENERGY CONSERVATION

The generation of new knowledge has a natural home in the R and D activities of federal laboratories, industries, and universities. The system is clearly responding to the nation's needs for better energy saving methods, new energy sources, and an improved understanding of the role of energy in our society.

Many of the Workshop discussions centered on current R and D programs and new ways to implement their results. For example, the life-cycles of home appliances need study. New labeling procedures need to be developed which enable the consumer to make choices on the basis of energy efficiency. The challenge of introducing a new technology, such as solar heating or the storage of ice sludge also was dealt with.

ENERGY CONSERVATION INFORMATION DISSEMINATION

The primary purpose of this Workshop was to review the ways in which the knowledge that has been accrued can be passed on to the people who need it, want it, and will use it. Such a network for dissemination is what is meant by an Energy Extension Service. Two approaches to this problem were identified:

- The *indirect* approach, which includes teacher education, curriculum changes, technician and professional skill updating, and similar long-range methods to use the multiplier effect of the classroom to produce changes.
- The *direct* approach of marketing and advertising. The person-to-person techniques of the county agent system of the agricultural extension have been copied by those utilities that have revamped their marketing from selling energy to selling conservation measures. Mass media advertizing, the introduction of "hot lines" to answer questions about energy, special courses at adult continuing education centers, and a host of other direct marketing techniques were discussed. In each case, the essential ingredient was identified to be the ability to provide believable and accurate information about energy conservation.

EVALUATION OF PROGRAMS FOR ENERGY CONSERVATION

Some utility companies have begun work on "energy audits" and on estimates of how much energy is actually saved by conservation programs of the kind discussed throughout this workshop. They are the first to say how difficult it is to obtain objective measures of the energy saved in a specific situation, much less in a national program. As the new Energy Extension Service begins to coordinate the individual programs of all fifty states, extreme care and judgment will be required to establish reasonable, and probably different, sets of criteria for program performance. These performance criteria will need to be changed as the programs mature and develop and as new technology and knowledge are applied. A major component of the new Service should be a flexible, sensitive, and diversified program of evaluation and assessment.

OTHER RECURRENT THEMES

Several other concerns were repeatedly mentioned. First was the question of whether the adoption of a "conservation ethic" will have an adverse impact on economic growth, jobs, and our standard of living; several speakers agreed that it will not. Next was the common belief of the participants that although conservation will help to solve our national energy problems, it will not obviate the need for continued efforts to develop new sources of energy. Most of the discussions tended to focus on methods to conserve energy and how to introduce them to the public.

WORKSHOP PAPERS

A series of background papers were presented on various topics related to the development of an energy extension service. These have been collected as the "Proceedings of the 1976 Workshop on an Energy Extension Service," which will be available late Spring 1977. Authors and titles appear belows:

Implementation of Water Conservation by a Public Water Utility
John Olaf Nelson

Electric Load Leveling by Chilled Water Storage
Arthur H. Rosenfeld, Fred S. Dubin

ENERGY CONSERVATION COST/SAVINGS TABLES FOR CALIFORNIA

A. H. Rosenfeld, K. Anderson, P. P. Craig, D. B. Goldstein, R. W. Kukulka

We have studied California's energy problems and have developed a methodology for presenting in tabular form the capital cost and annual savings of many conservation measures in the residential, commercial, industrial, and transportation sectors. A full account of this work may be found in the proceedings of the 1976 Workshop on an Energy Extension Service.[1] Here, however, we focus our attention on the residential sector to illustrate the usefulness of cost/savings tables; we also summarize the overall conservation potential in California.

RESIDENTIAL RETROFIT CONSERVATION OPTIONS

Data on residential retrofit measures — conservation options which residents can undertake for their own homes — are given in Tables 1a and 1b. Column 1 lists the capital cost to the consumer of each option, at current retail prices. If labor is involved in the option (e.g. for the insulation measures), this cost is included in the entry. For example, the entry for retrofit attic insulation, $275, is the current California price for contractor-installed attic insulation for a typical house of 1200 sq. ft.

Table 1a. California residential sector retrofit - natural gas. MBtu = 10^6. M$ = 10^6 $.

OPTION	COST AND SAVINGS PER UNIT				STATEWIDE POTENTIALS		
	1. COST	2. ANNUAL ENERGY SAVINGS	3a. COST SAVINGS (col.1/col.2)	3b. ANNUAL RETURN ON INVESTMENT	4. TOTAL UNITS	5. TOTAL CAPITAL	6. ANNUAL ENERGY SAVED
	[$]	[MBtu/yr]	$\left[\frac{\$}{\text{MBtu/yr}}\right]$	[%/]	[MILLIONS]	[10^6]	$\left[\frac{10^{12}\text{Btu}}{\text{yr}}\right]$
COLD WATER LAUNDRY	$0	5	-	-	4	-	20
SHOWER FLOW RESTRICTOR	$2	3.5	0.6	270%	6.25	$12.5	22
INSULATE WATER HEATER	$6	2.5	2.4	63%	6.25	$37.5	15.5
NIGHT-TIME THERMOSTAT SET BACK 70° TO 55° (AVERAGE OVERALL HOUSING)	$50	21	2.4	63%	6.25	$313	131
SOLAR POOL HEATERS	$1400	150	9	16%	.25	$350	38
THE FOLLOWING 3 NUMBERED MEASURES ARE ASSUMED TO BE PERFORMED IN SEQUENCE BEFORE NIGHT TEMP. SETBACK							
1. RETROFIT ATTIC INSULATION (R-19) (SINGLE FAMILY UNIT ONLY)	$275	30	9	16%	2.25	$620	68
2. RETROFIT WALL INSULATION (R-11) SINGLE FAMILY HOUSE	$450	29	15.5	10%	4.0	$1,800	116
MULTI-FAMILY UNIT	$250	22	11.5	13%	1.8	$450	40
3. STORM WINDOW SINGLE FAMILY HOUSE	$440	12	37	4%	4.0	[$1,800]	-
MULTI-FAMILY UNIT	$250	8	31	5%	1.8	[$450]	-
COMBINED HOUSEHOLD HEATING MEASURES INCLUDING NIGHT THERMOSTAT SETBACK SINGLE FAMILY HOUSE	$1,215	82	15	10%	-	-	-
MULTI-FAMILY UNIT	$550	36	15.3	9.8%	-	-	-
SOLAR HOT WATER HEATERS	$1000	18	55	2.7%	6.25	-	-
TOTAL RESIDENTIAL NATURAL GAS CONSERVATION POTENTIALS COMPARE WITH 1975 CONSUMPTION FOR THIS SECTOR						$3,583	379 675
TOTALS FOR: (INCLUDES STORM WINDOWS BUT NOT SOLAR HOT WATER) SINGLE FAMILY HOUSE	$1,223	93	$13.15	11.4%			
MULTI-FAMILY UNIT	$558	47	$11.90	12.6%			

Table 1b. California residential sector retrofit - electric. MBtu = 10^6 Btu; M$ = 10^6 $.

OPTION	COST AND SAVINGS PER UNIT				STATEWIDE POTENTIALS		
	1. COST [$]	2. ANNUAL ENERGY SAVINGS [MBtu/yr]	3a. COST SAVINGS [COL.1 / COL.2] [$/(MBtu/yr)]	3b. ANNUAL RETURN ON INVESTMENT [%/yr][2]	4. TOTAL UNITS	5. TOTAL CAPITAL [10^6]	6. ANNUAL ENERGY SAVED [10^{12} Btu/yr]
COLD WATER LAUNDRY	$0	11	-	-	500,000	-	0.5
SHOWER FLOW RESTRICTOR	$2	8.25	0.24	1350%	800,000	$1.6	6.6
INSULATE WATER HEATER	$6	3.5	1.70	190%	800,000	$4.8	2.8
NIGHT-TIME THERMOSTAT (SET BACK 70° TO 55°)	$50	24	2	160%	750,000	$37.5	18.0
STORM WINDOWS							
SINGLE FAMILY HOUSE	$440						
NORTHERN CALIFORNIA		39	11.3	29%	110,000	$48.4	4.3
SOUTHERN CALIFORNIA		23	19.1	17%	140,000	$61.6	3.2
MULTI-FAMILY UNIT	$250						
NORTHERN CALIFORNIA		21	11.9	27%	90,000	$22.5	1.9
SOUTHERN CALIFORNIA		11	22.7	14%	385,000	$96.3	4.2
KITCHEN FLUORESCENT LAMPS	$30	2.65	11.3	29%	4,000,000	$120	10.6
SOLAR HOT WATER	$1000	41	24.4	13%	[800,000	$800	33]
TOTAL (EXCLUDING SOLAR HOT WATER OPTION)						$413	52.1
COMPARE WITH 1975 CONSUMPTION FOR THIS SECTOR							478
" " " " FOR NON-APPLIANCE RESIDENTIAL USES							185
THE ITEMS BELOW HAVE ATTRACTIVE RATES OF RETURN, AND ARE SEPARATED ONLY BECAUSE WE HAVE NO DATA ON HOW MANY POTENTIAL UNITS EXIST.							
RETROFIT ATTIC INSULATION (SINGLE FAMILY HOUSE ONLY)							
R-0 to R-19 NORTH:	$350	107	3.25	101%	?	?	?
SOUTH:	$350	69	5.	65%	?	?	?
R-11 to R-19 NORTH:	$150	14	10.7	31%	?	?	?
SOUTH:	$150	9	16.7	20%	?	?	?
RETROFIT WALL INSULATION							
SINGLE FAMILY HOUSE	$500						
NORTH		85	5.9	56%	?	?	?
SOUTH		57	8.8	37%	?	?	?
MULTI-FAMILY HOUSE	$250						
NORTH		58	4.3	76%	?	?	?
SOUTH		33	7.6	43%	?	?	?

Column 2 gives the average annual energy savings in MBtu (10^6Btu) per year for each option. We have used the 1976 average California prices of $1.50 per MBtu for gas and $3.27 per MBtu for electricity in these tables. (The electricity price is equivalent to 3.6¢ per kWh at 11,000 Btu/kWh_e.)

The energy conservation options in the tables are arranged in order of increasing cost/savings ratio. This ratio, given in Column 3a, is the number of dollars of investment in the option required to save one MBtu/yr of energy. To put these numbers in perspective, we note that the alternative to increased energy *conservation* is increased energy *supply*. The 1976 estimates of the investment needs for a synthetic gas (syngas) manufacturing plant are about $16/(MBtu/yr) of capacity. This investment simply erects the plant; to produce gas one must also buy the coal, ship it to the plant, and pay operating expenses. New electricity supplies are comparably expensive. A new base-load electric power plant requires an investment of about $17/(MBtu/yr) of fuel burned; and again, one must then add yearly costs for fuel and operating expenses. In contrast, for conservation measures, the investment is the only cost to be paid; one is immediately able to start saving money from reduced utility bills.

Annual gross return on capital, in percentage of investment saved per year, is given in Column 3b. These percentages will rise as energy costs rise. For example, when gas prices have doubled, the return to a consumer who insulated his attic will have gone from 19% to 38%.

Columns 4 through 6 total the potential costs and savings on a statewide level. Column 4 gives the number of candidates for the conservation option. For example, for attic insulation, we estimate that there are 2.25 million uninsulated, gas-heated houses in California which can be insulated. We make no attempt to estimate how many of these houses actually *will* be insulated. Columns 5 and 6 give the potential capital costs and savings statewide.

Table 2. Summary of California conservation potentials. (We include options with an annual rate of return better than 8%).

Sector	1. Capital Investment (M$)	2. Potential Savings: Energy Gas (10^{12} Btu/yr)	Energy Electric[A] (10^{12} Btu/yr)	Energy Electric[A] (10^{9} kWh/yr)	Peak Power (MW)	% of 1975 Sector	3A. Cost Savings ($/MBtu/yr)	3B. Annual Return on Investment (Note G)	4. Jobs: Man Year, From New Investment in Col. 1. (1000)	Jobs from Annual Energy Savings in Col. 2 (1000)
Residential Retrofit										
Gas	3583	379	-	-		56%	$10	21%	210	20
Elect.	413	-	52	4.6	-	28%	$ 8	41%	24	5
New appliances, 10 years x current sales										
Gas	200	40	-	-	-	6%	$ 5	40%	12	2
Elect.	750	-	130	14.2	-	46%	$ 5.8	61%	44	12
Commercial Retrofit										
Gas	26.2	21	-	-	-	8%	$ 1.25	160%	2	1
Elect.	300	-	149	13.5	-	27%	$ 6.5	50%	18	13
New Commercial										
Econ. Sci. Corp[H]	+	-	88	8	-	20%	0		0	8
ADL,ASHRAE 90-75	0			-	-					
Industry				-	-	-	-	-	-	-
Electric Peak Power										
Residential	12	-	-	-	350	60%	3¢ add./watt			
New appliances	0	-	-	-	4480		-			
Comm'l retrofit	150	-	-	-	4257	75%	3¢ add /watt			5
New comm'l	0	-	-	-	2600		-			
Industry	-	-	-	-	-	-	-		—	—
Agriculture	—	—	—	—	850					
TOTALS	5400	431	419	40.3	12,500				310	66
COMPARE SUPPLY: 1975		1665	-	151	27,000					
1985 Utility Projections		shortage	-	244	50,000					
1985 ERDC Staff		"	-	214	42,000					

At the bottom of Tables 1a and 1b, (and gathered in Tables 2 and 3) are the statewide costs and fuel savings of retrofit options, totalled over all measures with an annual rate of return of over 8%. We believe these results are remarkable. In the case of residences, about one-half of the natural gas now used could be saved. This would require an outlay of $3.5 billion, and the creation of 210,000 man-years of jobs, but the annual return on investment would be 21%. For the *marginal* cost of new gas (about $3/MBtu), the rate of return is 32%. For residential electricity, the fuel savings are smaller than for residential gas but are still substantial, even though appliances are not considered in these tables. A total of $413 million of investment is warranted, and the percent savings for the electric options is 28%; the annual return on investment is 40% at the assumed price of 3.6¢kWh. This price will undoubtedly increase, thereby increasing the rate of return. In these calculations, we have not even included the promising, but still uncertain, solar hot-water options.

Table 3. Conservation potentials from Table 2.

	Natural Gas (10^{12} Btu/yr)	Electricity (10^{9} kWh/yr)	Peak Power (MW)
1. Potential Savings from Table 2	431	40.3	12,500
2. 1975 Consumption	1665	151	27,000
3. (Savings / 1975 Consumption)	26%	27%	47%
4. Potential Reduction in Annual Growth Rate (One Tenth of Line 3)	2½%	2½%	5%
5. Utility-Projected Annual Growth Rate	Short-age	4.9%	6.4%

SUMMARIES OF CONSERVATION POTENTIALS

The total statewide conservation potentials from all sectors are summarized in Tables 2 and 3. Table 2 lists required investments, savings in energy and power, cost/savings ratios, and returns on investment, in a format similar to that of the detailed option tables. Conservation potentials are arranged by fuel and by sector. In addition, Column 2 of Table 2 and Row 3 of Table 3 give ten-year savings potentials expressed as fractions of 1975 consumption or peak power; roughly 25% of present energy and 50% of peak power could be saved in ten years. If we want to restate these percentage savings as reductions in annual growth rates, we simply divide by 10 years; this shows that we could reduce annual energy growth by 2.5% and peak power by 5%, as shown in Row 4 of Table 3.

REFERENCE

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ENERGY CONSERVATION ASSESSMENT*

S. M. Berman, C. Blumstein, V. Adams, K. Block, R. D. Clear, D. B. Goldstein, B. A. Greene, M. W. Horovitz, E. P. Kahn, W. Klein, E. L. Krieg, R. Kukulka, I. Lasater, F. B. Lucarelli, C. Orloff, C. Schroeder,† L. Vincent, W. Walzer, W. W. Wilms†

In 1976 the Energy Conservation Assessment group concentrated its efforts on work for the California Energy Resources Conservation and Development Commission (CERCDC). The ERDA-sponsored effort reported in the 1975 Annual Report was terminated for budgetary reasons.

The focus of the work for the CERCDC was the "conservation plan," a part of the Biennial Report that must be prepared by the Commission. This plan is intended to set forth the State's program for energy conservation. The program is comprehensive in that all consuming sectors (i.e., residential, commercial, transportation, etc.) are involved and conservation efforts are aimed at both fossil fuels and electricity.

The development of such a program requires both the analysis of specific measures and the synthesis of a group of measures into a coherent plan. The LBL effort was concentrated on the former task. As a first step, an outline was developed by LBL and CERCDC staff members to serve as a framework for the analysis of conservation measures. This outline (presented below) is similar to that developed for the previous ERDA-sponsored program, but includes changes that reflect CERCDC's greater concern with implementation strategies.

Outline for Analysis of Conservation Measures

I. Title of program or measure

II. Summary

- A. Brief description of program or measure highlighting key issues and summarizing results on energy-saving potential and other costs and benefits
- B. Recommendations for implementation

III. Background

- A. Total current and projected energy use in affected sector(s) including information on loads curves where relevant
- B. Maximum "technical" potential for energy and/or capacity savings, given current or foreseeable technology or policies
- C. Previous conservation efforts

IV. Implementation Strategies

- A. Description of strategies
- B. Estimated actual energy and/or capacity savings (impact dates)
- C. Costs
- D. Side effects (positive and negative)
  1. Environment impact
  2. Economic impact (aggregate economic activity, employment, etc.)
  3. Social impact (quality of life, lifestyle changes, business-decision changes, etc.)
  4. Health and Safety effects
  5. Impact on other conservation programs
- E. Anticipated problems and constraints
  1. Regulatory, legislative
  2. Public acceptance

3. Technological

4. Resource requirements (materials and labor)

5. Economic, fiscal

6. Risk (consequences of failure or partial success)

F. Administrative requirements

1. Actions needed and responsibility for implementation

2. Program monitoring and evaluation methods

3. Coordination required (other agencies, private sector)

V. Information

A. Additional data needs and proposals for obtaining

B. Data sources and bibliography

Following this outline, we made preliminary analyses of six energy conservation measures;

- Retrofit ceiling insulation for gas-heated residences
- Retrofit insulation for electric water heaters
- Installation of shower flow restrictors in existing and new residences
- Reduction of lighting in commercial buildings
- Load management for agricultural (on-farm) irrigation pumping
- Cogeneration of electricity and process steam for industry.

Results of these first studies have been reported to CERCDC.[1] The topics of retrofit insulation, cogeneration, and commercial lighting are examined in more detail in reports now in preparation. Additional topics being studied include power pooling, professional education and licensure, "passive" solar heating and cooling, and load management on large water-delivery systems (e.g. the California aqueduct).

Recently, we have been exploring the possibility of undertaking continuing projects on some of the above topics. One that has been agreed upon is an effort to implement some of the recommendations developed in our study on professional education and licensure. In this project LBL will work with California boards responsible for licensing professionals (such as architects) in order to develop questions on energy conservation for inclusion in licensing examinations.

FOOTNOTES AND REFERENCE

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ELECTRICAL ENERGY CONSUMPTION IN CALIFORNIA: DATA COLLECTION AND ANALYSIS

S. M. Berman, M. W. Horovitz, C. Blumstein, V. A. Adams, K. B. Anderson, P. Caesar, R. D. Clear, D. B. Goldstein, B. A. Greene, D. M. Gustafson, E. P. Kahn, L. B. King, R. B. Weisenmiller

This project was performed on behalf of the California Energy Resources Conservation and Development Commission (CERCDC), which is required by law to develop a methodology for forecasting electricity sales and demand in the State. We have provided CERCDC with a data base on the patterns and efficiencies of electricity use in California that is flexible enough to be adapted to a variety of forecasting needs. In the course of gathering data and analyzing the components of end use, we also developed a model to account for historical trends and future changes in the pattern of electricity use. The model starts from an end-use accounting point of view, summarized in Fig. 1.

$$\begin{pmatrix}\text{End-use}\\ \text{electricity}\\ \text{consumption}\end{pmatrix} = \begin{pmatrix}\text{Total}\\ \text{households}\end{pmatrix} \times \begin{pmatrix}\text{Device}\\ \text{saturation}\\ \text{rate}\end{pmatrix} \times \begin{pmatrix}\text{Unit}\\ \text{electricity}\\ \text{consumption}\end{pmatrix} \times \begin{pmatrix}\text{Total}\\ \text{electricity}\\ \text{consumption}\end{pmatrix}$$

$$= \text{Sum of} \begin{pmatrix}\text{Consumption}\\ \text{by all}\\ \text{end uses}\end{pmatrix}$$

Fig. 1.

The accounting model can be adequately employed only for residential electricity consumption because data on the stock and efficiencies of devices in the other sectors are sparse or nonexistent. In the residential application, devices are household appliances.

Table 1. 1975 Electricity sales in the residential sector. $\overline{UEC}$ is the unit electricity consumption of a device type, averaged over the stock; UEC(75) is the unit consumption of new equipment sold in 1975; UEC(80) is an estimate of the unit consumption that would result from imposition of appliance efficiency standards and energy-conservation building codes.

	$\overline{UEC}$ (kWh/yr)	UEC (75) (kWh/yr)	UEC (80) (kWh/yr)	Lifetime (yr)	Saturation (%)	Total number of units ($\times 10^3$)	Total sales (kWh/yr$\times 10^6$)	Total sales (%)
Households (all devices)	5,881				100.0	7,441	43,517	100.0
Refrigerators	1,200	1,575	1,050	20.0	115.0	8,557	10,269	23.6
Lighting	1,130				100.0	7,441	8,408	19.3
Resistance heaters	5,330	5,040	2,750		10.0	752	4,006	9.2
Ranges	1,200	1,200	1,075	16.9	36.3	2,701	3,241	7.4
Water heaters	4,000				10.7	796	3,185	7.3
Central air conditioners	2,500	1,950	960		15.1	1,124	2,809	6.5
Color television	420	255	220	15.5	75.0	5,581	2,344	5.4
Freezers	1,400	1,400	1,050	24.5	22.2	1,652	2,313	5.3
Clothes dryers	950	875	825	15.3	29.1	2,165	2,057	4.7
Room air conditioners	900		640		23.6	1,756	1,580	3.6
Black & white television	140	60	35	13.8	80.0	5,953	833	1.9
Dishwashers	250	300		13.6	36.6	2,723	681	1.6
Clothes washers	70	70		12.3	64.7	4,814	337	0.77
Miscellaneous (residual)	195				100.0	7,441	1,454	3.3

To produce a model which fits historical data and which is suitable for forecasting, we developed a method to account for changes in the stock of appliances and changes in the efficiency of those devices. The central conceptual element in our model is the exponential lifetime assumption. This means that for every type of device, we assume that a constant fraction of the stock is removed (i.e. junked) in each unit time interval, independent of the age or year of manufacture. To apply this conceptual framework to the available data requires estimating the lifetime of each appliance. Studies have been done of retention times (how long one owner keeps an appliance); but the relevant information is the sum of all retentions, or the total lifetime. We developed a model which approximates this total lifetime from data on retention times of new and used appliances. The decay constant in our stock model then is simply the inverse of the device lifetime.

In any given year the unit electricity consumption of a device is an average weighted by the stock and efficiency of all existing devices of the given type. The unit energy consumption will change as the stock of a particular appliance turns over due to sales and removals. We collected data on the distribution of sales and efficiencies to produce average unit electricity consumptions ($\overline{UEC}$) over the stock for fourteen end-uses and two miscellaneous items. This is shown in Table 1, which also includes estimates of the unit electricity consumption that would result from the imposition of appliance efficiency standards and energy conservation building codes.

Data on heating and cooling energy requirements is disaggregated by single-family, multi-family, and mobile units. This type of disaggregation is very important when considering heating and cooling requirements, which differ markedly by unit type. The exponential lifetime model was applied to 1970 Census data and new construction figures for 1971-75 to calculate the 1975 stock of housing in our three unit-type categories. Unit electricity consumption for heating and cooling were determined using the LBL thermal load program TWOZONE. Loads determined by TWOZONE were weighted by the stock sizes of each housing type in each geographical region. The conservation measures evaluated were: (1) the requirement that housing units with central air conditioners or resistance heat have double-glazed windows, and (2) a 35% improvement in the efficiency of central air conditioners.

Two basic sources of appliance saturation data are the U. S. Census and utility company surveys. There are problems with both sources. Census questions are typically less detailed than utility questions and occasionally misleading. For example, the question "Do you have a refrigerator?" cannot reveal that a significant number of California households have more than one refrigerator. On the other hand, the Census data are more representative than utility surveys, which have no mechanism to assure responses from low-income groups. Spanish-speaking groups in Southern California utility areas probably were poorly represented.

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POWER SYSTEM RELIABILITY

M. Davidson, D. Levy, E. Kahn

Electricity consumers expect a certain degree of reliability from their power service. Although there are variations from one region to another on what the standard of service reliability should be, all power systems must plan to have some reserve generating capacity to insure reasonable service continuity. Utility companies have developed probabilistic methods to study how much reserve capacity is necessary to meet the goal they have set for reliability. Typically, these models require extensive computer implementation and provide very precise answers to very particular problems. Unfortunately, however, the reliability models are not well suited to the present power-system planning situation which requires great flexibility and the analysis of many alternatives. The electric utility is beset by a host of financial, environment, and resource constraints that have complicated the planning process considerably.

To meet the need for flexible planning tools, we have developed an analytic approximation to the most common reliability model, the loss of load probability (LOLP).[1] To simplify the analysis, we neglect several parameters employed in the standard computer calculations. Some of these factors are complementary. For example, utilities typically schedule maintenance on generators for the off-peak season; thus a fully accurate LOLP calculation is based on load variations during the day and over the year, as well as on a forecasted maintenance schedule. We neglect these factors and assume that the utility faces only a constant load at the peak level; this is a conservative assumption. The other main assumption in our model is that all generators have the same capacity and the same probability of random (forced) outages. This assumption is less realistic and is reasonable only if the generator mix under study does not change quickly over time. Future work will be devoted to dropping this limitation and generalizing the analysis.

The basic form of our approximation turns out to be a normal probability distribution for LOLP. From the expression for LOLP, we derive a formula

for the reserve margin which has the following form:

$$R = A + B/\sqrt{T} \qquad (1)$$

where A and B are constants, T is the total generating capacity of the system, and R is the reserve margin. We have shown that Eq. (1) fits data from a large power pool with good accuracy. In the future, we expect to develop a form of Eq. (1) in which the characteristics of the system under question appear in place of the constants A and B.

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Instrumentation Development Program

INTRODUCTION

Energy technologies emit pollutants that are potentially harmful to man and other forms of life. It is desirable to characterize these pollutants, to understand their fate, and to assess their biological impact.

In order to control these pollutants, it is necessary to find methods for monitoring the level of various substances that exist in low concentrations. The Energy & Environment Division instrumentation development program is designed to meet these needs. Emphasis is placed on the development of physical methods as opposed to conventional chemical analysis techniques. The widely recognized advantages include ease of operation and minimal sample preparation. Physical methods sometimes provide multi-parameter measurements, and are often the only means of achieving the sensitivity necessary for detecting trace elements.

The areas in instrumentation now being investigated include laser optoacoustic spectroscopy of gases, liquids, and solids; liquid crystal gas detectors; coherent forward scattering as a detector for atoms and molecules; advanced forms of atomic absorption spectroscopy; and X-ray fluorescence spectroscopy. Work is continuing on the Survey for Environmental Monitoring.

CHARACTERISTICS OF AN OPTOACOUSTIC DETECTOR

R. W. Gerlach,* G. T. Boyd,* M. J. Kelly,* H. Birecki,*, and N. M. Amer*

Laser optoacoustic spectroscopy is a refined version of infrared absorption spectroscopy. The only requirement for its use is that the spectral output of the laser matches one or more of the absorption bands of the gas to be detected. When this requirement is satisfied the incident photons can be absorbed and the temperature of the sample will rise. When the laser beam is modulated with a rotating shutter, the temperature change of the sample causes a time-dependent fluctuation of pressure which can be detected with a microphone placed in the sample cell. With proper electronic circuitry the microphone signal can be recorded and/or digitized.

This paper deals with the characteristics of a first-generation optoacoustic cell that uses methane as an absorber for 3.39 micron He-Ne laser light. Three parameters were used to evaluate the detector: the modulation frequency, the pressure dependence of the signal for a fixed percentage of methane in nitrogen, and the dependence of the signal on methane concentration at constant pressure.

A 3" long copper absorption cell with a 1" inner diameter was used. NaCl windows sealed the ends of the cell and a General Radio electret condenser microphone sensed the pressure fluctuations. The detector was also mounted on a lead brick base to ensure vibrational isolation.

The light source was a Spectra-Physics He-Ne laser with an output power of 6 mW at 3.39 μ. Phase-sensitive detection was used for the microphone output. A variable-frequency chopper was used, the chopping frequency being swept by applying a ramp voltage to the chopper control unit.

The frequency response of cylindrical cells was investigated using a mixture of 12 1/2% methane in nitrogen. The results are plotted in Fig. 1. The reason for the overall roll-off of the response with increasing frequency is that there is a long relaxation time for thermal conduction in the gas. One can estimate a single relaxation time of ∿10 seconds for the cell. The broad peak occurring around 80 Hz is due to mechanical resonance in the system. At higher frequency the first two longitudinal resonances of the cell are observed at

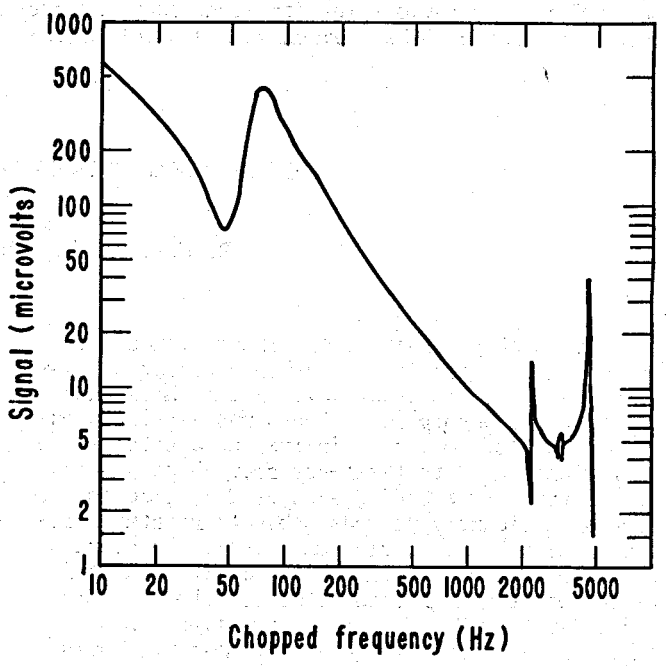

Fig. 1. Frequency response of the optoacoustic detector with 12.5% methane in nitrogen. (XBL 773-648)

2270 Hz and 4545 Hz. These resonances are associated with the velocity of sound in the mixture and correspond to solutions of the acoustical wave equation with the boundary condition that the pressure gradient must be zero at the walls of the cell. The second resonance is much stronger than the first because the microphone is situated at a pressure node for the first longitudinal mode whereas it is an antinode for the second one.

Using the 12 1/2% methane mixture we observed the change of the signal at several frequencies with pressure varying from atmospheric pressure to a fraction of a torr. If the laser was exactly coincident with the absorption line center, and if the absorption linewidth was dominated by pressure-broadening over the entire pressure range investigated, then the amount of power absorbed in the cell would have remained constant, independent of pressure, as long as the same fractional methane concentration was maintained. However, there is a 100 MHz offset between the laser line and the absorption line center. Doppler broadening begins to dominate over pressure broadening below 70 torr. As a result absorbed power is nearly constant down to roughly 150 torr, but then falls off rapidly for lower pressure. This falloff in absorbed power causes a corresponding falloff in optoacoustic signal for all chopping frequencies investigated. However, the signal per unit absorbed power has different behaviors for different chopping frequencies. For a 10 Hz frequency this quantity increases with decreasing pressure over the entire observed pressure range, while the signal at 1 kHz is virtually constant. The signal at the 4.54 kHz resonance is very nearly linearly proportional to pressure over the entire range.

We measured the signal for a 10 Hz chopping frequency for several different concentrations of methane in nitrogen at 1 atm total pressure. The lowest concentration investigated was approximately 120 ppm. At this concentration we measured a signal of 68.5 microvolts. Our noise level is now less than 100 nanovolts in a 0.03 Hz bandwidth. If the signal is assumed to be linear with concentration below 120 ppm, then the signal to noise ratio would be unity for a concentration of 180 ppb. Much smaller concentrations can be detected by acoustically shielding the detector.

We are currently conducting systematic studies on isolating noise sources (both mechanical and electrical). Preliminary results indicate that the elimination of these sources reduces the background signal by three orders of magnitude, thus enabling detection at the sub-ppb concentration levels.

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A CARBON MONOXIDE LASER OPERATING IN THE 1 → 0 BAND

R. W. Gerlach,*, M. J. Kelly* and N. Amer*

For highly sensitive and interference-free optoacoustic detection of carbon monoxide a laser is needed which emits at wavelengths where there is strong CO absorption. The strongest infrared absorption for CO occurs in its fundamental 1 → 0 vibrational band that extends from about 4.5 to 4.8 microns. Hot bands, such as 2 → 1, do not absorb significantly at reasonable temperatures because the v=1 level, 2100 cm^{-1} above the vibrational ground state, is not thermally populated except at very high temperatures. The overtone bands, such as 2 → 0, are not as strong as the fundamental because the diatomic molecule forms an approximation to a harmonic oscillator; the overtone transitions are completely forbidden for a perfect harmonic oscillator.

A carbon monoxide laser might be considered a likely candidate to provide wavelengths corresponding to strong CO absorption. However, conventional CO lasers operate only on hot bands at wavelengths greater than 4.8 microns. Although gas discharge[1,2,3] and chemical lasers[4,5] operating on the 1 → 0 of CO exist, they all exhibit a large degree of instability both in frequency and output power. In this paper we describe a stable electric discharge CO laser which lases on several bands including the 1 → 0 transition.

Several modifications were made to improve the previous scheme. A drawing of the laser discharge tube appears in Fig. 1. The double wall was constructed entirely of pyrex. As in Djeu's laser, helium passed through the outermost ports (A) so that CO molecules are swept out from the unexcited end regions in order to prevent self-absorption. N_2, CO, He, and Xe passed through the ports above the outer electrodes (B). All the gases exhausted through the center of the tube. The discharge tube was enclosed in a liquid nitrogen cooling jacket so that the laser operated on 1 → 0 band. Unlike earlier designs, the cooling jacket was completely closed off except for four 1-cm diameter tubulations. Liquid nitrogen flowed through one of these, and the boiloff exhausted through the other three. The liquid nitrogen cooling jacket was isolated from ambient room temperature by thermal insulation. This enhanced the output power stability of the laser and reduced the liquid nitrogen consumption by a factor of 2.

Another improvement was the large-area nickel electrodes that were mounted close to the main discharge section. This lowered the discharge voltage and reduced the amount of unneeded power dissipation.

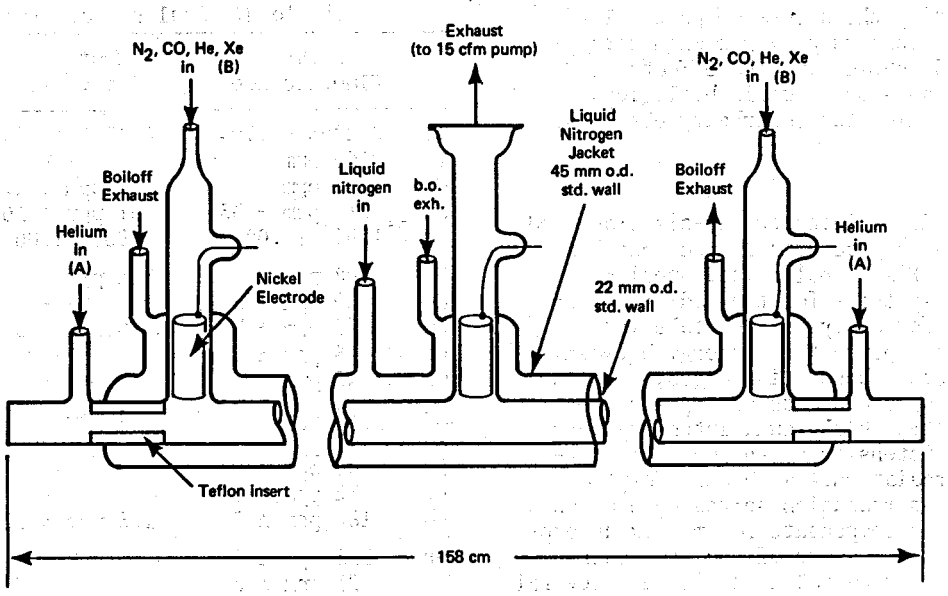

Fig. 1. Carbon monoxide laser tube. (XBL 773-654)

Teflon Brewster angle window mounts were used for the CaF_2 windows. These mounts slid over each end of the tube and O-rings were used to seal the vacuum between the windows and the Teflon mounts.

The mirrors used for multiline operation consisted of a 5 meter radius of curvature dielectric coated ZnSe output mirror having 98% reflectivity at 4.7 microns and a 6 meter radius ZrCu mirror. For single line operation, the latter was replaced by a 300 line/mm grating blazed for 4 microns.

Transitions P(8) through P(12) in the 1 → 0 band have been observed (wavelengths 4.734 to 4.773 microns) in multiline operation, but only P(8) through P(10) have been obtained in single-line operation. The maximum single-line power thus far observed has been 3mW on P(9) and P(10). In concurrence with Houston and Moore,[3] we have found that lasing on the 1 → 0 transitions is possible without the addition of xenon. In fact, the P(8) transition was obtained only when xenon was not added to the gas mixture.

As to the tunability of this laser, we found that without changing the gas mixture or the discharge current we can grating tune the laser on 70 transitions in the range from 4.7 to 5.4 microns. Increasing both the amount of CO in the mixture and the discharge current results in increased multiline output power and shifts the output spectrum toward longer wavelengths. By using NaCl windows for longer wavelength transition, we anticipate lasing action up to the 36 → 35 vibrational transition. This means that this CO laser provides a coarsely tunable coherent light source which covers the 4.7 to 8 micron region and thus is an extremely useful laser for detecting a wide variety of pollutants.

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DEVELOPMENT AND APPLICATION OF ENERGY DISPERSIVE X-RAY FLUORESCENCE ANALYTICAL METHODS

R. D. Giauque, R. B. Garrett, and L. Y. Goda

INTRODUCTION

There is an ongoing program within the chemical analysis group which involves the development and application of energy dispersive X-ray fluorescence (XRF) analytical methods. These methods are used by research programs funded through the Energy & Environment Division as well as by projects receiving outside government funding. During the past year we contributed to programs devoted to (1) studying physical and chemical processes which transform pollutants in an urban

plume, (2) estimating the amount of particulate sulfur emitted by vehicles equipped with catalytic convertors, (3) evaluating the effects of trace metal pollutants on specific biological systems, and (4) searching for superheavy elements.

METHOD DEVELOPMENT

A method for determining twenty-six trace and two major elements in geochemical specimens has been established. Finely pulverized specimens which are infinitely thick for the radiations of interest are used for analysis. We take into account that for any given X-ray energy between adjacent major element absorption edges, both the reciprocal of the specimen mass absorption coefficient and the spectral background intensity vary linearly with the intensity of the Comptom scattered excitation radiation.[1-4] Hence, Comptom scattered excitation radiation serves both as an internal standard to compensate for matrix absorption effects and as a measure of spectral background intensity as illustrated in Fig. 1. Several

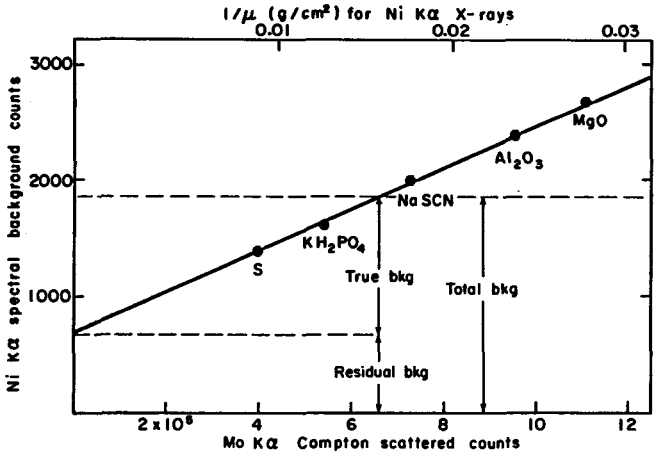

Fig. 1. Spectral background curve established for nickel using five powdered materials. (This curve serves to illustrate that the Comptom scattered excitation radiation intensity is directly proportional to both the true background and the reciprocal of the mass absorption coefficient.) (XBL 766-2932)

pure compounds, which have X-ray cross sections that vary over a wide range, are used to develop individual X-ray line spectral background curves. Standardization is achieved using geochemical reference standards. Fluorescent X-rays used for analysis are in the range of 4.5 to 32 keV. Since Fe is typically the only major constituent element present which has an absorption edge in this range, the specimen cross section curves vary smoothly at energies less and greater than the Fe K absorption edge. This considerably simplifies the overall matrix correction procedures required for analysis.

Each specimen is analysed for 20 minutes. Tables 1 and 2 list results obtained from French geochemical standards of granite and basalt, respectively, and serve to illustrate the capability of the method. The neutron activation analyses were carried out by Frank Asaro and co-workers.

Table 1. Analysis of Granite GA

	X-ray Fluorescence	Neutron Activation	Reported
Ti	0.226% ± .104	0.174% ± .042	0.228%
V	<160 ppm	---	36 ppm
Cr	<51 ppm	7.4 ppm ± 2.6	(10) ppm
Mn	712 ppm ± 33	631 ppm ± 16	665 ppm
Fe	1.94% ± .08	1.95% ±.06	1.98%
Ni	<8 ppm	<26 ppm	7 ppm
Cu	20 ppm ± 8	---	14 ppm
Zn	72 ppm ± 7	76 ppm ± 8	75 ppm
Ga	15 ppm ± 2	---	16 ppm
Ge	<2 ppm	---	(1.5) ppm
As	<3 ppm	<4 ppm	---
Se	<3 ppm	---	---
Br	<3 ppm	---	---
Pb	32 ppm ± 2	---	---
Rb	180 ppm ± 2	175 ppm < 12	175 ppm
Sr	313 ppm ± 4	---	305 ppm
Y	21 ppm ± 2	---	(18) ppm
Zr	123 ppm ± 11	---	140 ppm
Pd	<5 ppm	---	---
Ag	<5 ppm	---	---
Cd	<4 ppm	---	---
In	<5 ppm	---	---
Sn	<6 ppm	---	4 ppm
Sb	<7 ppm	<0.20 ppm	---
Te	<9 ppm	---	---
I	<11 ppm	---	---
Cs	19 ppm ± 15	6.6 ppm ± 0.4	(5) ppm
Ba	840 ppm ± 37	816 ppm ± 36	850 ppm

APPLICATION OF X-RAY METHODS

Our group as well as groups from other laboratories have participated in two ERDA sponsored Da Vinci ballon programs designed to study physical and chemical processes which transform pollutants in an urban plume. In these programs a manned balloon, carrying a sizeable package of sophisticated instrumentation and sampling equipment, was launched in St. Louis and traveled in the plume from a power plant for approximately 300 miles over a 16 hour time span. Atmospheric particulate sulfur levels were correlated with B_{scat} (optical scattering) measurements, which serve as indicators of the aerosol mass in the 0.1 to 1 micron particle size range, and were usually correlated with ozone levels (with a time lag).

During the past year a group of researchers at another laboratory reported that with XRF techniques they discovered new superheavy elements in microcrystalline monazite inclusions exhibiting giant halo formations in biotite mica.[5] Subsequently, we analyzed a large number of geological samples as part of an intensified laboratory effort to determine the validity of the reported existence of these superheavy elements. Our experiments, as well as those of researchers at other laboratories, produced results which suggest that the claim for the discovery is an erroneous interpretation of X-ray fluorescence data.

Table 2. Analysis of Basalt BR

	X-ray Fluorescence	Neutron Activation	Reported
Ti	1.57% ± .04	1.64% ± .05	1.57%
V	175 ppm ± 86	-	240 ppm
Cr	310 ppm ± 44	379 ppm ± 10	420 ppm
Mn	1587 ppm ± 36	1521 ppm ± 36	1600 ppm
Fe	9.13% ± .09	9.10% ± .22	9.01%
Ni	232 ppm ± 12	281 ppm ± 41	270 ppm
Cu	80 ppm ± 11	-	70 ppm
Zn	151 ppm ± 12	171 ppm ± 16	160 ppm
Ga	17 ppm ± 3	-	(20) ppm
Ge	<3 ppm	-	-
As	<3 ppm	5.5 ppm ± 3.2	-
Se	<3 ppm	-	-
Br	<3 ppm	-	-
Pb	6 ppm ± 4	-	(16) ppm
Rb	43 ppm ± 2	36 ppm ± 25	45 ppm
Sr	1326 ppm ± 9	-	1350 ppm
Y	35 ppm ± 2	-	(27) ppm
Zr	259 ppm ± 25	-	240 ppm
Pd	<7 ppm	-	-
Ag	<6 ppm	-	-
Cd	<6 ppm	-	-
In	<6 ppm	-	-
Sn	<7 ppm	-	(8) ppm
Sb	<8 ppm	0.28 ppm ± .26	-
Te	<11 ppm	-	-
I	<14 ppm	-	-
Cs	<30 ppm	0.65 ppm ± .50	-
Ba	1288 ppm ± 84	1095 ppm ± 50	1050 ppm

PLANNED ACTIVITIES

A XRF method is being developed for the determination of forty elements, Ti (Z = 22) through Ce (Z = 58) and heavy metals Ta, W, Hg, Pb, Th and U, in geochemical and industrial solid waste (e.g. sludge residues, coal fly ash, etc.) specimens. Relatively small sample sizes (100 mg) will be required for analysis. Matrix effects will be stabilized by diluting the samples with sulfur powder, a relatively high X-ray absorbing substance for this type of specimen. We plan to apply this method to determine the concentration of a broad range of metals in solid wastes, including those from energy generation, prior to disposal.

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DEVELOPMENT OF ATOMIC AND MOLECULAR DETECTOR BASED ON COHERENT FORWARD SCATTERING

T. Hadeishi

The main purpose of this project is to develop a technique to measure molecules with high sensitivity and specificity in the UV-visible region without the requirements of complex chemical pre-preparation. The importance of such a device cannot be overemphasized. Every year about 200 new compounds are introduced into the environment but there is presently no device available to make 200 molecular identifications per year. Our hope is that the coherent forward scattering technique may help to achieve this almost impossible task.

It is well known that most molecules have strong optical absorption in the ultra-violet region. Unfortunately, because of complex energy levels associated with molecules, the absorption spectrum is continuous even for relatively simple molecules such as SO_2 and NO_2. Thus, neither the absorption spectroscopy nor the fluorescence technique is suitable for molecular detection since it is not possible to make unique identification. This is especially true if we have several molecules having absorption in a particular spectral range. Thus, we must look for some other molecular characteristics. One such physical phenomenon is magneto-optical rotation. Another is magnetic double refraction. Both can be described by the theory first discovered by Faraday. These phenomena occur only when either the absorbing state or the excited state has a magnetic moment, that is, either the ground states or excited state must have finite Lande´g-value. Lande´g-value is large only for the state with a low total angular momentum quantum number. Since the total angular momentum of molecules could be quite large, only the smaller angular momentum state has appreciable g-value, resulting in the extreme simplification. This is the basis of the technique we are developing.

The magneto-optical rotation as well as the magnetic double refraction effect is due to interference between the primary light beam and the scattered beam. This phenomenon can be described in terms of propagation of electromagnetic wave through dielectric media. The experimental set-up consists of placing the media to be investigated between a pair of crossed polarizers in the presence of either a longitudinal or transverse magnetic field. When the wavelength of the primary beam is at the appropriate absorption wave-length so that there is a finite g-value associated with the transition, the linearly polarized light either rotates or becomes elliptically polarized. Thus, the scattered beam will transmit the second crossed polarizer. The intensity of the scattered beam is related to the concentration of scattering media.

The main advantage of this system, in addition to the simplification of the molecular spectrum, is that the primary beam is not detected. Thus, the signal to noise ratio is quite good. Any light source can be used. However, a laser light source is better because excellent extension between the pair of crossed polarizers can be achieved. Typical sensitivity which we have tested for in Na_2 is 1 part per trillion ($1/10^{12}$) with S/N=10 using a tunable laser.

At present we are testing the performance characteristics using atoms. So far the test has been conducted for Hg and Cd using electrodeless discharge lamps (EDL) and for Na using a tunable laser. We have verified that this technique is at least ten times more sensitive than the atomic absorption technique. The same scaling should apply to molecular detection so that a similar gain in sensitivity should apply over the molecular absorption.

So far the test on molecules has been limited to Na_2, I_2, NO, NO_2, SO_2, and OH. However, we have verified that expected simplicity can, in fact, be achieved by this method. We are in the process of making sensitivity tests at present. Additionally, we are using this technique to identify the molecular transitions in uranium compounds made at LBL. The main effort will be directed towards:

a) Identification of isotopic effect in molecules;

b) Study of Uranium atom formation by collision between the metastable state of mobile gas atoms and uranium compounds such as $UC(BH_4)_4$ and $U(COT)_2$.

The purpose of this work is to find a simple method for isotope separation. Uranium atoms can be detected by tuning a laser to 5915 Å resonance transition by means of the coherent forward scattering technique. At the same time quenching of metastable state is measured with the ZAA technique or by CFS. For the neon metastable state 6^3P_2, a dye laser can be conveniently tuned to 6143 Å ($2\ ^2P_{3/6}3\ ^2S_{1/2}$) → ($2\ ^2P_{3/6}\ 3\ ^2P_{1/2}$) transition to investigate the quenching due to collision of the neon metastable state with uranium compounds.

One possible application of this technique, which is superior to most other optical techniques, is to monitor atoms or molecules in the source which emits radiation. Typical examples are combustion sources and gas discharge sources. By using laser light the detector can be far enough away from the source so that source emissions will not be a problem. This is not the case with fluorescence, Raman effect and conventional atomic absorption. An additional advantage is that the light source need not be narrow as the crossed polarizers eliminate the primary light beam.

ZEEMAN ATOMIC ABSORPTION ANALYSIS

T. Hadeishi and R. D. McLaughlin

INTRODUCTION

This project deals with the utilization of the Zeeman effect as a tool in analytical chemistry. This idea was first demonstrated to be useful when atomic absorption analysis was modified so that the light source was contained in a magnetic field. This made available three closely spaced lines that could monitor the process of sample vaporization rather than the one line available in traditional atomic absorption analysis. Since one line coincided with the wavelength of absorption of the analyte and the other two did not, the Zeeman effect provided a method for essentially continuous background correction as the sample volatilized. The power of this method was soon demonstrated when the Zeeman split light beam was sent through the smoke and vapors given off while a piece of fish was being burned and the amount of mercury in the fish was immediately determined.

This proof of concept experiment occurred about five years ago. Since then efforts have been made to extend this technique to other sample types and to determine a large variety of elements.

ANNUAL ACTIVITIES

Last year's efforts can be divided into three categories: 1) The application of this technology to other projects designed to solve environmental problems; 2) The development of lamps that will produce spectra of different elements in a magnetic field; and 3) The design of a furnace that will provide an atomic vapor when various types of samples are raised to high temperatures.

Technology transfer has mainly involved three outside groups: The Environmental Protection Agency Laboratory at Las Vegas, Nevada; The U. S. Corps of Engineers Waterways Experimental Station at Vicksburg, Mississippi; and The N.S.I. Company at Mountain View, California. The Las Vegas Laboratory is interested in using the Zeeman atomic absorption (ZAA) technique for determining mercury, lead and cadmium in biological samples; the Vicksburg laboratory is interested in determining mercury, selenium and arsenic in water with high salt content; and the N.S.I. Company is interested in producing a ZAA machine commercially. Work with these groups resulted in the sale of prototype instruments to the Las Vegas and Vicksburg Laboratories.

In addition, samples were analyzed for groups at the University of Alaska, the University of California at Irvine, and two different groups at the Lawrence Berkeley Laboratory. (At LBL selenium was determined in approximately 250 samples.) We are analyzing samples to determine the environmental impact of oil shale processing. In this case, Hg, Pb, Cd, Zn, As, Sc, Cu, and Cr are of interest. Although a long lasting Cr lamp has not yet been developed this problem has been solved for the other seven elements. Plans have been made to present this work on oil shale analysis at the Second Pacific Area Chemical Engineering Conference in Colorado. The power of the ZAA technique will become known to more people in analytical chemistry through such activities.

The needs of the research groups mentioned have largely dictated the directions in which ZAA has been developed, both in terms of sample types to be analyzed and light sources to be fabricated. The need for light sources of copper and silver led to the development of a furnace assembly that is capable of holding the electrodeless discharge tube (EDL) at high temperature while located between the closely spaced poles of a permanent magnet. In order to obtain several hundred hours of service from EDL's in this configuration, the copper and silver iodide was sublimed into the region below the magnet poles, and the vapor pressure was controlled with a small air jet. Although this approach has been successful for copper and silver, a higher temperature is required for chromium. We are now investigating an assembly using heated air for this EDL.

It was necessary to make modification in furnace design in order to obtain optimum sensitivity for the different sample types that have been described. It was found that a dual chamber furnace could be packed with platinum and then used to determine mercury. This furnace was used in three configurations: 1) A liquid sample was injected directly; 2) A biological sample was burned in an oxygen stream in such a manner that the mercury was trapped by the furnace; and 3) Large volumes (several ml) of sample were vaporized in an external furnace, the vapors were condensed in a reducing solution and the mercury was swept from the reducing solution into the platinum lined furnace. The last approach was somewhat difficult because leaks kept developing in the system so that the mercury was not all transferred to the furnace.

Experience with the various sample types emphasized the need to develop a furnace that would break up inorganic molecules (i.e., PbS, Se_2) into atoms. This will occur if the molecule can be raised to a high enough temperature before passing into the central chamber of the dual chamber furnace. It was found that retention times in the outer chamber could be increased by using porous graphite construction. In addition this type of furnace is capable of reaching higher temperatures than the traditional dual chamber furnace. The development of this furnace is still under way.

PLANNED ACTIVITIES

The major goal for the future is to apply this technology as rapidly as possible to the field of analytical chemistry. An important part of this process is to increase the number of different

elements that can be determined and the number of different sample types that can be analyzed. Efforts will be made, through work with other groups, and by presenting talks and publishing papers, to make as many people as possible aware of the power of this technique.

PIEZOELECTRIC-TUNABLE MILLIMETER WAVE FABRY-PEROT RESONATOR IN INSTRUMENTATION FOR AIR POLLUTION RESEARCH

B. Leskovar, H. T. Buscher,* and W. F. Kolbe

INTRODUCTION

The technique of microwave absorption spectroscopy has been used for many years as a research tool to study the structure of molecules. Recently, these techniques have been shown to be useful in the detection of trace quantities of gaseous pollutants by means of their characteristic microwave line spectra.[1] Unfortunately, research spectrometers have not classically been designed to be both portable and highly sensitive. For this reason not much is known about optimizing such instruments for these characteristics.

It has been demonstrated[1,2,3] that significant improvements both in sensitivity and compactness can be made by using Fabry-Perot cavities as sample cells. This is especially true at high frequencies (above 30 GHz) where conventional absorption cells and cavities can become impracticably small.

ACCOMPLISHMENT DURING 1976

Of the several possible configurations which fall under the category of Fabry-Perot resonators, the most attractive for stable, high-Q microwave operation is the semiconfocal geometry. A new 70 GHz Fabry-Perot sample cell with variable microwave coupling and wide range piezoelectric tuning for use in a high-sensitivity microwave spectrometer was designed. The Fabry-Perot consists of a flat mirror facing a concave one, spaced as shown in Fig. 1. The radius of curvature of the concave mirror is exactly twice the mirror spacing. This semiconfocal geometry has the advantage that it is noncritical in alignment, is compact, and exhibits high Q. The Q of such a cavity is determined by reflection and diffraction losses as well as perturbations to the field structure due to coupling energy into and out of the resonator.

The desired cavity was expected to be part of a working prototype high sensitivity spectrometer which will be packaged as a portable air pollution detector. Therefore, the physical size of the entire spectrometer as well as the cavity size was limited. Mirrors were chosen primarily on the basis of compactness, having 5.08 cm diameters and a spacing of 7.43 cm. The spacing was such that diffraction losses could be assumed to be negligible compared to reflection losses.

To maximize the stability of the mirror surfaces, type 316 stainless steel was used for the blanks. Optical quality grinding techniques produced surfaces true to a few wave lengths of sodium light on both mirrors. To provide high surface conductivity at microwave frequencies, 75μ of silver was plated onto each mirror, followed by 1.5μ of gold as a corrosion inhibitor.

In order to couple energy in and out of the cavity, two small holes were drilled in the surface

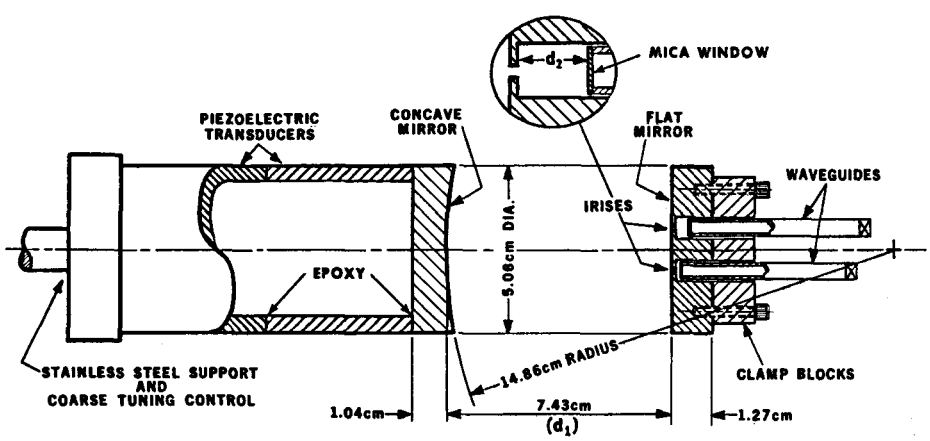

Fig. 1. Schematic View of Piezoelectric-tunable Millimeter Wave Fabry-Perot Resonator.
(XBL 766-8142)

of the plane mirror, and larger holes were bored from the rear to allow V-band wave guides to be positioned behind the small coupling holes as shown in Fig. 1. The positions of the input and output wave guides were made adjustable with respect to the irises, in order to allow the energy coupling to the cavity to be as varied as desired. To minimize microwave losses in the coupling structure, the irises should be as thin as is practicable. For the value of 0.13 mm thickness chosen, adequate coupling was obtained with a hole diameter of 0.64 mm. The separation between the input and output coupling holes was 6.2 mm. Under these conditions a measured (loaded) Q of 42,000 and a minimum transmission loss of 22 dB were obtained.

The mirrors were mounted in a fixture which allowed their spacing to be adjusted while enclosed in a vacuum chamber. For fine adjustment of spacing, a cylindrical piezoelectric transducer 7.62 cm long and coated with a low vapor pressure epoxy was used as the mount for the concave mirror. The transducer was designed to provide about 10μ of electrically-controlled tuning as compensation for thermal changes in the cavity and to allow it to track a frequency-swept and/or modulated microwave input.

Experimental data describing the electrical tuning characteristics and variable coupling performance are given in Ref. 4. The completed cavity has been successfully used in a high sensitivity laboratory-type millimeter-wave spectrometer. It has also been used to make absolute absorption coefficient measurements of a number of important pollutants and constituents.[5]

PLANNED ACTIVITY FOR 1977

A modified version of the Fabry-Perot cavity having little or no exposed metallic parts will be designed and fabricated to make possible the detection of unstable species such as O_3 and SO. We expect to use this cavity to study the techniques for making direct observations of the lifetimes of short-lived free radicals. Furthermore, a very high-Q cavity will be designed, increasing the conductivity of the mirror surfaces and decreasing diffraction and conductivity losses associated with the coupling structure. The high-Q potential of the resonator is an attractive feature contributing to the ultimate detection sensitivity of a high-sensitivity spectrometer and a pollutant monitor.

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DETECTION AND MEASUREMENTS OF AIR POLLUTANTS BY MILLIMETER-WAVE MICROWAVE SPECTROSCOPY

B. Leskovar and W. F. Kolbe

INTRODUCTION

Microwave rotational spectroscopy offers a highly specific and sensitive experimental research method for investigations of chemical kinetics and the monitoring of gaseous pollutants in the environment.

Previous investigations of the technique for pollutant monitoring have been restricted to the lower microwave frequency region below 40 GHz.[1] Our calculations have shown that larger absorption coefficients and hence greater sensitivity can be expected in the millimeter wave region above 40 GHz, provided that the spectrometer design can be optimized using state-of-the-art components. For this reason we have undertaken a program to develop a spectrometer operating at 70 GHz where favorable transitions exist for a number of interesting species.

The project has in the past included a study of the rotational transitions of the polar molecule SO_2.[2] Calculations were made of the transition frequencies and absorption coefficients of this molecule to determine the most favorable transitions. A cavity spectrometer capable of making absolute absorption coefficient measurements was constructed to verify these calculations. Theoretical criteria were established to determine the components necessary to construct an optimized spectrometer with high sensitivity.[3]

PROJECT ACCOMPLISHMENTS DURING 1976

Our major activity during the past year has been to develop a high sensitivity microwave spectrometer for the detection of low concentrations of gaseous pollutants. In addition, we have expanded our previous calculations and measurements of the frequencies and absorption coefficients to include a large number of important pollutants, free radicals and other atmospheric constituents.

Microwave Spectrometer Development

A superheterodyne microwave cavity spectrometer capable of detecting small quantities of pollutants diluted in air has been constructed. The major components of the system are shown in Fig. 1.

The sensitivity of such a spectrometer is determined by the total noise introduced during the generation of the microwave radiation, the absorption process in the resonant cavity, and the detection and amplification of the resulting signal.

The noise contributed by free-running microwave sources is primarily due to frequency fluctuations (FM).[3] To minimize these effects the Gunn diode source was phase-locked to the 76th harmonic of a high stability General Radio type 1062 frequency synthesizer. The frequency of the stabilized source was then doubled to produce the final signal.

In a cavity spectrometer the detected signal resulting from the gas absorption is directly proportional to the cavity Q. Hence it is desirable to make this quantity as large as possible. On the other hand frequency fluctuations will be converted to AM noise by a high-Q cavity if it is not accurately centered on the source frequency. This problem was alleviated by stabilizing the cavity resonant frequency to the microwave source frequency via the quadrature phase detector shown in the block diagram. A semiconfocal Fabry-Perot cavity with a loaded Q of about 42,000 was used and the cavity was tuned with a piezoelectric transducer.[4]

In order to minimize receiver noise contributions, a low noise mixer/preamplifier (TRG model V9125) was used. Local oscillator power was supplied by a reflex klystron which was also phase-locked to the primary frequency standard. Further improvements in sensitivity were obtained by using Stark modulation at 19 kHz or frequency modulation at 33 Hz followed by phase-sensitive detection and signal averaging.

Absorption Coefficient Calculations

Since the minimum detectable concentration of any species is dependent on the absorption coefficient of the transition selected, it is important to select those transitions for which the strongest absorptions are obtained. For this reason the previous calculations and measurements reported for SO_2[2] were extended to include a wide range of pollutant and constituent species. Absorption coefficients and transition frequencies have been taken for frequencies up to 140 GHz for SO_2, NO_2, H_2S, H_2CO, NH_3, CO, N_2O, H_2O, O_2, NO, O_3, SO, and OH. In addition, measurements in the vicinity of 70 GHz of a number of these species were made using the apparatus described above. Representative results are shown in Table 1 for several pollutants having favorable transitions near 70 GHz.

PLANNED ACTIVITIES FOR 1977

We plan during the next year to complete our optimization and evaluation of the performance of the low-noise spectrometer. Furthermore, the

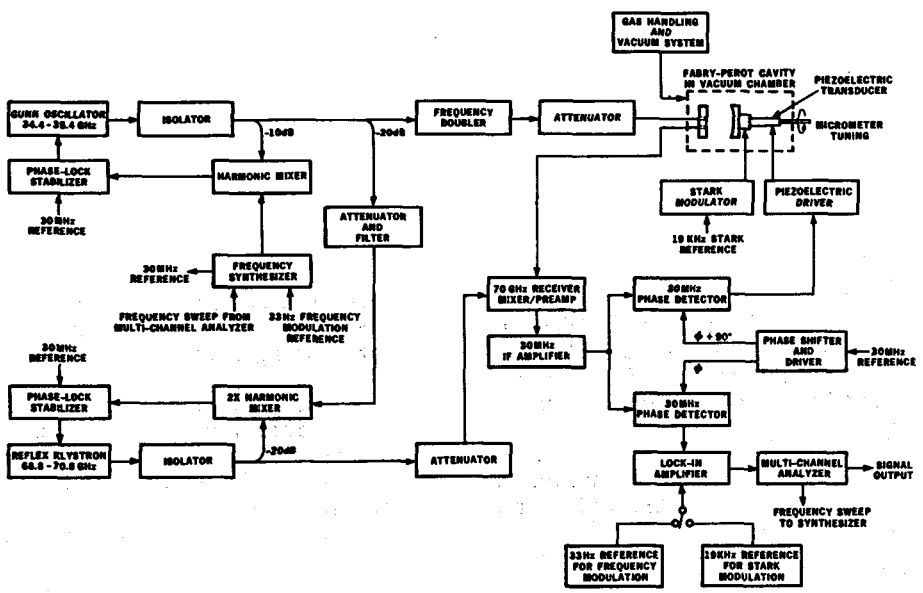

Fig. 1. Block Diagram of Microwave Spectrometer. (XBL 792-7501)

Table 1. Microwave Absorption Coefficients of Pollutants at 70 GHz

Molecule	Transition		Frequency	Calc. Abs. Coef.	Meas. Abs. Coef.	Meas. Linewidth
	Upper	Lower	MHz	cm^{-1}	cm^{-1}	MHz/Torr
SO_2	6(1,5)	6(0,6)	68 972.1	4.6×10^{-4}	4.5×10^{-4}	15.0
NO_2	5(1,5)	6(0,6)	70 589,7	1.7×10^{-5}	1.5×10^{-5}	4.0
O_3	6(0,6)	5(1,5)	67 356.2	1.5×10^{-4}		4.6
H_2CO	5(1,4)	5(1,5)	72 409.1	2.7×10^{-4}	2.6×10^{-4}	22.0
OCS	6	5	72 976.8	1.3×10^{-3}	1.2×10^{-3}	6.4

spectrometer will be modified to include a data processing system in order to permit more efficient signal averaging, digital filtering, lineshape fitting and automatic control of the spectrometer parameters. In addition, a new cavity having no exposed metallic parts will be constructed to make it possible to detect unstable species such as O_2 and SO. We plan to use this cavity to initiate a study of the lifetimes of these species as they react with other gases. Finally, we will continue to develop a high-sensitivity spectrometer using microwave solid state components.

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THE SURVEY OF INSTRUMENTATION FOR ENVIRONMENTAL MONITORING*

D. A. Mack, N. M. Amer, P. Bhardwaja, C. D. Hollowell,
M. J. Kland, R. A. McLaughlin, G. A. Morton, A. V. Nero, S. L. Phillips

In response to the need for up-to-date in information on pollution monitoring systems technology, Lawrence Berkeley Laboratory publishes the survey entitled Instrumentation for Environmental Monitoring (LBL-1) in a loose-leaf format that facilitates frequent up-dating. LBL-1 consists of four volumes: 1. Air (Parts 1 and 2), 2. Water, 3. Radiation, and 4. Biomedical. The contents of the most recent up-dates of these volumes are summarized in Table 1 and described in greater detail in a brochure published by the Technical Information Department.[1]

Since its inception LBL-1 has enjoyed recognition both in the United States and abroad as a source book for monitoring information in the four areas covered by its volumes. Over 4000 copies of LBL-1 have been purchased to date by both private and public laboratories and other agencies. In addition, some 450 copies have been distributed to environmental scientists in government agencies and laboratories.

The LBL-1 survey has also proven to be a pedagogic tool in the environmental monitoring field where textbook materials are as yet limited.

Sophisticated monitoring equipment needs reliable sampling materials and techniques as well as primary standardization and calibration methods to be most useful. Therefore, the principle focus of the past year has been in the area of instrument calibration, sampling, and standardization of analytical techniques, as well as in the

Table 1. Pollutants and Parameters covered in Survey of Instrumentation for Environmental Monitoring.

Vol. I AIR	Vol. II WATER	Vol. III RADIATION	Vol. IV BIOMEDICAL
SO_2 (updated)	Metals	Alpha Radiation	CO
NO and NO_2	Arsenic	Beta Radiation	SO_2
Oxidants	Cadmium	χ & Gamma Radiation	Asbestos
CO	Lead	Gamma Spectroscopy	Mercury
Hydrocarbons	Mercury	Neutrons	Cadmium
Particulates	Nitrogen	Personnel Dosimetry	Lead
Mass	Phosphorus	Radionuclides	Pesticides
Size	Sulfur	Tritium	Radiation
Opacity	Biochemical Oxygen Demand	Krypton-85	
Composition	Chemical Oxygen Demand	Strontium-89 & -90	
Mercury	Dissolved Oxygen	Iodine-129 & -131	
Asbestos	Total Organic Carbon	Radon 222 & its daughters	
Beryllium	Pesticides	Radium	
Lead	Phenolics	Uranium	
Noise	Petrochemicals	Plutonium	
Instrument Calibration	Oil and Grease	Microwaves	
Sampling Techniques	pH, Alkalinity, Acidity	Lasers	
	Radiation	Ultraviolet	
	Turbidity		
	Temperature		
	Instrument Calibration		

identification and evaluation of standards, both primary and derived, and their sources and availability particularly as they relate to the contents of the Air and Water volumes. The updating of all four volumes of LBL-1 is currently under way, including a substantial effort on the radiation volume.

FOOTNOTE AND REFERENCE

*Research supported by the National Science Foundation, Research Applied to National Needs and the U.S. Energy Research and Development Administration.

1. Available from the Technical Information Department, Lawrence Berkeley Laboratory, University of California, Berkeley, California 94720.

MEASUREMENT AND INSTRUMENTATION TECHNIQUES FOR MONITORING PLUTONIUM AND URANIUM PARTICULATES RELEASED FROM NUCLEAR FACILITIES*

A. V. Nero, D. A. Mack and R. J. Budnitz

Uranium and plutonium, the two basic elements of both commercial and military nuclear power, both pose important radiological dangers to man. Accordingly, standards have been set defining limits both to the amount of these materials that may be ingested by humans, and – considering the specific pathways for uptake – to the amount which may be present in various environmental media. It is important that ways be developed to monitor both the amounts of these materials that actually

escape into the environment and their concentrations in any environmental medium. The purpose of this work has been to scrutinize state-of-the-art instrumentation for monitoring release of uranium and plutonium into the environment, to compare the capabilities of this instrumentation with needs specified by current standards, and to identify ways to improve measurement capabilities. We have examined the types of instrumentation that are currently used at nuclear facilities, those that are planned for new facilities, developments which are now taking place in laboratory instrumentation, and techniques that warrant consideration.

The results of this investigation are presented in an LBL report.[1] The report discusses the occurrence of plutonium and uranium in the nuclear fuel cycle, the corresponding potential for radioactive releases, associated radiological protection standards, and monitoring objectives. Techniques for monitoring via decay radiation from plutonium and uranium isotopes are presented in detail, with an emphasis on air monitoring, but also including soil monitoring, as well as area and personnel survey methods. Additionally, activation and mass measurement techniques are discussed.

The work identified possible improvements in monitoring capabilities due to alterations in instrumentation, data handling systems, or overall monitoring programs. Improvement of instrumentation was emphasized, including refinement of current devices (such as large alpha-monitoring systems with more sophisticated data analysis), extension of specialized techniques (such as virtual impaction of particulate matter, and pulse shape discrimination) to a broader range of instruments, and application of additional techniques (such as mass spectroscopy or X-ray fluorescence) to the monitoring of plutonium or uranium.

FOOTNOTE AND REFERENCE

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Environmental Research Program

INTRODUCTION

The scope of the Environmental Research Program can be divided into three broad categories of projects on energy related environmental issues. The first category is composed of instrumental techniques and investigations of problems relating to marine and fresh water systems. For trace metal analysis by anodic stripping voltammetry, a method has been developed for the ozone oxidation of organic sequestering agents in fresh or marine water prior to analysis. Another project involves the use of flameless atomic absorption spectroscopy for the study of environmental impacts in the San Francisco Bay Area from future increases in energy production, transportation, and utilization. The ecosystem stability and dynamics project involves perturbation and other experiments on fresh-water microbiomes in order to study their nutrient regeneration and stability properties. The project goal is to develop stability indicators. Finally, a study is being done using gas chromatography techniques for the analysis of the methyl mercury content in various benthic organisms collected from the San Francisco Bay.

The next category includes atmospheric aerosol studies and investigations on indoor and outdoor air pollution. The atmospheric aerosol group is doing research on the formation and transport of particulate and gaseous pollutants from fossil fuel combustion. Their effort has been directed toward studies of certain atmospheric chemical reactions under laboratory conditions, application and development of techniques for the chemical and physical characterization of specific pollutants, and field studies of pollutant behavior. Another study, on indoor air pollution, is designed to study the chemical and physical behavior of indoor combustion-generated air pollution in residential and commercial buildings. This direct source of pollution has been preveiously neglected in air quality studies. The populations at risk to air pollution study involves the creation of a set of integrated primary air pollution data bases, the determination of populations at risk to air pollutants, and the analysis of associations between air pollutant levels and various indices.

The last category contains environmental projects relating specifically to solar, nuclear, fossil fuel, and geothermal energy development. A solar project assesses the environmental implications of the widespread application of the solar energy technologies being developed by ERDA. The health and safety impacts project has been performed in order to establish a methodology for the review of the health and safety aspects of proposed nuclear, geothermal, and fossil fuel electric generation sites and facilities in California. The cell membrane project is involved in studying the role of membranes in damage and protection of cells against environmental effects, including the determination of how and where various pollutants act on membrane structures. The study of water conservation with in situ oil shale development has objectives of identifying and assessing water related impacts of in situ oil shale development and developing control measures to mitigate adverse impacts. Finally, a study is being performed on the environmental impacts of the Geysers geothermal development and the proposed development at immediately adjacent Lake County.

OZONE OXIDATION OF ORGANIC SEQUESTERING AGENTS IN WATER PRIOR TO THE ANALYSIS OF TRACE METALS BY ANODIC STRIPPING VOLTAMMETRY (ASV)

R. G. Clem and A. T. Hodgson

There has long been a problem in sequestering trace metals, determinable with ASV, by naturally occurring weakly acidic, organic compounds in water samples such as humic and fulvic acids. Formerly, the only successful way of liberating these metals was through acidification to a pH of ≤ 2 so that the sequestering agents were converted to their molecular forms. Unfortunately, the presence of acid and mercuric-ion is required for the functioning of the ASV method, and this is precisely the condition which causes graphite electrodes to rapidly deteriorate.[1]

Previous workers recognized this problem and attempted to destroy the organic sequestering agents with persulfate[2], and with UV (ultraviolet) photolyzed hydrogen peroxide.[3] Both methods are effective but have serious drawbacks. Persulfate harbors trace metals impurities and the last trace which can also cause rapid deterioration of ASV electrodes, is difficult to destroy. UV photolyzed peroxide method is attractive because it is useable in neutral solutions. However, it also harbors metals impurities, is difficult to completely destroy, and the photolysis times exceed 5 hours.[3]

In view of the foregoing difficulties, ozone seems ideally suited to the oxidation of trace organic matter in water samples. It is a very strong oxident ($E^\circ = 2.07V - 0.06pH$) and reacts rapidly at room-temperature with organic matter. In addition it inactivates sequestering agents and compounds which are specifically absorbed at ASV electrodes over the pH range of from 2 to 10. High purity oxygen gas used in its generation is inexpensive, readily available, and does not harbor trace metal impurities. The decomposition product of ozone in aqueous solutions is oxygen which can be rapidly displaced with Ar, N_2, or CO_2, along with any dissolved ozone. Finally, the setup required for ozone

generation, a corona discharge tube and a high voltage transformer, is inexpensive and easy to build.

To develop the method, ozone was first used to destroy the compounds ethylene diaminetetraacetic acid (EDTA), ammonium pyrrolidine dithiocarbamate (APDC), and tannic acid.[1] All of these are known to be strong complexing agents for the metals, lead and cadmium, which are used in this study. The first substance is an amine with carboxyl groups, the second a thio compound, and the last is a phenolic compound with carboxyl groups. These three include all the groups thought to exist on the naturally occurring humic acid and are reported to be the most important for the sequestering of trace metals. At the levels of sequestering agent tested (3 ppm for EDTA to 100 ppm tannic acid) all the model compounds were destroyed within 1 hour or less when ozonized at pH2. Oxidation did proceed for all substances tested at pH9, but more time, perhaps several hours, was required at the higher pH. The oxidation potential of ozone drops to only 1.5V at pH9.

The humic acid received was quite impure. It contained over 11% ash and had very little exchange capacity for Pb and Cd. We devised a method for purifying it which involves repeatedly dissolving it with ammonia water and then precipitating it with HCL. Humic acid purified in this way had an ash content of 1%. Further purification with an HCL/HF mixture resulted in the virtually complete removal of ash. The ash content of the HCL/HF purified humic acid was <0.1%, a level of purity seldom mentioned in the literature.[4]

Ozonolysis of humic acid at the 25 ppm level required over 4 hours to complete, but this is not surprising considering that this level is one to two orders of magnitude greater than the levels that are present in natural waters. Data is being developed to illustrate the efficacy of the ozone method for bay water and sewage effluent samples. Ozonolysis for these samples requires one hour or less to obtain complete recovery.

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ENVIRONMENTAL ASSESSMENT OF SOLAR ENERGY CONVERSION

M. Davidson and D. F. Grether

INTRODUCTION

The objective of this project is to assess the environmental implications of the widespread application of the solar energy technologies being developed by ERDA. In pursuing this objective, the project is following the guidelines established by the Balanced Program Plan (BPP). This plan was developed during 1975 by the Division of Biomedical Research of ERDA in conjunction with the various ERDA laboratories. The solar input to the BPP[1] was coordinated by LBL. This document describes the status of the development of the solar technologies, identifies potential environmental problems, suggests research that would lead to a quantitative understanding of these problems, and estimates the cost and time required for the research. The potential environmental effects can be grouped into four broad categories:

1) Socio-economic Impacts of Widespread Utilization;

2) Alterations of Ecosystems and Climate;

3) Health and Ecological Effects of Effluents from Bioconversion Processes;

4) Health and Ecological Effects from Materials of Solar Devices.

These categories are described in detail in the 1975 Energy and Environment Division Annual Report.

The primary work on the project during 1975 (subsequent to the formulation of the BPP) was to identify selected areas from the above broad categories that could be studied with exisiting techniques and procedures. In order to focus the investigation, a particular solar technology was selected for initial concentration. The technology selected was the central receiver concept for solar thermal conversion to electricity since it is expected that future, commercial power plants will have the same basic properties as the currently evolving designs. In addition, these systems have the advantage, from an environmental analysis point of view, that the facilities will be large, isolated from other activities of our civilization, and probably of a limited number of designs.

ACCOMPLISHMENTS DURING 1976

There were three principal efforts during the year that fell under the above categories 1) and 2): a study of the socio-economic effects of solar thermal conversion, a survey of the ecological effects of all solar technologies, and an investigation of techniques for assessing climate modification by solar energy conversion (especially solar thermal).

Socio-economic Effects of Solar Thermal Conversion

For the purpose of studying the social and economic impacts of a given scenario of solar energy

plant production, a linear model of the U. S. economy was developed from several existing blocks. The core of the model is an input/output matrix constructed by the Bureau of Economic Analysis and put on the LBL computer by E. Schroeder of LBL. To this was added a matrix of jobs versus industries which was constructed by D. Merrill, also of LBL. A matrix of effluents was then constructed by aggregating the extremely detailed data of the SEAS model.[2] These matrices provide a simple and fast method of analyzing social and economic impacts, once one has first constructed a "bill of goods" for a scenario to be studied. For example the scenario might correspond to building some number of solar power plants per year of a particular design. The bill of goods would specify the tons of steel, glass, etc. and the cost of converting these materials into the solar devices. This bill is input to the model, which calculates the final demand in each of 93 industrial sectors, jobs in over 400 occupations by industry, and total effluents produced by the industries in meeting this bill of goods. All of the estimates are approximate and limited in accuracy by the nature of the models as well as by the uncertainties in the scenario. However they do give a rough idea of the implications of a particular energy strategy, and thus are a useful tool in decision making.

Some preliminary results of the model, based only on the materials requirements, were presented at a meeting of the International Solar Energy Society.[3] These results indicate that, for a construction scenario of 10 GW (electric) per year, the demands for steel, glass and concrete would be a few percent of the current yearly U.S. demand. Major air pollutants from production of the materials are estimated to be $\leq$ 1% of those currently released.

Ecological Effects of Solar Energy Conversion

At the request of the National Research Council's Committee on Nuclear and Alternative Energy Systems a report[4] was prepared that attempts to delineate the possible effects that the various solar technologies would have on ecosystems.

An effort was made to quantify effects. The most detailed consideration was given to solar thermal power because of its relatively advanced development and due to a concern for its impact on desert ecosystems. The report describes in some detail possible effects on such systems, and draws parallels to a particular modern technology (recreational off-road vehicles) which has already been very disruptive to the desert. Since pollution affects ecosystems as well as human health, the economic model described above was used to estimate the effluents which would be released in the refinement of the materials for the solar plants. Water requirements, a crucial factor for desert based systems, were estimated for the use of wet cooling towers. A comparison between these requirements and the anticipated supply in the Southwest's water resource regions indicated that extensive use of wet towers would necessitate a significant reallocation of the already scarce water.

The report discusses the other solar technologies in less detail with emphasis on the direct effects on ecosystems.

Techniques for Assessing Climate Modification

Studies of the climate are generally conducted on three scales: local or micro-climate, regional or meso-scale, and global. Since (with the possible exception of the micro-climate level) real physical experiments are ruled out, one must rely on analytic and computer simulation models. Many such models have been developed for purposes other than studying solar energy conversion. The approach of the project has been to construct a scenario appropriate to the scale under study, perform some simple analytic calculations to estimate the magnitude of the effect, and to investigate the applicability of existing computer models for examining the effects in more detail. This approach has been carried to a relatively satisfactory conclusion for solar thermal conversion on a global scale, as will now be described.

In collaboration with J. Weingart of the International Institute of Applied Systems Analysis (IIASA), a global scenario was developed for the central receiver concept supplying 100 Terrawatts (10^{15}watts) to a world population of 10 billion with an average energy consumption of 10 Kw each. This plan is detailed in Reference 5. For reasons given below, the scenaio was deliberately chosen to be a "worst case" that almost certainly overestimates the amount of land that would be devoted to the solar plants and the change in albedo of this land. In a simple black-body radiation model it was found that for this scenario the radiation temperature of the earth would increase by about .25°K.[3] This increase would appear to be rather modest for such a massive use of energy. However, the model provides no information on such possible effects as localized temperature changes or shifts in precipitation. A global climate model developed at Lawrence Livermore Laboratory was employed to estimate these effects. It is a two-dimensional model (latitude and altitude, averaged over longitude) known as ZAM2 and predicts climate change by latitude zone. Potter and McCracken[6] input the scenario outlined above into ZAM2 and observed considerable latitudinal dependence of temperature change, with the greatest changes occurring in the polar regions. They also found noticeable alterations in precipitation patterns in both the northern and southern hemispheres. Since the model is averaged over longitude, localized effects (e.g., in the vicinity of or downwind of the solar plants) are smeared out over a zone.

The next level of detail would be provided by three-dimensional models known as GCM's (usually indicating General Circulation Model). General Circulation Models currently have two difficulties that make their application to solar energy conversion of questionable value. First, the models are very costly to run. Second, the models are "noisy" in the sense that small variations in initial conditions for the control case lead to appreciable variations in the resulting climate. For a "signal" (real climate change) to show up for the perturbed

case (e.g., the above scenario) the perturbation must be quite large. The scenario was originally constructed for the GCM of the National Center for Atmospheric Research (NCAR), with the "worst case" approach taken to maximize the perturbation. The proposed computer run did not take place, partly because it was not clear that even this worst case would generate a signal.

The question of whether any reasonable solar scenario would be noticed by a GCM was the principal topic of a recent workshop on solar energy and the climate held at IIASA and attended by Davidson and Grether. Here the model under consideration was the British Meteorological Office version. Extensive discussion failed to resolve the issue.

The above stated approach has also been applied, although not as completely, to one aspect of the micro-climate of an individual central receiver plant. The question is whether the absorber unit and/or the cooling tower will generate an updraft that might carry with it dust from the surrounding area. A survey was made of existing models and a simple "Gaussian Plume" model for convection currents applied to a dry cooling tower sized for a solar plant generating 100 MW (electric). The results give convective velocities as a function of distance from the cooling tower and altitude.[5] The results suggest that the dust updrafting will not be a problem. The model does not include condensation and therefore cannot be used to study fogging or cloud formation induced by, particularly, wet cooling towers. Some work has been done on identifying more detailed models. One difficulty in applying these models to solar plants is in estimating how diffusion coefficients, used to parameterize atmospheric turbulence, will be affected by the plant. On site measurements may be necessary to overcome this difficulty. Miroscale climatology is in any event quite complicated and effects are likely to be site dependent.

PLANNED ACTIVITIES FOR 1977

The following activities are planned for 1977:

1. The socio-economic model will be applied to other solar technologies. The model will be updated as new information or data becomes available;

2. Work will continue on the assessment of techniques for studying climate modification for solar thermal conversion. As a result of collaborations with climatologists, the existing scenario will be modified to account more properly for global redistribution of the energy supplied by the solar plants. Studies will be continued on micro-climate effects such as condensation, changes in hydrology, and alteration of turbulent diffusion coefficients;

3. The climate change assessment approach developed for solar thermal conversion will be applied to other solar technologies. Prime candidates are the sea surface temperature effects of ocean thermal plants, and the atmospheric effects of solar satellites;

4. A few of the many possible alterations of ecosystems by solar facilities will be selected for further, more detailed study. One possibility is the site-dependent effects of solar thermal plants.

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ESTUARINE POLLUTANT INVESTIGATIONS

D. C. Girvin, A. T. Hodgson, R. N. Anaclerio, and M. E. Tatro

INTRODUCTION

Within the next decade, the San Francisco Bay area will be faced with massive environmental impacts from increased energy production, transportation, and utilization. Currently there are six oil

refineries and petrochemical plants operating in northern S. F. Bay with a total processing capacity of 823,000 barrels of crude per day. Although no plans have been announced for expansions of these existing facilities, their capacities are expected to increase due to the influx of Alaskan oil. In addition, new plants will be built. Already, a large petrochemical complex in Suisun Bay is being planned. These developments will result in increases in the pollutant loads discharged into bay and delta waters from process and cooling waste waters and in an increase in the probability of a major oil spill.

The biological significance of the S. F. Bay-Delta system is unquestioned. This environment supports commercial and recreational fisheries, serves as a nursery ground for numerous economically and ecologically important fish and invertebrates, and is a principal wintering ground for migratory waterfowl, including several rare and endangered species. Therefore, our estuarine pollutant research group has established long range objectives which hopefully will contribute to the understanding and assessment of the present and future impacts of an expanding energy related industry on the environment and biota of this important ecosystem.

These objectives are: (1) to establish a baseline for trace element and pollutant hydrocarbon levels in S. F. Bay-Delta waters and document large scale spatial and temporal variations in the concentrations of trace elements; (2) to investigate the chemical speciation of trace elements in estuarine waters as a function of salinity and other chemical parameters using chemical equilibrium models; (3) to document the concentration of trace elements and pollutant hydrocarbons in selected estuarine species from locations in S. F. Bay and compare these to levels in identical species from relatively uncontaminated locations outside of the bay; (4) to examine the trace element and pollutant hydrocarbon composition of waste waters from petrochemical complexes and municipal sewage treatment plants; and (5) to employ sensitive methods to detect and evaluate the biological effects of low level trace element and petroleum hydrocarbon contamination on selected estuarine organisms.

ACCOMPLISHMENTS DURING 1976

During the previous fiscal year we conducted a survey to determine the extent of trace element, chlorinated hydrocarbon, and total alkane and aromatic hydrocarbon contamination in individual species of shell-fish from nine locations within the S. F. Bay estuary and one location in Tomales Bay. Ag, As, Cd, Cr, Cu, Fe, Hg, Mn, Ni, Pb, Se, and Zn were analyzed in the clams Mya arenaria and Tapes japonica, the mussels Mytilus edulis and Ischadium demissum, the oysters Ostrea lurida and Crassostrea gigas, bottom sediment, and suspended particulates using X-ray fluorescence and atomic absorption spectroscopy. DDT metabolites and the PCB, Aroclor 1254, were analyzed in M. arenaria T. japonica, M. edulis, O. lurida, and bottom sediment by gas chromatography. Total concentrations of alkane and aromatic hydrocarbons were semi-quantitatively determined in M. edulis and O. lurida by thin layer chromatography.

The samples of C. gigas from South S. F. Bay and Tomales Bay demonstrate the dramatic difference between trace element bio-accumulation in a contaminated location and bio-accumulation in a relatively clean, non-industrialized location. For example, the hepatopancreas of S. F. Bay oysters had concentrations of Ag, Cd, Cu, Hg, and Zn which were respectively 103, 8, 31, 17, and 22 times higher than the concentrations observed in the hepatopancreas of Tomales Bay oysters.

Two major regional differences in trace element bio-accumulation were observed within the S. F. Bay estuary. Shellfish populations along the northeast bay shoreline had distinctly higher concentrations of Pb than did south bay populations of the same species. On the other hand, substantially higher concentrations of Ag occurred in south bay populations than in north bay populations.

The presence of biologically available Ag in South S. F. Bay, as indicated by Ag accumulation in adult shellfish, may be having an adverse effect upon the biota. Other researchers have shown that Ag, which is one of the most toxic metal cations, is lethal to molluscan embryos at low part per billion concentrations. Therefore, the possibility exists of diminished shellfish reproductive success in South S. F. Bay.

Pollutant hydrocarbons were not differentiated from naturally occurring hydrocarbons by our method. However, general hydrocarbon contamination in S. F. Bay is suggested by the consistantly high total alkane and aromatic levels observed in shellfish from five S. F. Bay locations. In M. edulis the average alkane and aromatic concentrations were 25 and 200 times higher than the respective concentrations found in M. edulis from Tomales Bay.

During the current fiscal year an intensive effort is being made by our LBL group, in collaboration with Dr. E. A. Jenne of the U. S. Geological Survey (USGS), Menlo Park, CA, to document large scale spatial and temperal variations in dissolved and suspended particulate associated trace element concentrations in the S. F. Bay-Delta system and in the Gulf of the Farallones. Beginning in March 1976, water and suspended particulate samples for trace element analyses were collected at 20 stations throughout the bay and delta and at several offshore stations. Subsequent sampling at these locations has been made at approximately three month intervals and will continue until October 1977. Ship time for these collections and access to routine water quality data is generously being provided by D. H. Peterson and T. J. Conomos of the USGS, Menlo Park.

Dissolved Ag, Cd, Cu, Fe, Mn, Ni, Pb, and Zn in shipboard filtered water samples are solvent extracted and analyzed by flameless atomic absorption spectroscopy. Suspended particulate samples are collected on filter membranes and analyzed for the same elements by X-ray fluorescence spectroscopy. In addition, shipboard measurements are conducted by USGS personnel for salinity, temperature, pH, partial pressure of dissolved carbon dioxide, and concentrations of suspended particulates, dissolved oxygen, nitrate-N, nitrite-N, ammonia, phosphate, and silica. In the laboratory, total carbonate al-

kalinity and concentrations of dissolved organic carbon, Na, K, Mg, Ca and sulfate are determined. This detailed water quality characterization is essential for our inorganic modeling of soluble trace element speciation using a version of the USGS chemical model, WATEQ II.

Initially we used WATEQ to determine whether specific chemical data, necessary for the modeling of trace element speciation had been overlooked. For example, we had not initially considered H_2S to be an important parameter since in well mixed, aerobic waters it is highly unstable. However there is evidence in the literature suggesting that H_2S may coexist with dissolved oxygen in estuarine waters. Preliminary tests with WATEQ, using typical Bay-Delta Ag concentrations and our March 1976 water quality data, have shown that an extremely low concentration of H_2S (approximately 0.4 nanogram/ℓ) significantly alters the speciation of Ag as the salinity of the water decreases (Fig. 1). At a salinity of 8°/oo, $AgHS^o$ emerges as an important fraction of the total dissolved Ag, and below 3°/oo, $AgHS^o$ dominates the various chloride complexes. In the absence of H_2S, chloride complexes dominate throughout the entire salinity range. It is therefore apparent that either analytical measurement or reliable estimates of H_2S concentrations are necessary.

The USGS group is currently proposing to evaluate and update the existing thermodynamic data used in the model and to incorporate data for more trace elements. Additionally, the model could quantitatively treat soluble organic ligands if their identities, environmental concentrations, and stability constants for trace elements could be determined. Continued experiments with the ozone destruction of organics (see Clem and Hodgson, this annual report) may provide insight into the importance of dissolved organic ligands in the speciation of trace elements in natural waters.

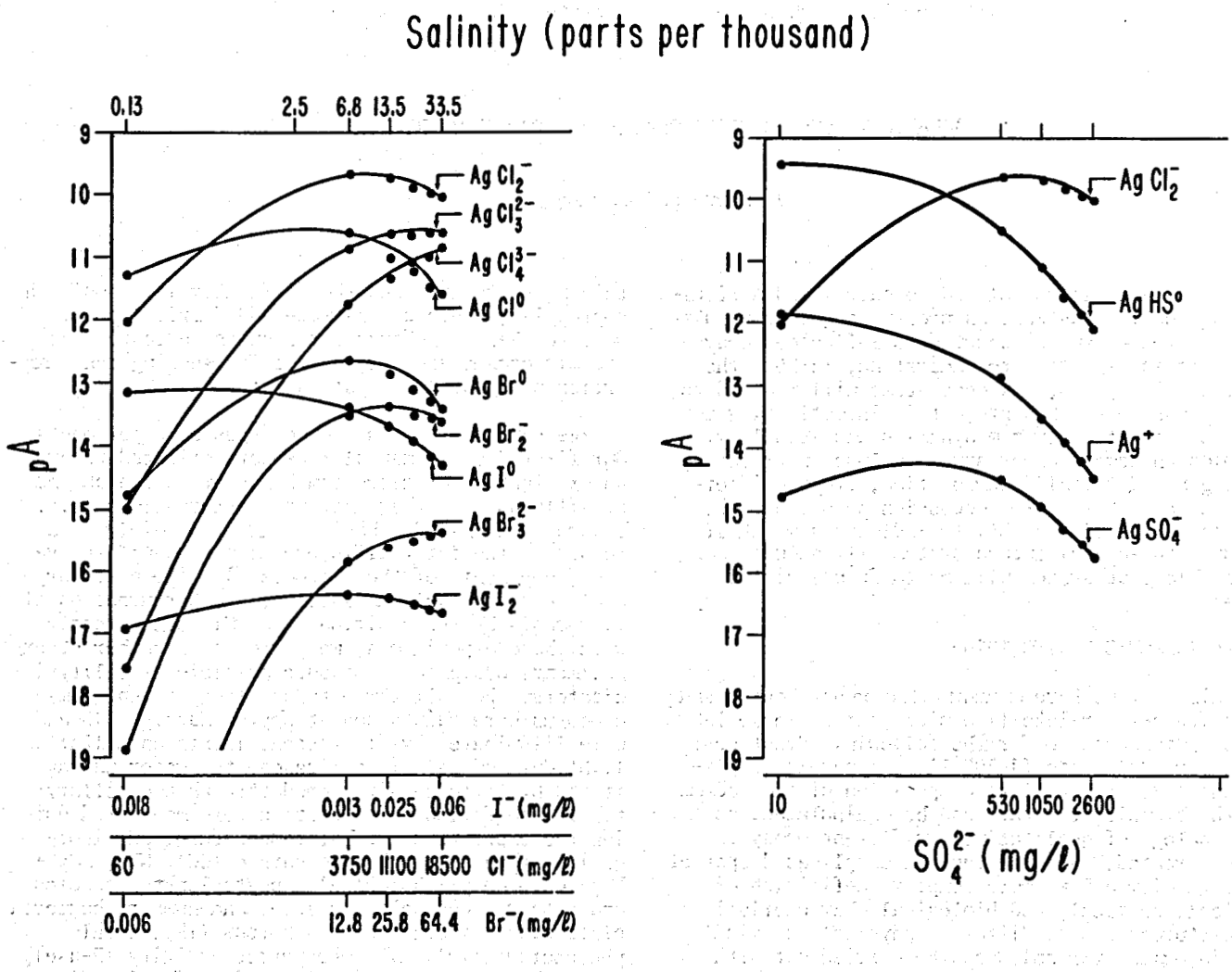

Fig. 1. Activities of soluble Ag complexes versus the concentrations of four anionic ligands (I^-, Cl^-, Br^-, and $SO_4^=$) at salinities measured along a transect from the Sacramento River to the open ocean. Ag and H_2S concentrations were held constant at 40 µg/1 and 3×10^{-11} molal, respectively. The distribution of Ag among its complexes was determined in the presence of all other competing cations. (XBL 773-486)

The joint LBL-USGS modeling of S. F. Bay trace element data should ultimately enable us to predict which soluble complexes predominate in bay-delta waters and how variations in chemical parameters, such as salinity, alter speciation. In the future, we would like to incorporate the predictive capabilities of WATEQ into laboratory accumulation and toxicity experiments to investigate the hypothesis that the biological effects of trace elements are dependent upon chemical speciation. This hypothesis is based upon the findings of other researchers that the toxicity of soluble trace elements is significantly altered by variations in salinity, alkalinity, hardness, pH, and other chemical parameters.

PLANNED ACTIVITIES FOR 1977

In addition to continuing the Bay wide trace element data collection and chemical speciation modeling efforts, our LBL group plans to initiate a preliminary search for specific pollutant hydrocarbons (e.g., polynuclear aromatic compounds) in S. F. Bay waters. This work will be done in collaboration with Dr. A. S. Newton of LBL and Dr. R. W. Risebrough of Bodega Marine Laboratory following the installation of a gas chromatograph/mass spectrometer system at LBL this summer. Eventually, pollutant hydrocarbons will be examined in selected estuarine species and possibly in waste waters entering the Bay from petrochemical complexes and municipal sewage treatment plants.

We also plan to investigate the biological effects of trace elements and pollutant hydrocarbons. One of our initial objectives is to examine the potential use of hepatic microsomal enzyme induction in fish and possibly invertebrates as a sensitive biological monitor for estuarine hydrocarbon contamination. As a preliminary step, we intend to measure the specific activities of mixed function oxidases in the livers of several fish species collected from locations adjacent to and remote from suspected petroleum discharges. Another anticipated biological effects study is a laboratory investigation of the toxic effects of several trace elements and pollutant hydrocarbons on the sensitive embryonic and larval stages of selected estuarine invertebrates.

AQUATIC ECOSYSTEM MICROCOSMS AS STABILITY INDICATORS

J. Harte and D. Levy

INTRODUCTION

Future activities related to energy and agriculture production, as well as pressures due to population increases, can be expected to influence ecosystems. It is important to understand, in both the short and long term, how ecosystems will respond to these pressures. This project is investigating certain aspects of ecosystem dynamics and stability. Dynamics phenomena under study include; nutrient cycling and detrital decomposition, trophic interactions, and short term succession phenomena. We are also developing stability indicators which if measured in an undisturbed system will suggest how vulnerable that system will be to future disturbances.

ACCOMPLISHMENTS DURING 1976

This year we have concentrated on developing and using fresh-water lake-like microcosms. These laboratory microcosms offer the following advantages: (1) their small size (4-700 liters) permits replication; (2) the chemical composition of the medium and the trophic structure can be manipulated, so that analogs of qualitatively different ecosystems can be created; (3) the lack of complicated spatial heterogeneity allows more complete definition of physical, chemical, and biological characteristics; (4) perturbations of different physical, chemical, and biological variables can be carried out with little effort and expense; and (5) causal relationships often are easier to deduce in the laboratory than in natural systems, where the complicating factor of environmental variability cannot be eliminated. On the other hand, there are a number of drawbacks inherent in the use of aquatic microcosms, such as the high surface-to-volume ratio of the containing structure, and the difficulty in choosing an appropriate benthic substrate and detrital pool. Despite these drawbacks our results indicate that the microcosms are very useful for showing many properties of natural ecosystems.

We have carried out three types of experiments. Our first 2 experimental runs were oriented toward an examination of microcosm behavior in the absence of effluents or other external perturbations (i.e., toward patterns of behavior generated solely as a result of the internal interactions among the various components of the microcosms). The next large scale experimental run involved the perturbation of microcosms by the addition of NH_4Cl. Concurrently with these experiments, we performed a number of experiments designed to measure possible stability indicators. For all three types of experiments, microcosms were maintained at approximately 19°C and were illuminated by fluorescent lights on a 12h:12h light:dark cycle. In all cases, the water was agitated by filtered air pumped through a capillary tube. The following quantities were monitored during the experimental runs; temperature, pH, inorganic carbon (IC), organic carbon (OC), NH_4, NO_3 + NO_2, chlorophyll a (Chl a), phytoplankton species and number, zooplankton species and number, bacteria plate count, inorganic phosphorous (IP), total phosphorous (TP), ATP, phosphates activity (P-ase), and net community respiration and production (i.e., net dark and light CO_2 evolution) using the pH method.

The first run lasted 117 days and involved four 700-liter microcosms (A,B,C,D). The microcosms were identically initiated by addition of inorganic en-

richment medium (Table 1) adjusted so that the molar N:P ratio was .5 (i.e., systems were nitrogen limited). For each tank, 3.5 liters of local lake water were added to this. After day 26, 2 Gambusia (mosquito fish) were added to tanks A and C. Tables 1 and 2 summarize the time averaged values of various quantities measured in this run. They clearly demonstrate the differences induced by the fish in initially similar systems. Namely, in the fish systems there were significant increases in phytoplankton, bacteria, and the rotifer lecane; while there were significant decreases in NH_4, NO_3 + NO_2, and the large cladoceran Simocephalus vetulus. These results agree with our intuition that the fish would graze on the larger zooplankton, and this in turn would result in reduced grazing pressure on the phytoplankton and therefore an increase in phytoplankton.

Table 1. Microcosm chemical data from Run 1. N is the number of times duplicate measurements of the parameter were taken in each system. The entry for each pair of systems (A,C and B,D) is the mean ± standard error of the average value of the parameter for each member of the pair. The value of t is the t-statistic for the null hypothesis that the 2 pairs of systems (A,C with Gambusia and B,D without Gambusia) have equal means.

Parameter (units)	N	Mean ± standard error A,C	B,D	t
IC (mmol liter^{-1})	12	0.21 ±0.04	0.23 ±0.04	0.57
DOC (mmol liter^{-1})	11	0.32 ±0.01	0.31 ±0.01	1.34
POC (mmol liter^{-1})	11	0.076±0.011	0.022±0.001	6.70**
POC:DOC	11	0.29 ±0.01	0.090±0.003	19.61***
NH_4 (µmol liter^{-1})	14	2.2 ±0.2	5.6 ±1.5	3.21*
NO_3 + NO_2	12	0.50 ±0.05	0.90 ±0.14	3.82*

*Null hypothesis rejected at the 80% level of significance.
**Null hypothesis rejected at the 90% level of significance.
***Null hypothesis rejected at the 95% level of significance.

Table 2. Microcosm biological data from Run 1. N is the number of times measurements of the parameters were taken in each system. Only bacteria were duplicated. The entry for each pair of systems (A,C and B,D) is the mean ± standard error of the average value of the parameter for each member of the pair. The value of t is the t-statistic for the null hypothesis that the 2 pairs of systems (A,C with Gambusia and B,D without Gambusia) have equal means.

Parameter (units)	N	Mean ± Standard Error A,C	B,D	t
bacteria (10^4ml^{-1})	17	16±4	5.0 ±1.4	3.90*
Phytoplankton (10^6µm^{3}ml^{-1})	21	3.4±0.1	0.69±0.37	10.05**
Chl a (µg liter^{-1})	11	5.4±2.0	5.1 ±0.7	0.20
phyto C:Chl a[1]	11	113±27	21±7	4.68*
Rotifera (ind liter^{-1})				
Anuraeopsis sp.	17	0.12±0.00	0.59±0.83	1.00
Keratella cochlearis	17	4.5 ±4.4	66±93	0.94
Keratella quadrata	17	130±120	6.2 ±6.7	1.48
Lecane sp.	17	42±3	6.4 ±6.4	7.15**
Trichotria sp.	17	23±31	0.60±0.85	1.00
Cladocera (ind liter^{-1})				
Alona guttata	17	20±4	15±7	0.82
Simocephalus vetulus	17	0.80±0.71	6.8 ±1.0	6.96**
Copepoda (ind liter^{-1})				
Cyclops vernalis	17	1.7 ±0.1	7.2 ±3.3	2.39
Diptera (ind liter^{-1})				
Tanytarsus sp.	17	0.59±0.83	1.8 ±0.8	1.41

*Null hypothesis rejected at the 80% level of significance.
**Null hypothesis rejected at the 90% level of significance.
[1]Assuming that phyto C is 10% of fresh weight.

Table 3. Enrichment levels of inorganic C, N, and P in the 4 700-liter microcosms (A,B,C, and D).

Nutrient	Run	Microcosm concentrations (mol liter^{-1}) A	B	C	D
$NAHCO_3$	1	2.1×10^2	2.1×10^2	2.1×10^2	2.1×10^2
$NA_2HPO_4\cdot7H_2O$	1	3.4	3.4	3.4	3.4
$NaNO_3$	1	1.7	1.7	1.7	1.7
$NaHCO_3$	2	6.3×10^2	6.3×10^2	6.3×10^2	6.3×10^2
$Na_2HPO_4\cdot7H_2O$	2	1.2	4.8	19	4.8
$NaNO_3$	2	19	77	3.0×10^2	77

The second run lasted 188 days and used four 700-liter tanks to which a benthic substrate of acid washed sand (average particle diameter 1.5 mm) was added. Initial enrichment of the water resulted in a molar N:P ratio of 16:1, with different absolute amounts of N and P in tanks (Table 3). As before, an initial inoculum of local lake water was added to each tank. Trophic manipulation of the systems was carried out by the selective addition of mosquito fish (Gambusia affinis), South American catfish (Placostomas placostomas), oligochaetes (Pristina sp.), midge larvae (Tanytarsus sp.), and snails (Physa sp.). (See Table 4.) Figures 1,2 & 3 describe the time evolution of tank D's parameters. Although it had the simplest trophic structure (no fish), the qualitative behavior of its phytoplankton and zooplankton blooms, and the attendant chemical changes was similar to the other tanks.

Perhaps the most significant aspect of this run was the occurrence of a "spring" phytoplankton bloom on days 28-42 followed by a "late summer" bloom on days 168-189 despite the absence of external seasonal variations (Fig. 1). This suggests that so called seasonal behavior may be generated by the internal interactions of a lake's various components. The

Table 4. Manipulation of the biological structure in the four 700-liter microcosms.

Run no.	Date	Day	Manipulation
1	12-03-75	0	Inoculation of each of A,B,C,D with 3.5-liter sample of lakewater
1	01-08-76	36	Addition to each of A,C, of 2 Gambusia of length 2.5 cm
2	05-06-76	0	Inoculation of each of A,B,C,D with 3.5-liter sample of lakewater
2	05-21-76	15	Addition to each of A,B,C,D of 5 Pristina and 5 Tanytarsus larvae
2	06-09-76	34	Addition to each of A,B,C,D of 5 Gambusia of length 1.2 cm
2	06-24-76	49	Addition to each of A,B,C,D of 5 Physa of length 2.5-5.0 mm
2	07-04-76	59	Addition to A of 4 Placostomas of length 1.0 cm
2	08-15-76	101	Transfer of 3 Placostomas from A to B

initial bloom consisted mainly of diatoms and green algae. The secondary bloom consisted almost completely of cryptophyte. Blue-greens were only important in between the two blooms on day 84, when they represented 18% of the phytoplankton volume. Examination of the protozoa and zooplankton blooms (Figs. 1 and 2) combined with changes in the organic carbon levels indicates that the zooplankton limit the blooms by their grazing. Here protozoa blooms preceed while rotifer and bacteria blooms coincide with the phytoplankton bloom. Figure 3a resolves the crustacea into 3 groups: cladocera, copepoda, and ostracods, while Fig. 3b breaks out the cladocera into their component species. Each group has a peak separated in time as does each species of the cladocera. This detailed temperal resolution may not always be observed in natural systems due to spatial mixing. The chemical data is consistent with the taxonomic data. In particular, there were increases in organic carbon and decreases in inorganic carbon during the blooms, followed by increases in NH_4 and $NO_3 + NO_2$ after the bloom indicating organic decomposition. Between days 42 and 49 a formerly light side growth consisting of Oscillatoria and Cladophora increased substantially. Subsequent grazing by 5 adult snails and their offspring removed this growth by day 199. Taken in

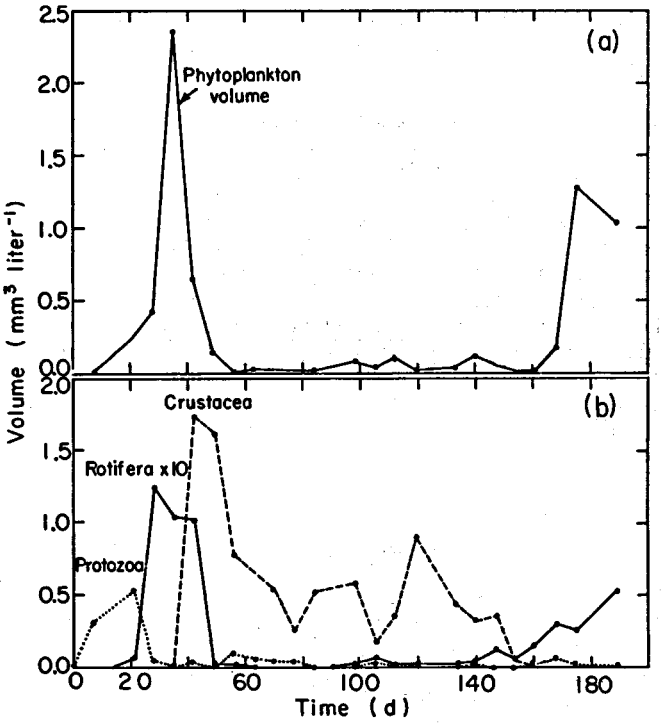

Fig. 1a. Phytoplankton volume, bacteria volume, and chlorophyll a (µgm/ℓ) plotted as a function of time.

1b. Protozoa, rotifera, and crustacea volumes plotted as a function of time.

(XBL 771-119)

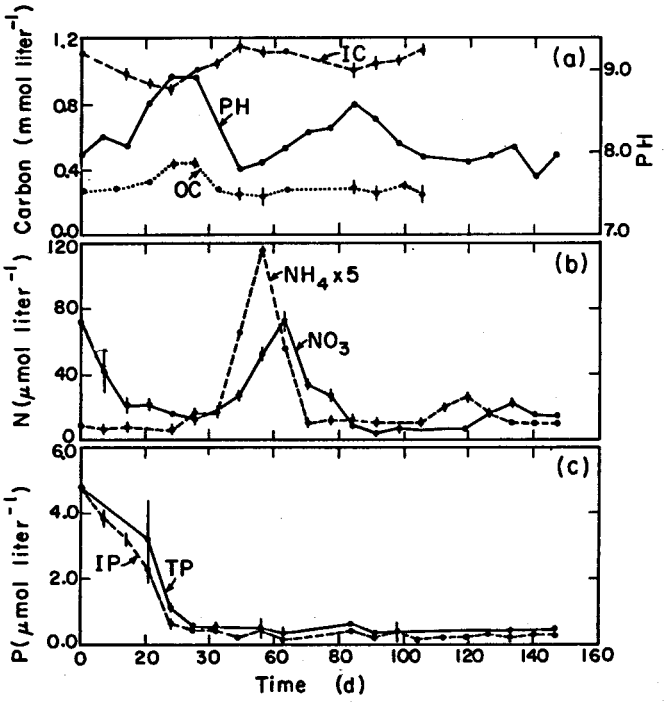

Fig. 2. Chemical parameters plotted as a function of time. (XBL 771-120)

toto, the taxonomic and chemical data suggest that the microcosms behave in a manner very similar to that of natural lake systems between spring and fall

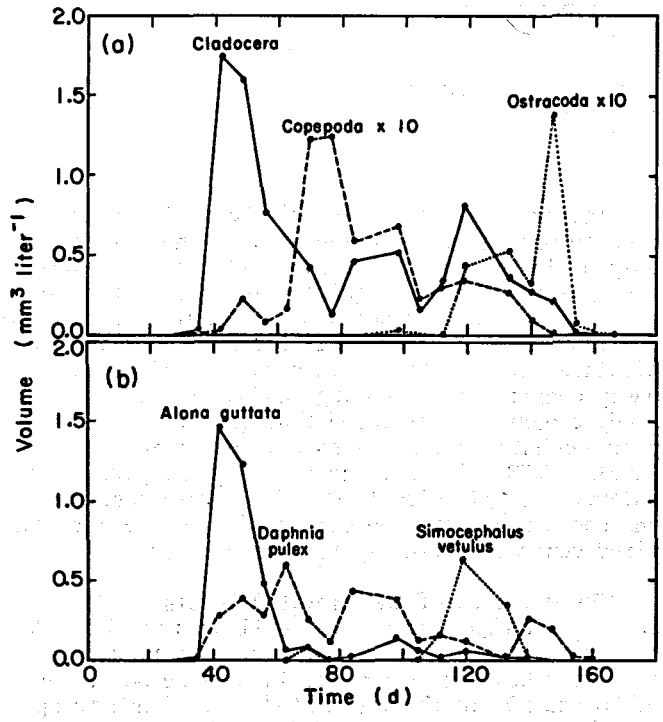

Fig. 3a. Resolution of crustacea into cladocera, copepoda, and ostracoda as a function of time.

3b. Resolution of cladocera in 3 most prevalent species as a function of time.

(XBL 771-121)

and provide extremely useful tools for the study of ecosystem response to perturbations.

Our third extended run is a perturbation experiment and uses 24 50-liter microcosms (A1, A2, A3, B1, B2, B3, C1,...H3). To initiate this run, we added 25ℓ of tank A water from the second run plus 25ℓ of deionized water to each 50-liter tank. We also added varying amounts of N and P in inorganic form to each set of 6 tanks with the idea of creating 4 different types of initial nutrient conditions (Table 5). Fish were initially added but subsequently removed after day 58. On day 60, we perturbed half of these systems by the addition of NH_4Cl (100 ppm). Both the control and perturbed systems will be monitored over a 4 month period. (At the writing of this report, this run was not completed.) Just prior to the perturbation, water samples were removed from the tanks and a series of mini-perturbation experiments performed on them.

These mini-perturbation experiments are designed to indicate the stability properties of the parent systems. Previous theoretical work suggests that an ecosystem's short term response to a detrital pulse can be used to predict its long term stability properties (see 1975 Energy and Environment Division Annual Report).

These experiments are carried out in 4 liter beakers. A detrital-like spike composed of either concentrated freeze-dried E. coli, concentrated freeze-dried algae, or a mix of organic chemicals (similar to enrichment broth), is added. The amount of spike added is selected so as to increase the beakers' organic carbon by approximately 50%. The beakers are then closely monitored over 21 days, and the induced pulses in dark and light CO_2 evolution, NH_4 production, $NO_3 + NO_2$ production, phosphotase activity, bacteria, phytoplankton, and zooplankton tracked and compared with the controls' behavior. In addition to providing measures of our stability indicators, these miniperturbation experiments are a useful tool for studying detrital decomposition and trophic interactions. This is because the induced pulses and relatively rapid changes in the treated systems' various biotic and abiotic components allow certain dynamic relationships and interconnections among the various components to be exhibited. Replication in these mini-perturbation experiments is generally excellent. After introduction of the spike, the initial decomposition (first 3 days) results in increased dark CO_2 evolution (crudely respiration) and increased NH_4 production. Using either of these quantities and comparing treatments with controls, one of our hypothesized stability indicators is readily calculated. Values of this stability indicator soon will be compared with results of the perturbation run. As results of the first perturbation experiment are analyzed, other correlations with stability obtained from these mini-perturbation experiments will be searched for.

PLANNED WORK FOR 1977

Future work will emphasize perturbation experiments and empirical correlations of stability, as well as experiments designed to probe basic aquatic freshwater ecosystem dynamics. To aid these studies, we will probably work on techniques for doing further in situ enzyme assays and for performing rapid suspended particle size concentration measurements. Eventually, we plan to extend our stability work to include the study of terrestrial systems. We also are beginning development of a trace gas flux detection system which can be used in the field at both aquatic and terrestrial interfaces with the atmosphere. We plan to apply this system to the study of a number of trace gases including N_2O and H_2S.

Table 5. Inorganic nitrogen and phosphorus levels in tanks before start of perturbation experiment.

	(A1,2,3:B1,2,3)	(C1,2,3:D1,2,3)	(E1,2,3:F1,2,3)	(G1,2,3,H1,2,3)
μm(N)/ℓ	.9	10.9	100.9	<0.1
μm(P)/ℓ	<0.1	1.0	20.0	10.9

COMBUSTION-GENERATED INDOOR AIR POLLUTION

C. D. Hollowell, R. J. Budnitz, G. W. Traynor,
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INTRODUCTION

Air pollution research has focused almost exclusively on pollution in the outdoor environment and has virtually neglected the indoor environment, even though the major portion of the population spends far more time indoors than outdoors. The importance of indoor air pollution is only now being recognized. Its significance is expected to have a large impact (1) on the overall assessment of the effect of air pollution on human health, (2) on the design of epidemiological studies that must consider indoor as well as outdoor air pollution, (3) on energy conservation strategies for buildings that might restrict indoor-outdoor air exchange, and (4) on the need for more stringent control of air pollution from indoor combustion sources.

The LBL indoor air pollution research project, initiated in 1975, is designed to study the chemical and physical behavior of indoor combustion-generated air pollution in residential and commercial buildings. The broad goals of this project are (1) to characterize indoor air pollution; (2) to identify the important sources, abundance, and fate of indoor air pollutants; (3) to study the abatement of indoor air pollutants; (4) to characterize exposures of the occupants to the important air pollutants; (5) to study the health and welfare effects; and (6) to assess the impact of various energy-conservation strategies on indoor air quality.

The Energy Conservation Standards for New Buildings Act of 1976[1] calls for promulgation of performance standards for all new residential and commercial buildings by 1980. It is expected that the results of this LBL project will provide valuable insight into the impact of various energy conservation measures for buildings on indoor air quality. It is essential that this impact be considered in the development of energy conservation performance standards for new and existing buildings required by this Act.

The work reported here represents the current status of ongoing field and laboratory studies of this project. The initial goal of these studies has been to examine in detail the sources, rates of emissions, dispersion, transformations, and fates of gaseous and aerosol air pollutants in residential buildings. Laboratory and field measurements are conducted with the LBL Mobile Atmospheric Research Laboratory (MARL),[2] which is capable of remote, multipoint sampling for such pollutants as SO_2, NO, NO_2, CO, O_3, and for aerosol size and chemistry. Measurements on laboratory- and field-collected aerosol samples are performed by X-ray fluorescence (XRF), photoelectron spectroscopy (also known as electron spectroscopy for chemical analysis--ESCA), infrared spectroscopy (IR), combustion, and wet chemistry techniques to characterize particulate species such as total sulfur, total nitrogen, SO_4^-, NO_3^-, NH_4^+, Pb, Fe, Zn, and total carbon. Aerosol size measurements for the range 0.01-1.0 μm are performed by condensation nuclei formation and electrical mobility techniques.

The principal objective of the field study has been to obtain quantitative data on the relationship of indoor to outdoor air pollutant concentrations as a function of gas cooking and heating appliance use. Six occupied single-family residential buildings were studied in 1975 for gaseous and particulate air pollutant levels under typical occupancy conditions of cooking and heating.[3] This field study clearly demonstrated that gas stove use under poor ventilation conditions can result in elevated levels of CO, NO, NO_2, and even SO_2 and particulate sulfur. High levels of NO and NO_2 were observed in the one house where the effect of a forced-air gas-fired central heating system was studied.

The duration of the elevated levels of CO, NO, and NO_2 from gas combustion appliances may be under 1 hour for gas stove use but may be continuous for gas-fired heating system use in cool seasons. Levels of CO and NO_2 in the field study were found to approach or exceed existing U.S.A. ambient air quality standards. Nitrogen dioxide levels in kitchens of houses with gas stoves were observed to be as high as 1000 $\mu g/m^3$ with one top burner operating for less than 30 minutes and as high as 1700 $\mu g/m^3$ with the oven operating for 20 minutes. Concentrations of NO_2 were observed to be as high as 1200 $\mu g/m^3$ for 8 hours in the bedroom of a house with a forced-air gas-fired heating system operating under normal conditions. These NO_2 concentrations can be compared with the short-term recommended U.S. and promulgated foreign NO_2 air quality standards (~400 $\mu g/m^3$ for 1 hour).[4]

ACCOMPLISHMENTS DURING 1976

Laboratory studies now in progress in experimental rooms and buildings are designed to identify various parameters which affect rates of emissions from gas-fired cooking and heating appliances and short- and long-term air pollution levels in the indoor environment from such appliances. The parameters include appliance type and its operating characteristics (for example, fuel/air mixture, flame temperature and geometry) and reduced ventilation and air infiltration rates expected to be imposed because of energy conservation measures. Work in progress concerns the dispersion, transformations, and ultimate fate of combustion-generated indoor pollutants. The physical and chemical transformations depend on the many constituents (gaseous and particulate) present in the air, on temperature and humidity, and on the effects of walls and other materials on the ultimate fate of various species. This phase of the study involves detailed analysis and experiments with various ventilation and air circulation systems.

Studies using an experimental room with an air volume of 27 m^3 have characterized the emissions from a new gas stove operating in the room with air exchange rates from 1/4 to 10 air changes per hour. Well-constructed new single-family houses have air exchange (ventilation and infiltration) rates on the order of 1 air change per hour (ACPH). Older houses

and most new houses have air exchange rates of 2 ACPH or higher. Energy conservation measures which would limit the air exchange rate in new houses to 1/4 to 1/2 ACPH are now being considered by state governments and the Federal government.

These laboratory studies have shown that gas stoves generate extremely high concentrations of such species as CO, NO, NO_2, respirable aerosols (size <1.0 μm), and particulate sulfur when the air exchange rate is controlled to less than 1 ACPH. The results of one such experiment are given in Table 1 and are compared with typical polluted urban outdoor air. This experiment was conducted with the air exchange rate at 1/4 ACPH and with the oven of a new gas stove on for the first hour of a 3-hour measurement period. While these laboratory studies do not necessarily duplicate "real world" situations, they clearly demonstrate the types and levels of air pollutants one could expect under low air exchange rates for buildings; these rates may be required in order to meet new energy conservation performance standards for buildings. Such "real world" findings have already been demonstrated in field experiments with six "leaky" houses where air exchange rates were on the order of a few air changes per hour.

PLANNED ACTIVITIES FOR 1977

Laboratory investigations now in progress include detailed studies of nitrogen compounds in the indoor environment. Of particular interest are the high NO_2/NO ratios observed in the laboratory and field studies. In addition to NO and NO_2, considerable attention is being given to such gaseous species as HCN and NH_3 and particulate species as NO_3^-, NH_4^+, and organic nitrogen compounds. Analytical procedures for HCN and NH_3 are currently being developed. Gas chromatography/mass spectrometry (GC/MS) analyses for organic aerosol species will also be explored in future studies. Detailed air circulation, ventilation, and infiltration measurements will be performed in future field and laboratory experiments using air flow sensors and sulfur hexafluoride as a tracer gas for air exchange rate determinations.

Combustion-generated indoor air pollution will be studied in several occupied residential buildings in 1977. The buildings will be selected on the basis of residential building type, indoor combustion sources, occupancy patterns, and air circulation, ventilation, and infiltration factors.

Other indoor environments in which people spend considerable time are commercial buildings such as office buildings, and schools and other public or semipublic buildings. Modern commercial buildings are usually engineered so that the circulation and infiltration of air are controlled, and public health regulations often require certain minimum air-circulation rates, usually for the purpose of decreasing transmission of infectious disease. However, significant attention is seldom, if ever, given to the public health role of air pollution generated by indoor sources. Combustion-generated indoor air pollution in these buildings will be studied in subsequent phases of this project.

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Table 1. Air pollutants observed from a gas stove operating in an experimental room at a controlled air exchange rate of 1/4 air changes per hour.[a]

Parameter measured	Background		3-hr measurement period		Typical peak polluted urban levels
	Indoor	Outdoor	Gas oven on (1-hr average)	Gas oven off (2-hr average)	
CO (ppm)	.8	.8	35	60	10-20
NO (ppm)	.005	.040	0.8	1.2	.2-.5
NO_2 (ppm)	.045	.050	2.5	2.5	.2-.5
SO_2 (ppm)	.005	.005	.010	.020	.1-.5
S (as SO_4^{--}) ($\mu g/m^3$)	<1	<2	13	14	10-20
Aitken nuclei (no./cm^3)	20K	40K	3000K	200K	100-4000K
Submicron aerosol mass median diameter (μm)	.2-.3	.2-.3	.08	.2	.2-.4

[a]Measurements at center of 27 m^3 room for 3-hr period (gas stove oven operating for first hour only).

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POPULATIONS AT RISK TO AIR POLLUTION

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INTRODUCTION

A project to assess the populations at risk to various air pollutants was initiated in July, 1976, under funding from the U. S. Environmental Protection Agency (EPA). This 2-year research project is divided into three main tasks, the first to be completed by July, 1977, and the second and third to be completed by July 1978.

Task One involves the creation of a set of integrated primary data bases containing data on socio-economic and demographic characteristics, air pollution levels for several important pollutants, meteorological parameters, and the development of morbidity and mortality statistics for the United States on a county basis. Task Two involves the determination of the populations at risk to various air pollutants, and Task Three involves the analysis of associations between air pollutant levels and various indices.

The set of data bases to be created in Task One will be interfaced to efficient and sophisticated computer information storage, retrieval, and display systems (including computer-generated color maps, charts, and graphs). The four categories of data bases to be created are:

1. Socio-economic and demographic data base. The socio-economic and demographic data base known as Socio-Economic Environmental Demographic Information System (SEEDIS)[1] has been developed at LBL and is available for use. The SEEDIS system contains most of the 1970 Census of Population and Housing for the nation in detail, as well as a variety of other data on employment, manufacturing, agriculture, water resources, cause of death, transportation, income, economic factors, and a large geographic data base of state, county, and census tract boundaries.

2. Air quality and emissions data bases. The SAROAD (air quality and NEDS (emissions) data banks of EPA for 1975 will be obtained in machine-readable form for total suspended particulates, SO_2, NO_x, photochemical oxidants, carbon monoxide, hydrocarbons (methane and nonmethane), sulfates, and nitrates. Extrapolations and interpolations in space and time will be required to fill gaps in the air quality data. It is expected that only straightforward techniques using the above data banks will be applied, without recourse to auxiliary data sources. As it is most likely that the above data bases contain adequate information on only three or four of the pollutants, only limited analysis can be done on the others.

3. Meteorological data base. Limited meteorological data from the U. S. Weather Bureau are available at LBL and will be processed if appropriate to this project. The summary meteorological data base from EPA's Human Studies Laboratory will be acquired and processed.

4. Health statistics data base. The 1970 and 1975 mortality data will be acquired from the National Center for Health Statistics. Geocoding these data by SMSA and county will be undertaken in order to correlate them with the air quality and socio-economic and demographic data. Morbidity data will be analyzed from small area surveys, including the 3rd National Cancer Survey. It will be possible to integrate such heterogeneous data with the above-mentioned data bases only with additional support.

The geographical subunits to be used in the initial populations-at-risk assessments of Task Two will be counties of the entire United States. Wherever there are multiple sampling sites within a limited geographical area (for example, states or counties), optimum data utilization will require knowledge of the latitude and longitude coordinates of individual monitoring sites, emissions sources, and approximate centroids of sub-county geopolitical units (for example census tracts). Computer programs developed at LBL will be used for this purpose. Extrapolations and interpolations in space and time may be used to estimate air pollutant concentration data and correlate these data to observed and extrapolated air quality data.

When all of the geographical subunits have been identified and a particular distribution of air-pollutant concentration has been assigned, it will be possible to estimate directly from the SEEDIS data base the populations exposed to various air pollutants. These estimations will be broken down by a variety of census-determined characteristics, including such parameters as age, sex, indices of economic status, occupational history, ethnicity, and nativity. Having identified the population sub-

units and air pollution characteristics, we will then estimate various high-risk groups by geographical area for the entire country.

Task Three will entail the analysis of the disease effects of air pollution through the use of step-wise multiple regression analyses. The dependent variables will be (1) general mortality as well as disease-specific mortality, and (2) disease-specific morbidity, if available. Using the census data for each of the geographical subunits, normalized self-weighting age-adjusted indices will be computed. These indices will be used as the dependent variables in a series of step-wise multiple regression analyses of 1970 census tract characteristics divided into five groups consisting of ethnic, industrial, social, physical, and economic factors. The physical factors may include meteorological data as well as air pollution data.

ACCOMPLISHMENTS DURING 1976

Specific project goals have been clearly identified, with initial attention focused on the creation of the data bases of Task One.[2,3]

Sources of mortality, air quality, and emissions data within various ERDA laboratories as well as the EPA have been identified. Several computer-related tasks were begun in 1976; these tasks are in various stages of completion and are described below.

In order to facilitate communication between LBL, EPA, and other institutions, a computer teleconference has been established in the DEC PDP-10 computer of Bolt, Beranek, and Newman in Cambridge, Massachusetts. The teleconference program, named PLANET, is the product of Institute for the Future, in Menlo Park, California. Participants having MODEM-equipped 30 char/sec computer terminals may access the teleconference directly via either TELENET or the ARPANET.

In order to facilitate access to data files in many different locations, account numbers have been established in computers at the following locations:

- (LBL) Lawrence Berkeley Laboratory, Berkeley, California
- (EPA) Environmental Protection Agency, Research Triangle Park, North Carolina
- (BNL) Brookhaven National Laboratory, Upton, New York
- (BBN) Bolt, Beranek, and Newman, Cambridge, Massachusetts
- (ANL) Argonne National Laboratory, Argonne, Illinois
- (ORNL) Oak Ridge National Laboratory, Oak Ridge, Tennessee
- (LLL) Lawrence Livermore Laboratory, Livermore, California
- (PNL) Pacific Northwest Laboratory, Richland, Washington
- (LASL) Los Alamos Scientific Laboratory, Los Alamos, New Mexico
- (MIT) Massachusetts Institute of Technology, Cambridge, Massachusetts
- (SRI) Stanford Research Institute, Menlo Park, California
- (STAN) Stanford University, Stanford, California
- (UCLA) University of California at Los Angeles
- (UCB) University of California at Berkeley
- (NYU) New York University, New York, New York
- (BCL) Battelle Columbus Laboratories, Columbus, Ohio
- (TYM) TYMSHARE, Inc., Cupertino, California
- (ABAG) Association of Bay Area Governments, Berkeley, California
- (CCA) Computer Corporation of America, Cambridge, Massachusetts
- (SLAC) Stanford Linear Accelerator Center, Stanford, California

Computer accounts have been officially opened at the first four locations, which will be heavily used in this project. Accounts at the other locations have been provided free of charge on a limited-use basis, for exploratory use and the retrieval of small files that may be required. A Textronix 4923 cassette recorder has been connected to a computer terminal and successfully used to retrieve small data files from all of the above computer installations. Several files to be used directly in this project have already been transferred. These include the following:

- (from EPA) conversion dictionary, SAROAD to FIPS county codes
- (from BNL) portions of MEDABA medical data base
- (from EPA) portions of APPAR population-at-risk data base
- (from EPA) portions of EDS Energy Data System data base
- (from EPA) portions of AEROS, from AEROS Terminal System (ATS)
- (from BNL) UTM to latitude-longitude conversion programs
- (from ABAG) programs for conversion of geographical data bases
- (from BNL) portions of NEDSNE (NEDS data for New England)
- (from ORNL) specifications for IWGDE data exchange standard
- (from ORNL) RUSTIC technical memo
- (from BBN) transcripts of PLANET teleconferences
- (from TYM) transcripts of PLANET teleconferences
- (from ORNL) portions of LLL survey of data bases
- (from ORNL) bibliographic data from ERDA-RECON
- (from ORNL) descriptions of software for geographical data bases
- (from ANL) descriptions of software for geographical data bases

Two data sets on cancer incidence and mortality have been loaded into the LBL system. They are (1) the U. S. Cancer County Mortality data for 1950-1969 used recently by the National Cancer Institute to generate an "Atlas of Cancer Mortality," and (2) the Third National Cancer Survey, 1969-1971, which contains complete cancer incidence data for nine areas of the U. S.

PLANNED ACTIVITIES FOR 1977

Several items are on the agenda for the coming year. These include:

1. Completing the loading of the required data bases;

2. Putting subsets of the data base into CARTE input format for production of selected black-and-white and color maps (U. S. by county). These maps will provide the basic guidance necessary in planning detailed studies of the project and include:

   a. Maps of air quality data for examining the validity of various measurement methods. For example, it would be useful to prepare maps of SO_2 obtained with the EPA reference method (pararosaniline 24-hour manual method) and equivalent instrumental methods (FPD, UV fluorescence, coulometric) in order to estimate the severe temperature dependence of the EPA reference method recently recognized;[4]

   b. Maps of mortality data for 1969-1971, including the National Cancer Institute's county cancer mortality data as an initial examination of the pattern of mortality due to various disease outcomes;

   c. Maps by county of 1970 census variables of primary interest such as age, sex, race, education, income, housing characteristics, and occupation;

3. SAROAD air quality data from 1975 will be investigated for measurement techniques, quality assurance, and completeness. It is expected that NEDS data will be used extensively to estimate air quality with simple models for those counties where no measurements or unacceptable measurements have been made. Black and white maps will be used extensively in making decisions regarding adequacy of air quality estimates based on the NEDS data.

4. Certain preliminary statistical analyses are planned but may be revised depending upon the content of the final data bases. These preliminary analyses include:

   a. Examination of mortality data for every city with a population of 250,000 or greater in relation to the pollutant data available for these urban areas;

   b. Calculation of correlations between specific causes of death and various pollutants. High correlations will initiate further investigation of subsets of these data;

   c. Comparison of mortality rates of nonurban areas. Important variables such as age, race, sex, socio-economic status, as well as pollutant level, will be taken into account.

FOOTNOTES AND REFERENCES

*Energy & Environment Division.

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HEALTH AND SAFETY IMPACTS OF NUCLEAR, GEOTHERMAL AND FOSSIL-FUEL ELECTRIC GENERATION IN CALIFORNIA*

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INTRODUCTION

The Health and Safety Impacts project has been performed for the State of California Energy Resources Conservation and Development Commission (ERCDC) primarily to support the effort of the ERCDC Facilities Siting Division to establish a methodology for the review of the health and safety aspects of proposed electric generation sites and facilities. The work has involved two closely related aspects. The first has been to assemble information on applicable health and safety standards and to review the present understanding of the impacts which nuclear, geothermal and fossil-fuel power plants may have on the health and safety of the public and of employees. The second has been to set forth detailed methodologies which may be employed in the review of proposed facilities. An important result of this dual effort has been to identify areas where new information or new standards should be developed in order to establish a satisfactory review methodology.

The project began on July 1, 1976 and has been essentially completed except for possible modification of the project reports, now in draft form, which should be available in final form by April 1, 1977.[1]

ACCOMPLISHMENTS DURING 1976

The three technologies treated in this work; nuclear, geothermal, and fossil-fuel, have substantially different potential impacts. For this reason, much of the work and many of the resulting reports have drawn a conventional distinction between nuclear power plants and geothermal and fossil-fuel power plants, and, by association, between radioactive pollutants and conventional pollutants. However, as much as possible, the resulting review methodologies have used similar structures.

Health and Safety Impacts and Related Standards

The major emphasis has been on potential impacts on the public, which occur largely through emissions of radioactive or conventional pollutants into the air. Known and possible health effects of these emissions have been identified and discussed, and related standards for the protection of the public have been examined for their effectiveness considering the control technologies which are currently, or may shortly be, available.

A strong distinction may be drawn between the effects of routine emissions and accidental releases from these plants. For all the technologies considered, substantial regulatory apparatus and standards exist for control of routine emissions, and, although there are areas where improvements should be made, this structure provides a substantial and largely adequate measure of protection for the general public. In each case the standards are based on large amounts of research, either epidemiological, clinical, or biochemical. For radioactive pollutants the results of this work have been adequate to establish standards that are closely related to actual estimates of the health effects of these pollutants. For conventional emissions the information is generally not adequate to make such estimates, but it is adequate to support the establishment of standards which would effectively protect the public health. Based on the rough estimates which have been made, it appears that the public health effects of conventional emissions from a fossil-fuel plant are more substantial than the radioactive emissions from a nuclear plant of similar size.

However, a nuclear plant has the potential for causing considerable harm to the public, should a large accidental release of radioactivity occur. Accidents of corresponding severity, in their effects on the public, cannot be associated with geothermal and fossil-fuel plants. A substantial portion of the work, therefore, has been devoted to an examination of the probability and consequences of nuclear plant accidents and to consideration of the means for mitigating the potential danger to the public. While the present work has not been extensive enough to make important independent contributions to the understanding of these matters, it has served to clarify the manner in which previous work may be used in establishing a structure for an ERCDC review of the safety of proposed facilities.

The potential effects of noise production and of power plant emissions into water are less important than emissions into air, and have been treated only briefly. Moreover, the impacts of plant operation on workers are controlled via occupational safety and health regulations common to all industrial facilities. Although in some cases the overall impact on workers may be more severe than on the public, occupational exposures are not considered in the same light as public exposures because of the increased benefit the worker gains from operation of the facility. Nevertheless, control of these impacts through the implementation of OSHA standards is a subject of review by the ERCDC.

The engineering of the plant facilities may also be examined to minimize either routine emissions or the potential for accidents. For nuclear power plants, these matters are reviewed in detail by the Nuclear Regulatory Commission. The extent to which the ERCDC might eventually involve itself in plant engineering is uncertain and greatly affects the nature of the review process. Many engineering standards (as distinguished from regulatory standards) are available for use in the design of plants and in their review, but a substantial effort would be necessary to select standards for use in the regulatory process.

Methodologies for Review of Proposed Sites and Facilities

Based on existing information on the health and safety impacts of nuclear, geothermal and fossil-fuel power plants, and on related standards, we have formulated possible methodologies for review of proposed sites and facilities. These methodologies rely as much as possible on regulatory standards, particularly for emissions from the plants. Even in these instances, compliance with certain types of standards, such as air quality standards, can only be checked on the basis of detailed analysis by the ERCDC staff of related agencies. In many areas, such as those related to site characteristics, the staff may have to rely on expert advice in reaching a judgment on site suitability.

The form of the methodologies has been determined by the structure of the ERCDC review process, which is divided into a Notice of Intention (NOI) review, wherein a number of sites are examined as to suitability for generic plant type, and an Application for Certification (AFC) review, wherein the details of the proposed facilities may be examined. At the various stages of proposed NOI methodologies, the subjects examined are: air emissions, water emissions, noise, waste disposal, and geophysical and developmental site characteristics. The possible AFC methodologies involve methods for assuring compliance in the matters reviewed at the NOI, examination of the performance of emission control equipment, and review of the safety and general engineering of the facilities.

Areas Where Further Work is Required

Existing health-related standards are largely adequate for the general protection of the public. In specific areas, such as standards for conventional particulates, considerable improvements are possible. For radioactive materials most of the ev-

idence suggests that only minor adjustments in standards for individual radioactive species will take place.

For conventional pollutants a substantial effort will be required to develop the information to make an actual assessment of health impacts. (For radioactive emissions, estimates of such impacts may be made now.) Such assessments will be very useful for choosing between alternative sites or, ultimately, between alternative technologies.

For nuclear power plants further work is required to develop the capability to perform site-specific analyses of the potential impacts of large accidental releases of radioactivity. Such analysis may serve as a basis for establishing and maintaining low population zones near nuclear power plants. Both this analytical capability and the tools for controlling population growth must be developed.

The alternative manners in which the ERCDC may involve itself in the engineering review of proposed facilities needs to be examined carefully. For either a few or many engineering areas, this may involve establishing standards and a corresponding review process that relies heavily on a quality assurance program, or leaving review to other agencies or to the plant designers.

In any case, it is clear that although enough information presently exists to establish an initial review process, this process will be improved as work in the above areas, and others is carried out.

FOOTNOTE

* Supported by the State of California Energy Resources Conservation and Development Commission, Contract No. 4-0123.

REPORTS RESULTING FROM THIS WORK

A. V. Nero, et al., "Health and Safety Impacts of Nuclear, Geothermal,and Fossil-Fuel Electric Generation in California: Overview Report", Lawrence Berkeley Laboratory Report LBL-5924. Includes "Executive Summary" for the project.

A. V. Nero and Y. C. Wong, "Radiological Health and Related Standards for Nuclear Power Plants", Lawrence Berkeley Laboratory Report LBL-5285.

A. V. Nero and M. R. K. Farnaam, "A Review of Light-Water Reactor Safety STudies", Lawrence Berkeley Laboratory Report LBL-5286

W. W. S. Yen, "Radiological Emergency Response Planning for Nuclear Power Plants in California", Lawrence Berkeley Laboratory Report LBL-5920.

A. V. Nero, C. Schroeder, and W. W. S. Yen, "Control of Population Densities Surrounding Nuclear Power Plants", Lawrence Berkeley Laboratory Report LBL-5921.

C. C. Case, T. A. Bertolli, J. Bodington, T. A. Choy, and A. V. Nero, "Health Effects and Related Standareds for Fossil-Fuel and Geothermal Power Plants", Lawrence Berkeley Report LBL-5287.

A. V. Nero and I. N. M. N. Bouromand, "Power Plant Reliability-Availability and State Regulation", Lawrence Berkeley Laboratory Report LBL-5922.

L. C. Rosen, "A Review of Air Quality Modeling Techniques", Lawrence Berkeley Laboratory Report LBL-5923.

M. S. Quimby-Hunt, A. V. Nero, and staff, "Methodologies for Review of the Health and Safety Aspects of Proposed Nuclear, Geothermal, and Fossil-Fuel Sites and Facilities", Lawrence Berkeley Laboratory Report LBL-5923.

ATMOSPHERIC AEROSOL RESEARCH GROUP

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INTRODUCTION

The principal goal of the Atmospheric Aerosol Research Group's program is to understand the formation and transport of particulate and gaseous pollutants from fossil fuel combustion. During 1976 our major efforts were directed toward (1) studying certain atmospheric chemical reactions under laboratory conditions, (2) applying and developing techniques for the chemical and physical characterization of specific pollutants, and (3) studying pollutant behavior in the field.

Sulfur, nitrogen, and carbon compounds constitute up to 80% of the dry mass of atmospheric aerosol particles. It is therefore important to understand the chemical mechanisms responsible for their formation. It is also important to examine the relative significance of homogeneous (gas-phase) and heterogeneous (gas-particle) reactions in the formation of major pollutants. Most studies in the past have emphasized gas-phase reactions in general and photochemical reactions in particular. Considerably less effort has been devoted to studies of nonphotochemical heterogeneous reactions. Such reactions seem to be important, however, because episodes of heavy aerosol pollution do occur under typically nonphotochemical conditions, that is, when the concentrations of photochemical reaction products such as ozone are low or negligible.

Under such conditions the aerosol particles should consist of primary particles and secondary species produced in nonphotochemical, probably gas-

particle, reactions. We have therefore begun a systematic field study, using our newly equipped Mobile Atmospheric Research Laboratory, to characterize the frequent wintertime pollution episodes in the Berkeley area. These studies will be extended into the summer when the manifestations of photochemical smog-type reactions become pronounced. A careful comparison of aerosol behavior under these two distinctly different situations will enable us to differentiate the relative contributions of photochemical and non-photochemical reactions to the formation of specific pollutants.

These field studies are intimately connected with our ongoing laboratory experiments on the formation of pollutants. Because most of the air pollution is caused by the combustion of fossil fuels, it is of interest to investigate the formation of particles in flames and to study the chemical interactions between these particles and the principal pollutant gases. The results of two such studies are reported here. One deals with the production of carbon particles in well-defined premixed flames, while the other deals with the chemical reaction of carbon particles with ammonia.

We have continued to place heavy emphasis on the chemical characterization of aerosol species by physical methods. Two novel methods have been under development during the past year. A nuclear activation method for the determination of total particulate nitrogen was developed and tested with both synthetic and ambient particulates. We have also investigated the feasibility of using optical attenuation by ambient particulates to determine total particulate carbon concentration.

The chemical characterization of ambient, source-enriched, and synthetic aerosol particles by means of vibrational spectroscopy provides a promising way of obtaining molecular and structural information about these materials. We are using both Raman and infrared spectroscopy for this purpose. The two techniques are complementary. A newly acquired rapid-scan Fourier-transform infrared spectrometer has greatly expanded our capabilities. The applications of these methods to laboratory studies and to analysis of ambient particulates are described in this report.

Photoelectron spectroscopy for chemical analysis (ESCA) has continued to play an important part in our work as a convenient method for the chemical characterization of ambient and other particulates. The results obtained by this technique are presented for samples collected in Berkeley and in a collaborative ERDA project known as the Da Vinci Experiments. These experiments refer to two manned balloon flights, Da Vinci II and Da Vinci III, carried out during the spring and summer of 1976. The purpose of these flights was to follow the St. Louis, Missouri, mixed urban-industrial plume. Samples collected in these flights were analyzed by X-ray fluorescence and X-ray photoelectron spectroscopy. The principal results of these analyses are outlined in this report.

POLLUTANT FORMATION STUDIES

1. Studies of Carbon Particle Production from Well-Defined Flames

Understanding soot formation phenomena and properties of soot particles produced in flames is of considerable importance from both the industrial and the environmental point of view. Knowledge of the radiation properties of particles formed in flames is important for improving thermal efficiencies of power plants and industrial furnaces. Soot particles are a major source of air pollution in themselves, and they also affect the rate of NO, CO, and hydrocarbon formation.[1] Furthermore, catalytic reaction on suspended soot particulates plays an important role in oxidation of SO_2 to sulfate.[2] Reactions between nitrogen oxides and carbonaceous solids are also of interest for control of NO_x emissions.[3] This suggests that fine particles (about 70-100 Å)[4] generated in nonluminous, "clean" flames can be very important in these reactions because of their large surface area.

There is not much information on the properties of these particles because of the many parameters that influence combustion processes. Most of the reports on this subject concern the initiation and characterization of the soot particles within the flame, or the soot emitted by flames as carbon black. This characterization was usually done by measuring the amount of scattered light or by probing the gases and analyzing deposits with the electron microscope.[5] These techniques do not give much information on the properties of soot particles from the "nonsooty" flames, and the question of what happens to these nuclei after they leave the flame remains unanswered.

A water-cooled porous-plate flat-flame burner was used in the study of a premixed acetylene-air flame. Figure 1 shows a schematic of the experimental setup. The burner is located in a stainless steel combustion chamber which prevents entrainment of combustion products with dirty laboratory air. A sheath of nitrogen gas around the burner minimizes the mixing of fresh gases with old combustion products. Part of the burned gases is probed and then diluted with clean air used for different gas and solid phase analyses. Flames obtained in this burner are stable and well characterized for a large range of combusion parameters. Acetylene was used in this study because its flammability limits are wide (2.5-80% acetylene in an acetylene-air mixture)[6] and the flames are very stable. The acetylene was purified and metered before mixing with filtered dry compressed air. Perfectly flat flames were obtained for a range of equivalence ratio (ϕ) of 0.7 to 1.4. Flames richer than this tend to become polyhedral. At $\phi = 1.8$, the flame becomes luminous and carbon particles are detectable to the eye. Flame temperature was measured using a 0.0076-cm diameter Pt-Pt, 10% Rh thermocouple. The maximum flame temperature was 1794°K for a stoichiometric mixture ($\phi = 1.0$) at a flame velocity of 21 cm/sec. Flame temperature remained uniform to ±1% of maximum temperature ex-

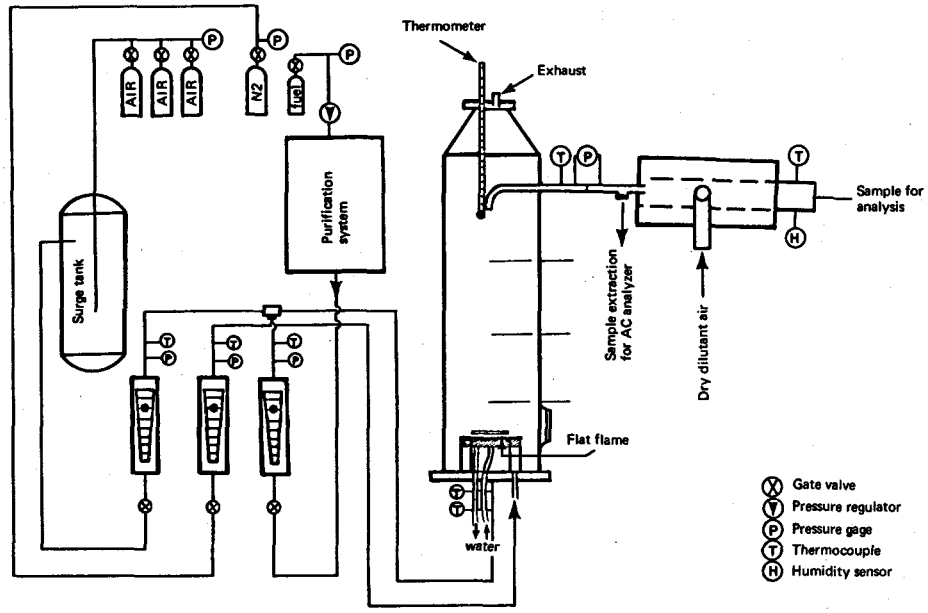

Fig. 1. Schematic of experimental setup. A mixture of dried purified air and acetylene is metered and then burned, producing a flat flame. Part of the combustion product is sampled at different locations and diluted before analyses. (XBL 773-652)

cept at the very edges where mixing with the cool ambient air occurs. Heat losses to the burner were measured for different flow rates and equivalence ratios. Adiabatic flame temperature and flame velocity were calculated by extrapolating data to zero heat loss. Maximum adiabatic flame velocity of 135 cm/sec at $\phi = 1.0$ was found. Assuming flow is controlled by a single overall reaction obeying the simple Arrhenius rate expression, the activation energy of E = 48±10) kcal/° K was obtained (Fig. 2). Experiments were repeated for total flow ratios of 10-35 liters/min. Increasing the total flow rate increases the distance of the flame relative to the burner surface. Heat removal becomes less efficient and the flame becomes more adiabatic.

Elementary studies of number and size distribution were made using an Electrical Aerosol for Mobility Analyzer (EASA) and a Condensation Nuclei Counter (CNC). Based on these studies, particles of 50-200 Å and concentrations of 10^8-10^{12} particles/cc are detected. We are also investigating the effects of humidity and other combustion parameters on the particle size distribution using X-ray photoelectron spectrometry to study the surface chemistry of carbon deposits.

2. Surface Reactions of Carbon Particles with Ammonia

The surface of a carbon particle contains many active sites as a result of the unsaturation in valency of surface atoms and can therefore readily react with many chemical species, resulting in the formation of surface functional groups. These surface species can modify the catalytic activity of the carbon particle. Therefore it is important to identify the surface species in order to understand the catalytic nature of the carbon particle.

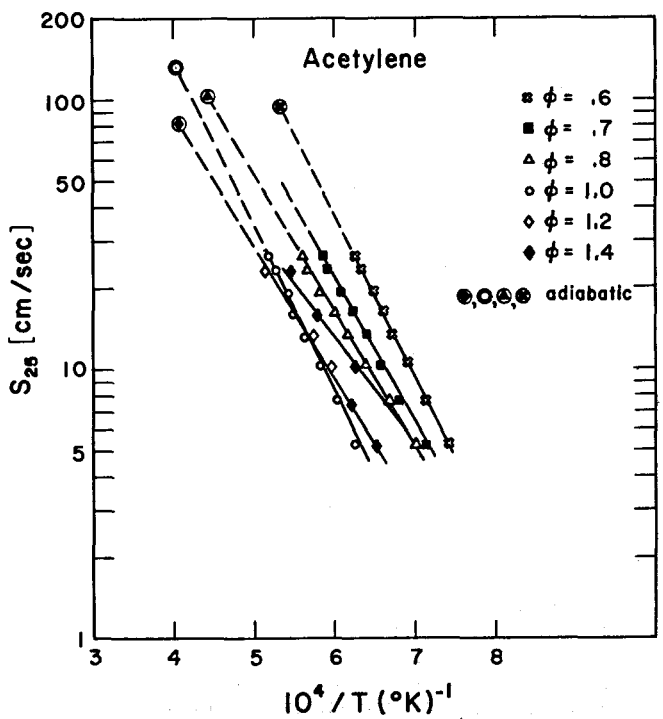

Fig. 2. Flame velocity of the flat acetylene flame S_{25} (normalized to 25° C unburned gas) as a function of inverse temperature. An Arrhenius-type equation $S_{25}^2 = ke^{-E/RT}$ when E = 58±10 kcal/° K fits the data. Adiabatic flame velocities are obtained by extrapolating the data to equilibrium adiabatic flame temperatures. (XBL 773-650)

It is difficult to apply optical spectroscopy to uncover the structure of surface species on carbon because of the high absorption coefficient of the carbon particle. We have employed a technique to increase the surface area per unit mass of carbon to enrich the concentration of surface species in question. This is done by grinding a graphite sample in the presence of a desirable chemical reactant. After extensive grinding the carbon particles are mixed thoroughly with KBr powder and pressed into a pellet for infrared analysis.

With the use of ESCA, we have been investigating the structure of surface nitrogen species that can be produced after exposure of a fresh graphitic carbon particle surface to NH_3 at room temperature. This nitrogen species could be in the following chemical forms: an intercalation compound, a heterocyclic compound, a coordination compound, and/or a dissociative chemisorbed species on the particle surface. X-ray diffraction technique has been applied to these samples and the results seem to rule out the possibility of the existence of an intercalation compound. Mass spectrometer analysis of the species coming off at high temperatures is in progress. Investigation of the chemical reactivity of this nitrogen species is also under way.

Infrared spectra of the graphitic particles after extensive grinding in an atmosphere of ammonia have been successfully obtained as shown in Fig. 3a. For comparison, infrared spectra of the particles ground under identical conditions in an atmosphere of air and Xe have also been made, as shown in Fig. 3b and 3c. The vibrational frequencies observed are summarized below, with (S), (M), and (W) indicating strong, medium, and weak absorptions: (1) grinding in ammonia, 1160(S), 1320(W), 1400(W), 1450(W), 1580(S), 1660(W), 2840(W), 2910(W), 3200(M), 3350(M) cm^{-1}; (2) grinding in oxygen, 800(M), 1380(S), 1580(S), 1700(W), and 1720(W) cm^{-1}; and (3) grinding in Xe, 1580(W) cm^{-1}. These frequencies will be assigned when the isotope study now in progress is finished.

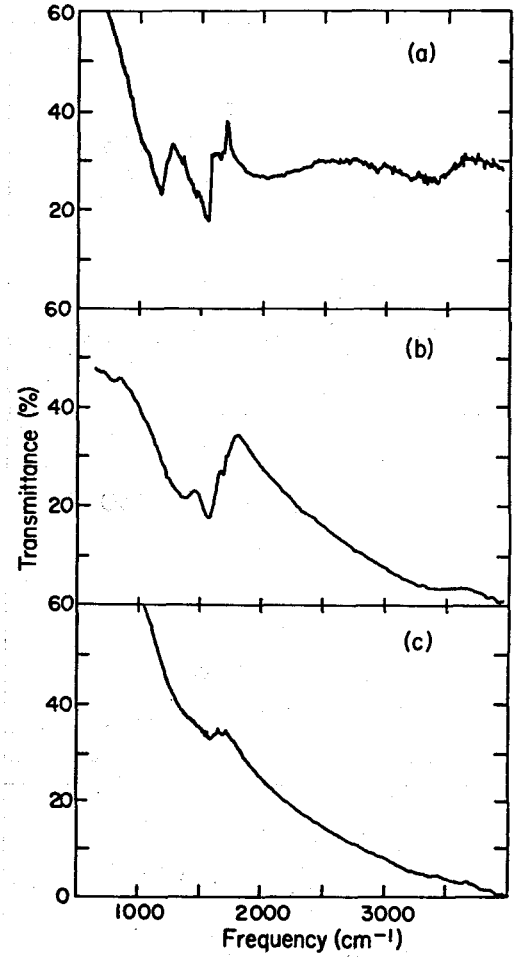

Fig. 3. Infrared spectra between 600 and 4000 cm^{-1} of: a) Graphite ground in an atmosphere of ammonia. b) Graphite ground in an atmosphere of air. c) Graphite ground in an atmosphere of Xe. (XBL 772-424)

3. Study of the Activation of Graphite Using Raman Spectroscopy

Activated carbon is a well-known surface chemical and catalytically active material used in many important industrial processes. It can be viewed as being made up of small crystallites of the order of 25 Å in size, which have layered graphitic structure. The chemical activity of the material is thought to be due to functional groups containing oxygen and hydrogen that are attached to the surface of these crystallites. However, the nature and the formation mechanism of these species are not well understood. Such an understanding could help to tailor the catalyst for particular needs.

There have been several investigations of these species using the infrared technique, but these have had only limited success because of the difficulty in taking spectra on the highly absorbing carbon substrate. Our initial attempts in using the Raman scattering technique, which in many ways is complementary to the infrared technique, have been encouraging. We believe that this is the first attempt to apply this spectroscopic technique to the characterization of surface species on activated carbon.

Our approach is to use polycrystalline graphite as a model substrate and to study its Raman spectrum as a function of activation temperature. The activation procedure involves exposure of the sample to $O_2 + H_2O$ for a period of 1/2 hour at various temperatures. Our results in Fig. 4 clearly show changes in the Raman spectrum as the activation temperature is varied. As the oxidation threshold for polycrystalline graphite is approached, the Raman mode near 1320 cm^{-1} begins to decrease in intensity and a new sharp mode near 1620 cm^{-1} appears. This behavior continues up to about 675°C. As the temperature is raised beyond this point to 900°C, the 1350 cm^{-1} mode grows in intensity and the 1620 cm^{-1} mode disappears. If we can assume that there are no large changes in the graphite substrate at these temperatures, then these spectral changes must be due to changes in surface species. It would be expected that the intensity variation of these modes would be a function of activation temperature if one assumed there is competition between two species for a fixed number of sites on the crystallite boundary. This picture is also quite consistent with the observation that the intensity of the 1350 cm^{-1} mode varies inversely with the crystallite size as determined from X-ray data. We are presently involved in

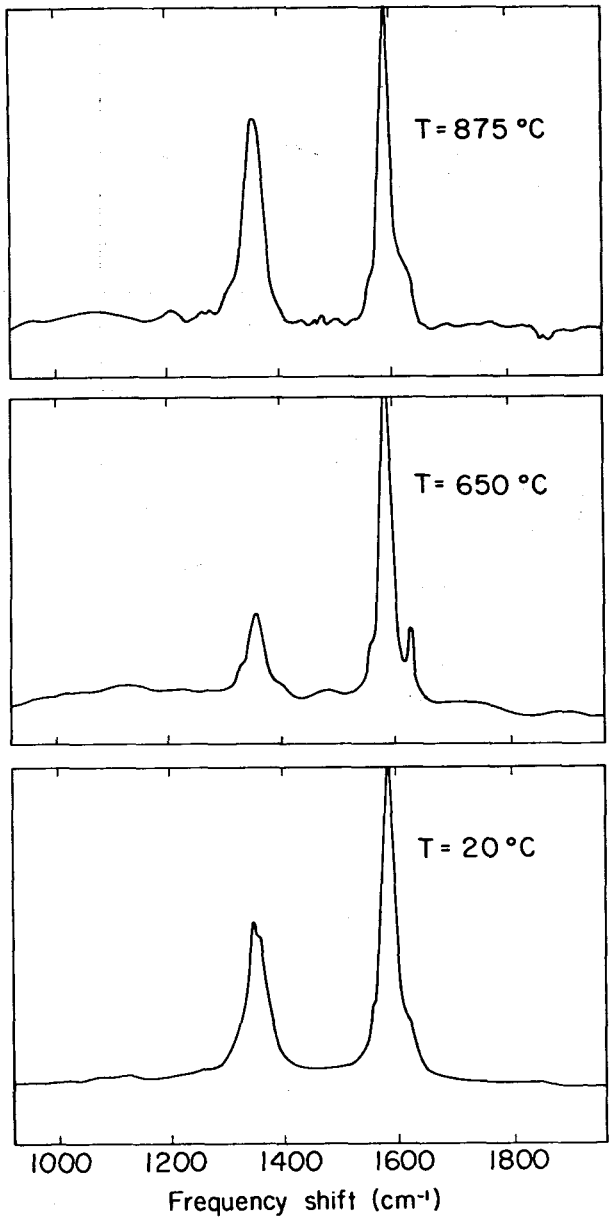

Fig. 4. Raman spectra of polycrystalline graphite between 920 and 1950 cm^{-1} as a function of activation temperature. (XBL 772-359)

trying to establish that these modes are definitely due to surface species. We believe these experiments in combination with parallel measurement using photoelectron spectroscopy will help clarify the surface chemical properties of activated carbon.

ANALYTICAL METHODS DEVELOPMENT

1. Determination of Nitrogen in Atmospheric Aerosols by Nuclear Reactions

Low-Z elements such as carbon, oxygen, nitrogen, and sulfur constitute the major fraction of urban atmospheric aerosols, yet there is presently no method available for a rapid and nondestructive analysis of these elements. The X-ray fluorescence technique, an important tool in the determination of heavy element concentrations, is of little use for low-Z elements due to large X-ray absorptive effects and low fluorescence yields. Some other methods, such as combustion, are destructive and thus do not allow other analyses to be performed on the same sample. We are presently developing a technique which uses activation analysis for the determination of the concentrations of these elements in aerosols. Experiments are almost complete in the development of the technique to determine elemental nitrogen concentrations, the first low-Z element which we investigated. The technique involves using protons to induce the nuclear reaction $^{14}N(p,\alpha)^{11}C$ and then following the decay of ^{11}C, a radioactive nuclide with a half-life of 20.4 minutes.

A stacked foil technique was used for the irradiation of the aerosol samples. A typical stack included a nitrogen standard, the aerosol sample to be analyzed, and aluminum beam degraders. The nitrogen standard used in our experiments, melamine ($C_3N_6H_6$), was prepared by vacuum sublimation onto a 0.001-in. aluminum foil. The maximum beam energy used in these experiments was 16.0 MeV; and by the use of known range-energy relationships, aluminum degraders were placed in the stack so that the proton energy at the standard was 9.2 MeV and at the aerosol sample, 6.0 MeV. The cross section for the $^{14}N(p,\alpha)^{11}C$ reaction at these energies was determined in a previous experiment. Previous experiments also determined that the preferred collection filter was the silver membrane filter. A proton energy of 6.0 MeV was chosen for the aerosol sample for several reasons:

1. There is no interference from the $^{12}C(p,pn)^{11}C$ reaction which has a 20.3-MeV threshold energy;

2. There is minimum interference from other reactions that produce activities with half-lives close to that of ^{11}C;

3. This energy is below the classical Coulomb barrier of 8.4 MeV for protons on silver.

The target stacks were irradiated for 1 minute at a beam intensity of 1 μA at the LBL 88-inch cyclotron. The decay of the ^{11}C and other positron-emitting species produced in the irradiation of the aerosol sample was followed by counting their 511-

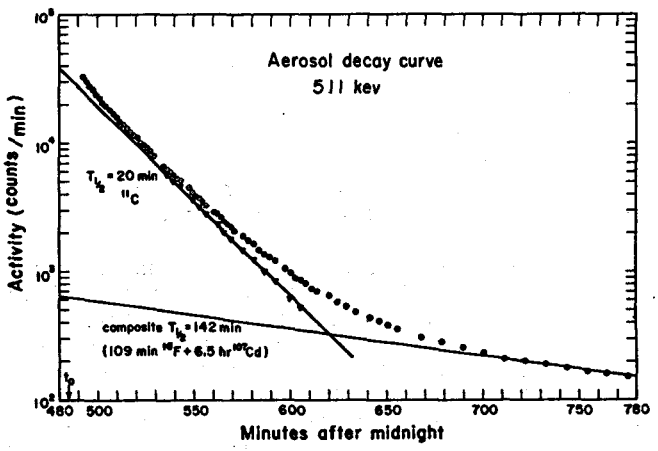

Fig. 5. Decay curve for a typical Bay Area aerosol. (XBL 772-333)

keV annihilation radiation by means of a Ge(Li) multichannel spectrometer. The decay of the integrated intensity of the 511 peak for a typical Bay Area aerosol with a loading of 1 mg/cm^2 is shown in Fig. 5. The four major components have been identified in this decay curve as 10.0 min ^{13}N, 20.4 min ^{11}C, 110 min ^{18}F, and 6.5 hr ^{107}Cd. The ^{13}N is produced from ^{16}O and ^{13}C in the aerosol, the ^{18}F is produced from ^{18}O in the aerosol, and the small amount of ^{107}Cd is produced from the proton reaction on ^{107}Ag in the silver filter. The dominant component by far is the ^{11}C produced from the ^{14}N in the aerosol. The components can be resolved either by graphical methods or by a more exact computer treatment using the CLSQ program. A computer treatment of the decay curve shown in Fig. 5 yields the counting rates at the end of bombardment, A_0, for each of the components shown in Table 1. We note the good agreement between ^{11}C A_0 values given by the computer

Table 1. A_0 values for the resolved components of Figure 5.

Component no.	Half-life	A_0 (counts/min)
1	10.0 min	$1.17\pm0.03 \times 10^4$
2	20.4 min	$3.21\pm0.01 \times 10^4$
3	109.8 min	$5.06\pm0.07 \times 10^2$
4	6.5 hr	$1.23\pm0.01 \times 10^2$

($3.21\pm0.01\times10^4$ c/m) and by graphical analysis ($3.2\pm0.2\times10^4$ c/m). The ^{11}C activity in the sample at the end of bombardment is corrected for the ^{11}C activity due to nitrogen in the silver filter. This was determined in a separate experiment and is typically a small correction. The $A_0(^{11}C)$ due to just the nitrogen in the aerosol and the $A_0(^{11}C)$ for the nitrogen standard are used to determine the amount of nitrogen in the aerosol by use of the following equation:

$$\text{aerosol nitrogen thickness } (g/cm^2) = N_{std} \times \frac{14.007}{6.02\times10^{23}} \times \frac{A_0(^{11}C,\text{aerosol})}{A_0(^{11}C,\text{ std})} \times \frac{\sigma(9.2\text{ MeV})}{\sigma(6.0\text{ MeV})}$$

where $\sigma(9.2\text{ MeV})/\sigma(6.0\text{ MeV}) = 0.91$ is the ratio of the cross sections for the ^{14}N(p,α)^{11}C reaction at the standard bombarding energy and at the aerosol bombarding energy, and N_{std} is the number of nitrogen atoms per centimeter squared in the standard.

Various experiments were carried out to determine the reliability and accuracy of our technique. The first such experiment involved the nebulization of a known amount of $(NH_4)_2SO_4$ onto a silver filter and the comparison of the nitrogen determined by activation analysis with the known nitrogen content. The results are shown in Table 2. The next experiments involved the analysis of an unknown nitrogen-containing compound by activation analysis and by combustion analysis. Our analysis was carried out on three separate samples from the same batch to check our reproducibility. The results of these experiments are also shown in Table 2. Our most recent experiments have involved the analysis of four aerosol samples collected at LBL during an air pollution episode in the first week of November 1976. These results are also shown in Table 2. Parallel quartz filters were sent out for separate combustion analysis, but the results are not yet available.

Table 2. Summary of experimental results for nitrogen.

Sample	Proton activation analysis	Independent check
$(NH_4)_2SO_4$	69 ± 5 µg/cm^2	70 µg N/cm^2 [known weight $(NH_4)_2SO_4$]
FN1	5.3±0.3%	
FN2	5.4±0.3%	4.3% N (combustion)
FN3	5.4±0.7%	
11-5-5	16±2 µg/cm^2	
11-4/5-2	59±7 µg/cm^2	combustion of parallel quartz (not available)
11-5-8	36±5 µg/cm^2	
11-5-11	46±3 µg/cm^2	

The activation analysis technique appears to work quite well for nitrogen determinations in aerosol samples, but further experiments are needed to refine the technique and to verify this conclusion. The sensitivity of the technique for the determination of nitrogen is ~1 µg/cm^2 for the experiments as carried out. Other future experiments will deal with developing a method for the determination of other low-Z elements in atmospheric aerosols.

2. Determination of Particulate Carbon by Optical Attenuation

The total carbon content of atmospheric particulates can readily be determined by combustion techniques.[7] This method of analysis is rather time consuming and is destructive of the sample. It also requires a special substrate with virtually no carbon content. We have investigated the use of optical attenuation by ambient aerosol particulates collected on Millipore cellulose ester filters to determine total carbon. This method is quick, nondestructive, and correlates well with carbon as determined by combustion analyses. This correlation would be expected if a large fraction of the carbon content in these samples were "graphitic soot," which has a very large optical absorption cross section. Preliminary theoretical calculations indicate that this correlation can be explained quantitatively.

Samples of ambient aerosol in Berkeley were collected simultaneously on 1.2-μm Millipore filters, and on quartz fiber filters that had been prefired to remove all combustible carbon. Collection times were adjusted to yield a wide range of particulate loadings. Total carbon was determined from the quartz fiber filters by combustion in an oxygen atmosphere, followed by separation and measurement of the evolved CO_2 with a gas chromatograph/thermal conductivity detector system. (Mueller et al.[7] describe a similar system.) The values thus obtained were used to calculate the total carbon loadings on the corresponding Millipore filters. Optical attenuation measurements were made with an apparatus incorporating a photomultiplier as a detector and a 1-mW He-Ne laser as a light source ($\lambda = 0.6328$ μm). A blank filter was assigned 100% transmission (I_0) as measured with this system. The loaded filters were then sequentially placed in the beam with the loaded side toward the laser, and the transmission of each (I_T) was measured. The ratio of I_T/I_0 vs the carbon content as determined from combustion is shown in Fig. 6. A linear least-squares fit to all data points below 40 μg of carbon has a correlation coefficient, r, of 0.944. Data points above that loading show a saturation effect which is predicted from theoretical considerations.

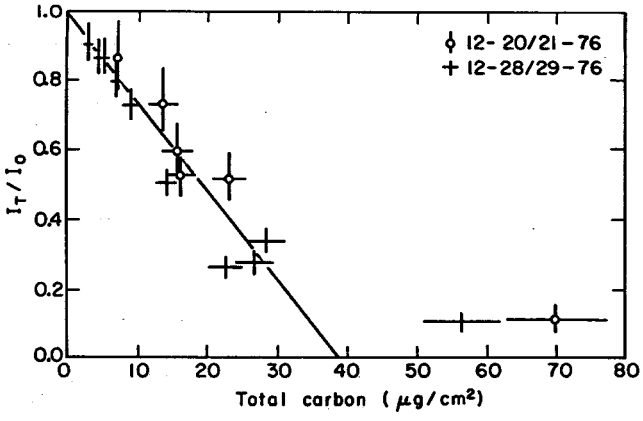

Fig. 6. Optical transmission of ambient samples as a function of carbon content.
(XBL 772-361)

CHARACTERIZATION AND TRANSFORMATION OF AMBIENT AEROSOLS

1. Application of Raman Spectroscopy to the Characterization of Atmospheric Particulates

In order to better assess the origin and the environmental effects of airborne particles, it is important to explore new techniques for their chemical characterization. During the past year, we have successfully obtained Raman spectra of both ambient and source-enriched particulate samples. As far as we know, this is the first application of this method to the characterization of pollution particulate samples.[8,9] Although the Raman scattering technique is in its early stages of development, it seems to hold considerable promise as a nondestructive, sensitive, and highly selective method for the characterization of pollution particulates.

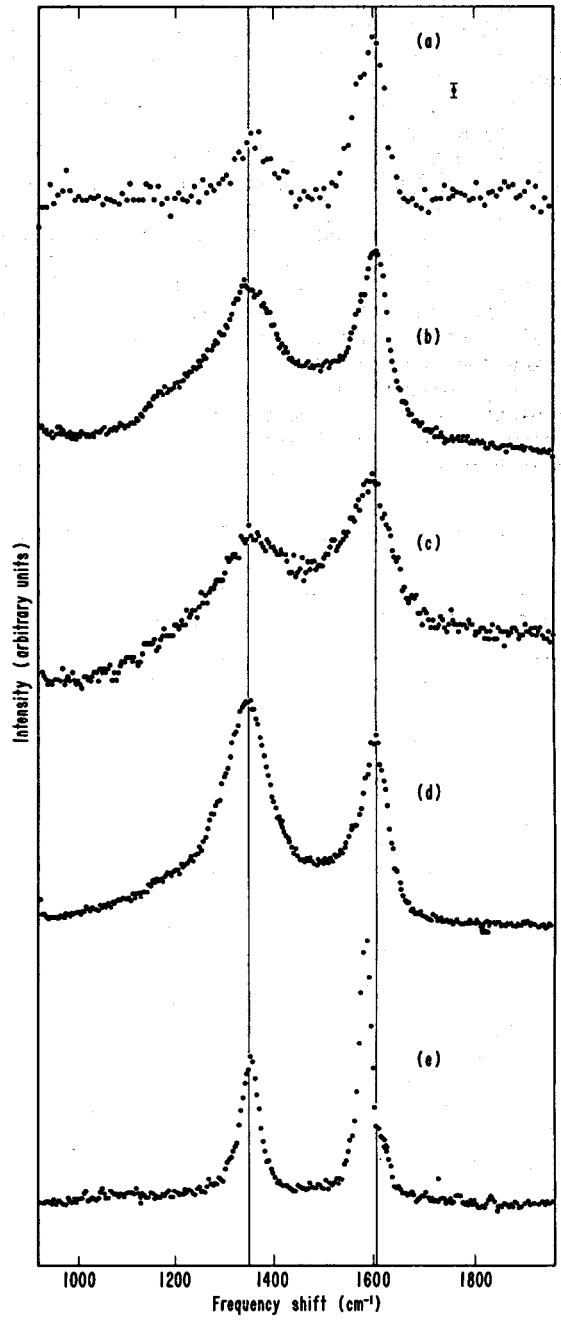

Fig. 7. Raman spectra between 920 and 1950 cm^{-1} of: a) Ambient sample collected in 1975 as part of EPA's RAPS program. The sample was collected on a dichotomous sampler and was in the small size range fraction. The slit width was 8 Å (~25 cm^{-1}) and the integration time was 0.2 min/ch. b) Automobile exhaust collected from a number of cold starts of a poorly tuned automobile using lead-free gas and having no catalytic converter. c) Diesel exhaust. d) Activated carbon. e) Polycrystalline graphite. The slit width for samples b-e was 3 Å (~10 cm^{-1}), and the integration time was 0.1 min/ch. (XBL 767-3091)

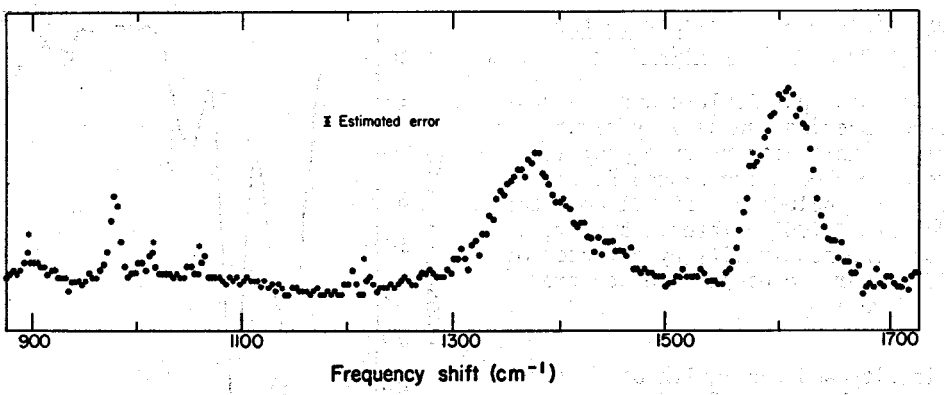

Fig. 8. Raman spectrum of an ambient sample collected in 1975 as part of EPA's RAPS program in St. Louis, Missouri. The sample was collected on a dichotomous sampler (Loo et al., 1976) and was in the small size range fraction. The spectrum was obtained with a slit width of 3 Å (~10 cm^{-1}) and integration time of 2 min/ch. The lines denoted by an asterisk correspond to grating ghosts.
(XBL 7612-4489)

The Raman spectra between 900 and 1950 cm^{-1} of ambient, automobile exhaust, and diesel exhaust particulates are compared with the spectra of activated carbon and polycrystalline graphite in Fig. 7. The close correspondence of the spectra strongly suggests the presence of physical structures similar to activated carbon in both source-enriched and ambient samples. These graphitic species are presumably of primary origin, and throughout the text we shall use the term "graphitic soot" to describe them.

Typically about 10% of the weight in the small particle size fraction ($\leq 2.4\,\mu$) of the ambient samples studied is sulfur. Therefore if the Raman cross section for sulfur species is comparable to that of "graphitic soot," we would expect to observe such species. In Fig. 8 we show the Raman spectrum of a heavily loaded ($\simeq 400\ \mu g/cm^2$) St. Louis sample taken with longer integration times than in the previous runs. The spectral lines characteristic of "graphitic soot" are again evident. However, a sharp line is also observed near 976 cm^{-1}, which we assign to sulfate species. The position of the sharp line was compared with that of the ν_1 vibration of $(NH_4)_2SO_4$ which was used as a standard. The peak position was coincident to within $\pm 2\ cm^{-1}$, which is the estimated experimental error. This suggests that the line is indeed due to $(NH_4)_2SO_4$. It is clear from Fig. 9, which shows the Raman spectra of sulfuric acid, ammonium bisulfate, and ammonium sulfate, that the Raman technique is highly selective and can certainly distinguish between these species.

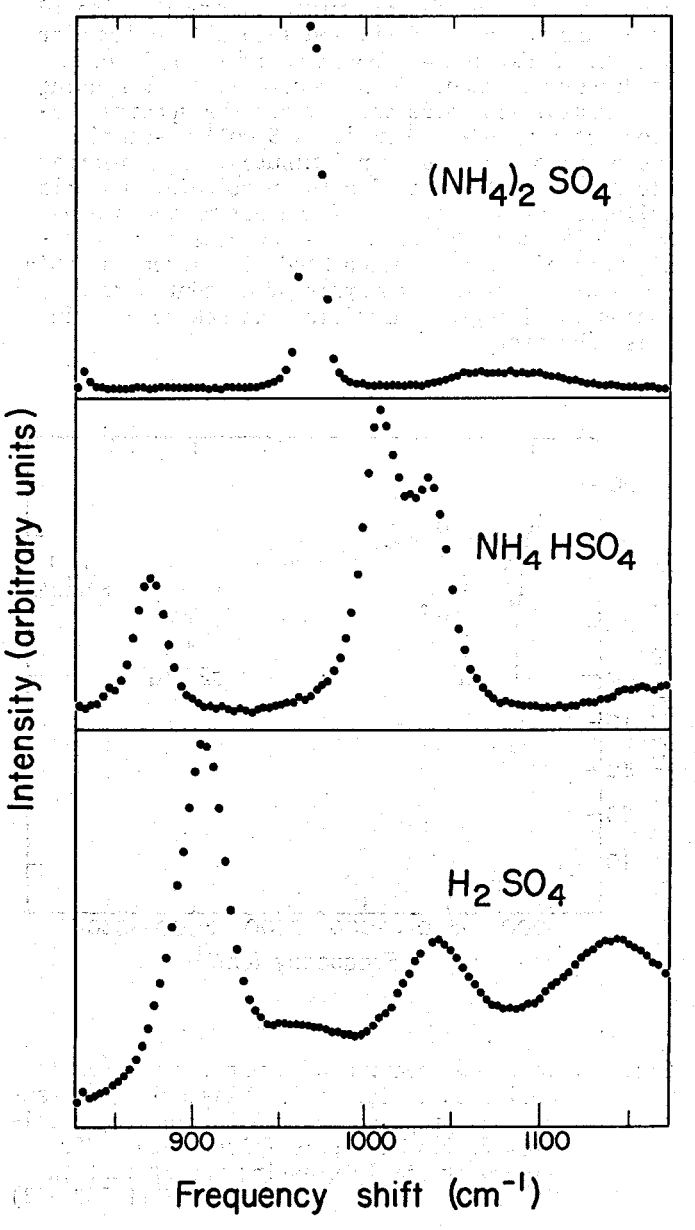

Fig. 9. Raman spectra of $(NH_4)_2SO_4$, NH_4HSO_4, and H_2SO_4 in the spectral region between 850 and 1150 cm^{-1}. These spectra were obtained with a slit width of 3 Å (~ 10 cm^{-1}).
(XBL 7612-4487)

2. Application of Infrared Spectroscopy to the Characterization of Atmospheric Particulates

The amount of airborne particulate and the concentration of surface species can be very minute, and therefore a high sensitivity spectrometer is desirable. We have assembled a rapid-scan Fourier transform spectrometer, including a PDP-11 computer and an EOCOM Model FMS^{TM} 7001 P interferometer, which could increase the sensitivity by a factor of between 100 and 1000 over the dispersive spectrometer in the infrared region.

The high sensitivity and the wealth of chemical information which could be obtained by this technique are illustrated in Figs. 10 and 11. The spectrum shown in Fig. 10 is from particles collected in St. Louis, Missouri. The sample was prepared by transferring the particles from a Millipore filter onto a KBr window by simply pressing one against the other. In Fig. 11 the spectra of a sample collected in a winter episode in Berkeley is shown. Fifty micrograms of particulate matter were removed from a silver membrane filter, mixed thoroughly with 10 mg of KBr powder, and pressed into a 3-mm diameter pellet. A Harrick 4X TBS-VA variable angle beam condenser was used. Both spectra were taken using the transmission mode and covered the spectral region between 500-4000 cm^{-1}. A 5-cm^{-1} resolution was obtained in less than 5 minutes. The spectra clearly indicate that airborne particulate material collected at both St. Louis and Berkeley contains NH_4^+, SO_4^{--}, and NO_3^- species among others. The assignment of the absorption bands is listed in Table 3. Routine infrared analysis of ambient particulates in microgram quantities can now be made in this laboratory.

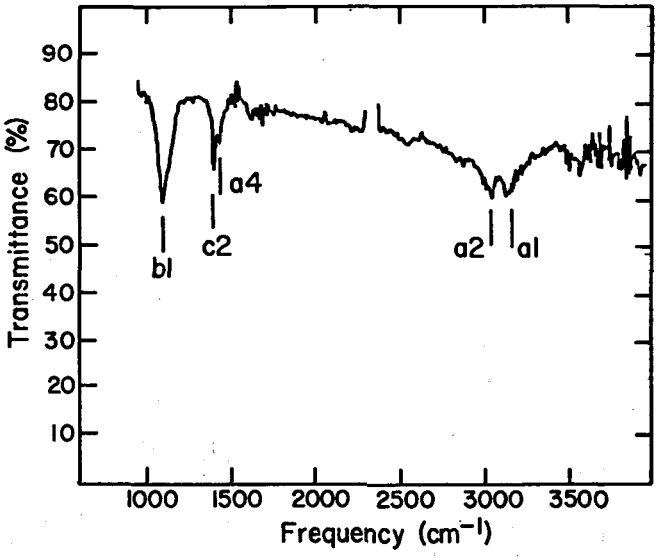

Fig. 10. Infrared spectrum of a particulate sample collected in St. Louis, Missouri. The sample was prepared by transferring the particles from a Millipore filter onto a KBr window by simply pressing one against the other. (XBL 722-422)

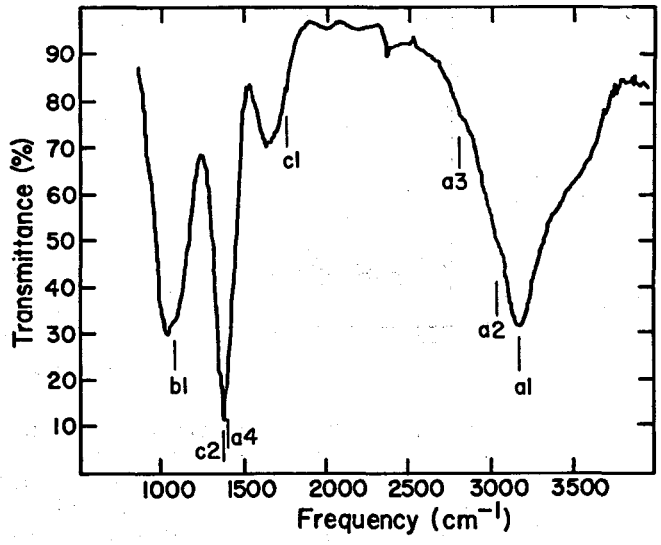

Fig. 11. Infrared spectrum of a particulate sample collected in a winter episode in Berkeley. The sample was prepared by the microsampling technique. Fifty micrograms of particulate matter were mixed thoroughly with 10 mg KBr powder and pressed into a 3-mm diameter pellet. A Harrick 4X TBS-VA variable-angle beam condenser was used. (XBL 772-423)

Table 3. Listing of assigned infrared bands observed in particulate samples.

Frequency (cm^{-1})	Assignment		Designation
	Species	Normal mode	(Figs. 10 and 11)
3160	NH_4^+	ν_3	a1
3040	NH_4^+	$\nu_2 + \nu_4$	a2
2800	NH_4^+	$2\nu_4$	a3
1760	NO_3^-	$2\nu_2$	c1
1400	NH_4^+	ν_4	a4
1385	NO_3^-	ν_3	c2
1090	SO_4^{--}	ν_3	b1

In order to minimize the perturbation of the particulate samples during their preparation, one may use the external reflection technique. Here, one measures the reflected intensity versus wavelength at the desired angle of incidence and polarization. However, caution must be taken in the interpretation of the reflection spectra since the reflectivity might be dependent on a number of parameters such as particle size, shape, polarization,

and angle of incidence. The reflection technique could be very powerful. We believe that it has not been applied elsewhere to ambient particulates.

3. Chemical Characterization and Transformations of Automotive Sulfur Emissions

The chemical characterization and transformations of gaseous and aerosol species emitted by highway vehicles have been investigated in a series of experiments conducted in the Caldecott Tunnel on a major highway near Berkeley. Initial studies focused on the emission rates and particle size distribution of species emitted by diesel and nondiesel vehicles.[10] Recent studies have investigated the chemical transformations of sulfur species emitted by vehicles traveling through the tunnel.

Considerable controversy surrounds the mechanism and rate of oxidation of SO_2 to aerosol sulfur species in the atmosphere.[11] Two processes are thought to be involved in the oxidation of SO_2: oxidation by components derived from photochemical reactions, and catalytic oxidation by certain types of particulate aerosols. The relative humidity has been shown to be an important parameter in the oxidation processes especially at levels greater than 70%. There has also been considerable interest in the question of primary aerosol sulfur directly emitted from vehicles equipped with catalytic converters.[12]

Tunnel roadway air containing fresh vehicular emissions was sealed in a 600-m^3 room for 3-1/2 hours and analyzed for CO, SO_2, total particulate sulfur, and total particulate lead. The relative humidity and temperature were increased during this measurement period from 65% and 15°C to 100% and 18°C. The results shown in Fig. 12 illustrate the 20% decrease observed for all four chemical species in the 3-1/2-hr measurement period; this decrease is attributed to the air leakage of the "sealed" room. Sulfur dioxide and aerosol sulfur decreased at the same rate as the unreactive species, CO and Pb, indicating no apparent conversion of SO_2 to aerosol sulfur, even under high humidity conditions. The ratio of particulate to gaseous sulfur, S_p/S_g, was observed to be 3%. Earlier experiments in the tunnel when the relative humidity was 65%±5% gave S_p/S_g ratios of 1 to 5%. The results of this 3-1/2-hr experiment indicate that the oxidation of SO_2 to sulfur is less than 0.1% per hour. Other work has estimated the rate of oxidation of SO_2 in urban atmospheres and power plant plumes to be from 1.5% to 5% per hour or even higher at very high relative humidity levels.[13-15]

Earlier studies in the Caldecott Tunnel found the SO_2 emission rate to be 0.15±0.05 g/mile (as sulfur) averaged for all vehicles. The present work, assuming $S_p/S_g = 3\%$, gives a particulate sulfur emission rate for vehicles equipped with catalytic converters of 0.025±0.015 g/mile when it is assumed that aerosol sulfur is emitted only from catalytic converter-equipped vehicles, estimated to be 20% of the vehicle population at the time of the experiment. This aerosol sulfur emission rate, 0.025±0.015 g/mile, can be compared with other work reporting estimated and measured aerosol sulfur emission rates from 0.006 to 0.02 g/mile.[12,16,17] The value reported here, considering the several assumptions made, is in general agreement with other work.

4. Summary of ESCA Results for Da Vinci II and III

The filters collected for ESCA analysis were very lightly loaded, especially from Da Vinci III.

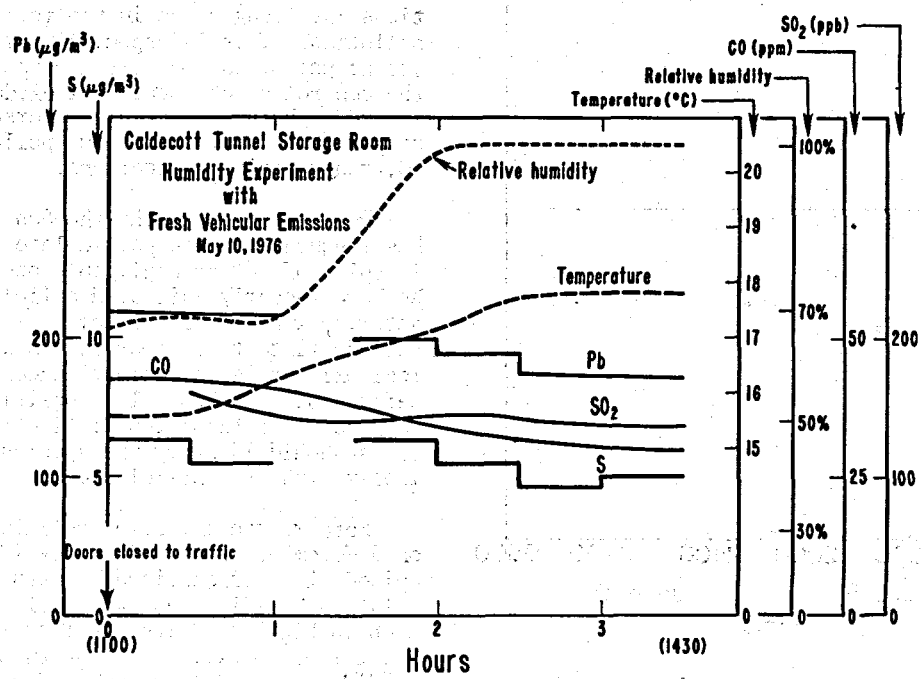

Fig. 12. Characterization of vehicle emissions in the Caldecott Tunnel at high relative humidity levels. (XBL 7611-4375)

A detectable amount of sulfur as sulfate was present in all samples from each flight. Da Vinci II filters also showed varying amounts of nitrogen, primarily ammonium nitrogen but with some indication of the presence of more reduced forms. Lead concentrations on the filters were small.

Vacuum volatile components of the particulate loading cannot be excluded, and because of the long periods in vacuum (up to 18 hr) necessary to obtain reasonable spectra, the volatile components could be lost.

Da Vinci II (8-9 June 1976). All sulfur observed was in the form of sulfate, which had a binding energy (b.e.) of 169 eV. There was apparently some increase in sulfate concentration during the flight, but intersample quantitation is hazardous at best.

No nitrate or other oxidized form of nitrogen was observed. This is not surprising since such species in atmospheric samples are usually volatile in vacuum, and the time necessary to obtain reasonable statistics was relatively long.

Ammonium nitrogen (b.e. = 402 eV) is noticeable by 1400 of June 8 and increases with time relative to the observed sulfate by approximately a factor of 2, with the final observed ratio being more ammonium-rich than NH_4HSO_4 but less than $(NH_4)_2SO_4$ as shown in Fig. 13. This behavior could be explained as the neutralization of acidic sulfate species by ammonia entering the air parcel. The total particulate sulfur as determined by X-ray fluorescence on parallel samples shows that the increase in ammonium relative to sulfate exceeds by approximately 10% the increase which could be brought about by injection of stoichiometric ammonium sulfate into the aerosol.

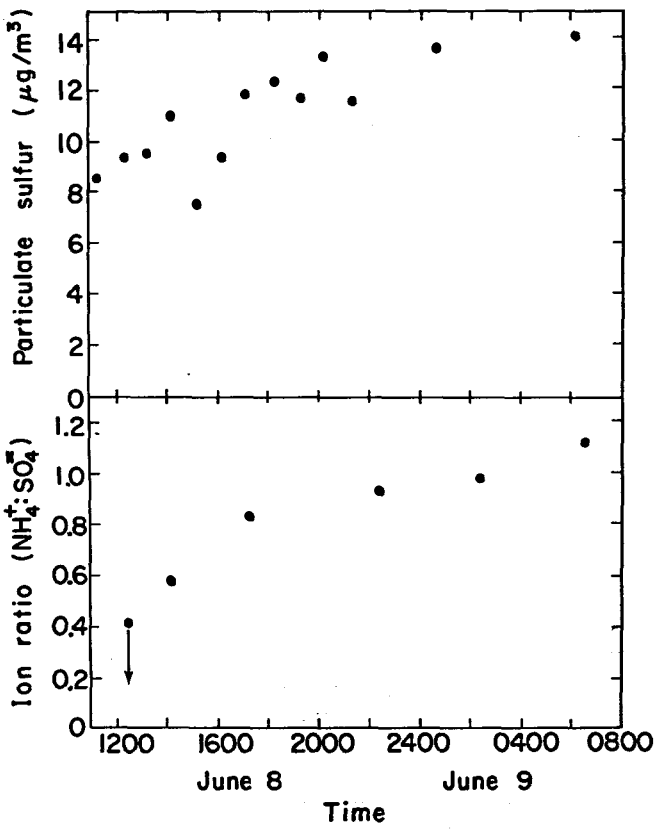

Fig. 13. Da Vinci II results as a function of flight time: a) Total particulate sulfur concentration by X-ray fluorescence. b) Ammonium-to-sulfate ratio by ESCA. (XBL 772-362)

Da Vinci III (23-24 July 1976). Da Vinci III filters were very lightly loaded and showed little except the general presence of sulfur as sulfate. There was no apparent change in the amount of sulfate detected on the various filters.

Method sensitivity. Using X-ray fluorescence results for lead and sulfur and experimentally determined relative atomic sensitivities for sulfur and nitrogen, we estimate that loadings of approximately 0.5 μg S/cm^2 would be necessary to obtain reasonable semiquantitative results, although some speciation should be possible as low as 0.1 μg S/cm^2. Because of the interference of the silver energy loss spectrum in the nitrogen region, approximately 1 μg N/cm^2 would probably be necessary to obtain reasonable results. Oxidized nitrogen species should be somewhat easier to detect than reduced species because of the shape of the background curve, but they are also generally more volatile when they are observed in ESCA spectra of ambient particulates. Lead was not measurable in any of the spectra taken from any of these samples, and as a consequence, lower limits for reasonable results can only be estimated at 0.5-1.0 μg Pb/cm^2.

5. Characterization of a Bay Area Air Pollution Episode Under Conditions of Low Photochemical Oxidant

It is important to understand the relative contributions of nonphotochemical reactions and reactions involving ozone in the formation of aerosol air pollution. This is especially important because existing pollution controls are specifically aimed at the control of photochemical oxidant, which is believed to be an essential precursor for the formation of particulates from gaseous pollutants such as SO_2, NO, and certain hydrocarbons.

During winter months the San Francisco Bay Area has frequent intense particulate pollution episodes in spite of low or negligible ozone concentrations. We have recently initiated a field program to characterize wintertime aerosols. The program will be extended into the summer months when the photochemical oxidant is at maximum concentrations. A comparison of the chemical composition of the aerosol sampled under these two distinctly different conditions should identify the species associated specifically with oxidant-related aerosol-forming reactions.

Here we present some preliminary results obtained on 5 November 1976 in Berkeley (Figs. 14-17). This episode is characterized by warm temperatures, low relative humidity, and generally stagnant air, as seen in Fig. 14. The light-scattering coefficient b_{scat} reached extremely high values during midday, as did the particle volume and concentration of condensation nuclei (Fig. 15). The most striking feature in the gas data (Fig. 16) is the high NO_2 and very low NO concentration. NO_2 exhibits maximum

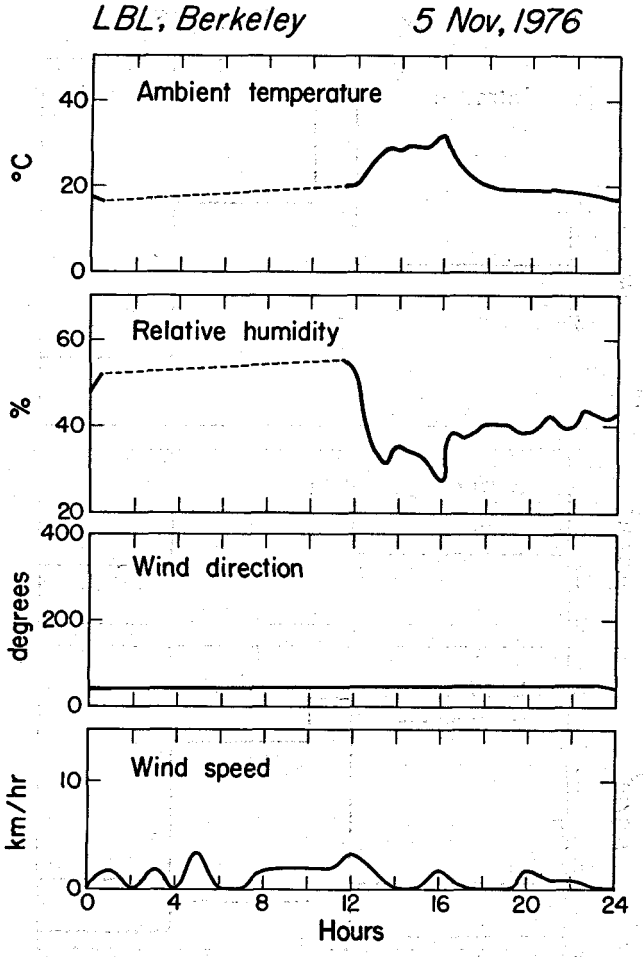

Fig. 14 Variations in temperature, relative humidity, wind direction, and wind speed.
(XBL 771-222)

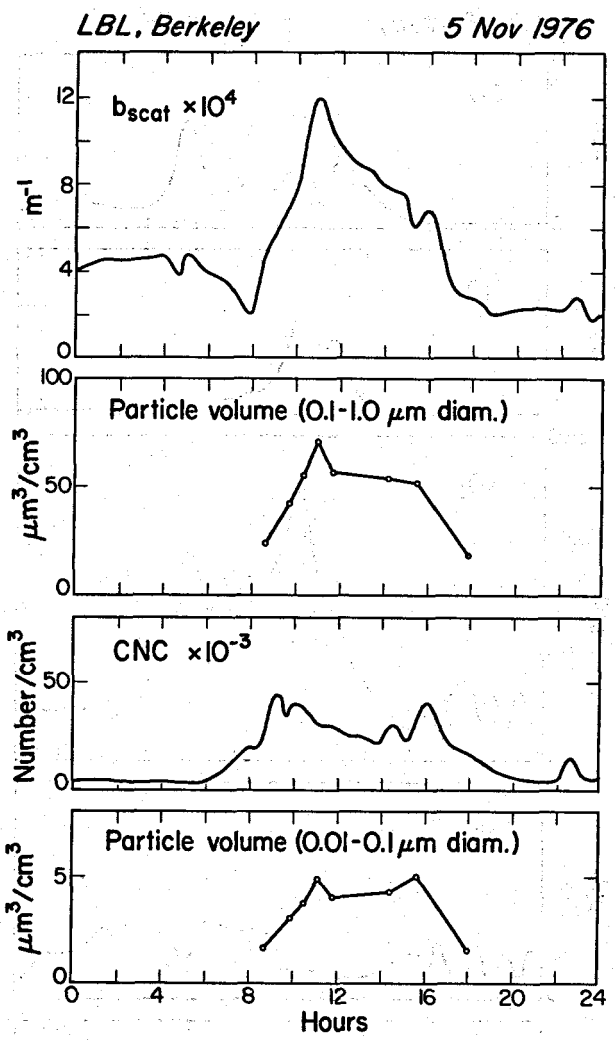

Fig. 15. Variations in b_{scat}, particle volume, and condensation nuclei concentrations.
(XBL 771-223)

concentrations at midday, concurrent with the concentrations of primary gaseous pollutants such as CO and SO_2. Ozone concentrations remained at the background level throughout the day. The diurnal concentration variations of particulate nitrogen, sulfur, lead, and bromine are shown in Fig. 17. The nitrogen concentrations were obtained by the proton activation analysis as described above in this report. Sulfur, lead, and bromine concentrations were obtained by X-ray fluorescence. It is of interest to note that the nitrogen concentrations are higher by about a factor of 5 with respect to sulfur.

ESCA measurements on the collected samples have shown that the particulate sulfur was in the form of sulfate. About 80% of the total nitrogen was in the reduced chemical state with ammonium and compounds having amino-type functional groups as the principal components. About 20% of the particulate nitrogen was in the form of nitrate. No major changes in the relative concentrations of these species were observed during the 24-hour period.

The total sulfur, that is, gaseous and particulate sulfur, is observed at relatively low concentrations, indicating that no major high sulfur-burning source contributed to this episode. Thus the described episode corresponds to a situation where the fuels used are low in sulfur. The sulfate-to-SO_2 ratio indicates significant SO_2-to-sulfate conversion.

The low oxidant concentrations and the predominant use of low sulfur fuels did not alleviate the problem of high concentrations of particulate and gaseous nitrogenous species. Complete interpretation of the data will follow the results of chemical analyses now in progress.

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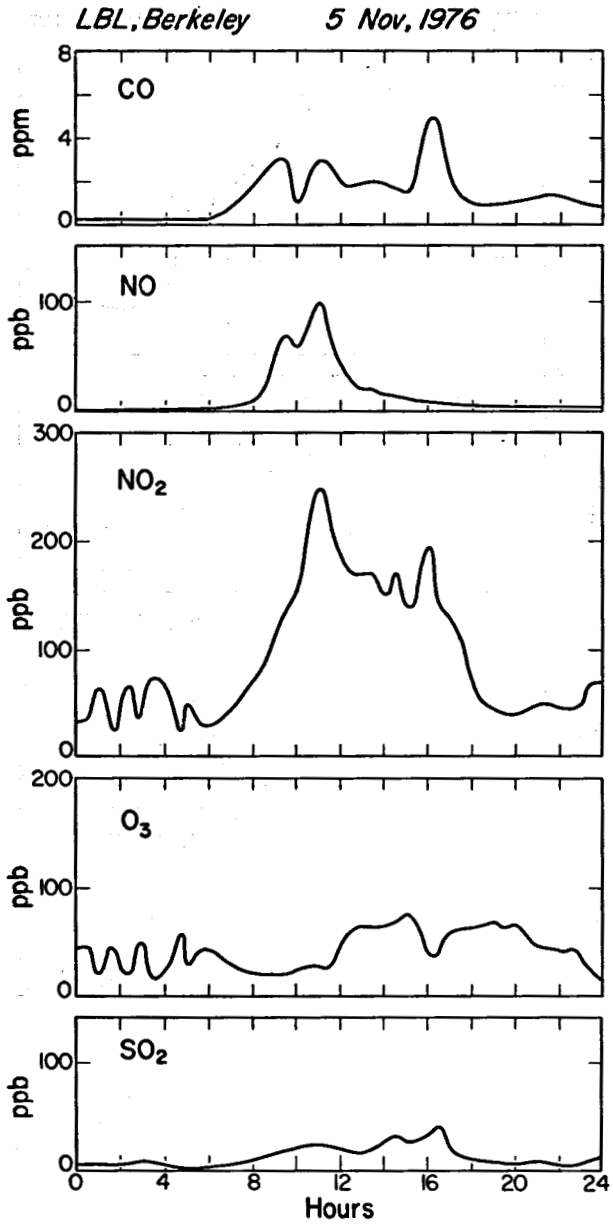

Fig. 16. Diurnal variations in CO, NO, NO_2, O_3, and SO_2 concentrations. (XBL 771-221)

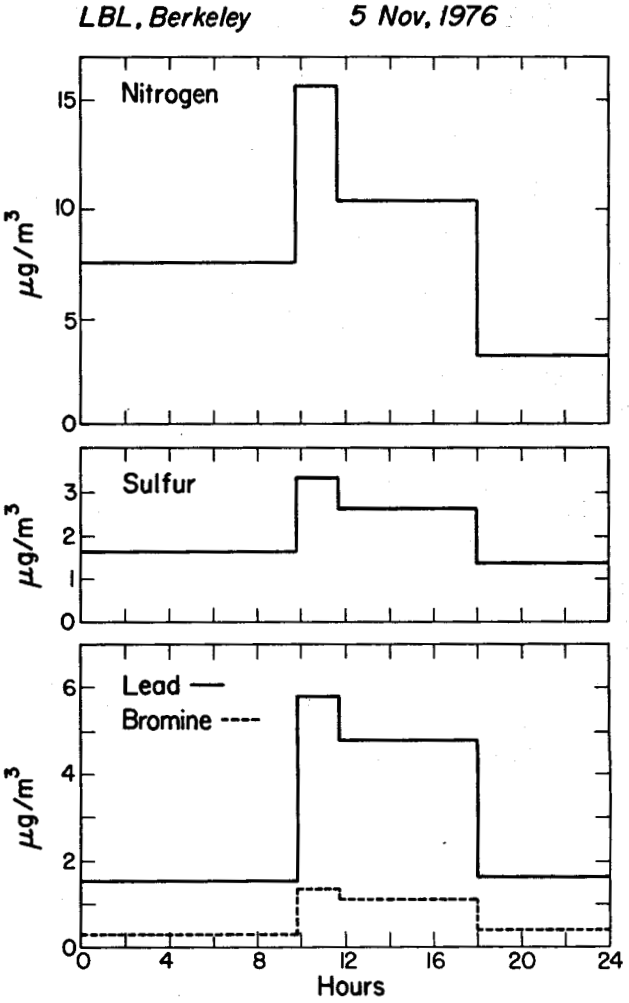

Fig. 17. Concentrations variations of particulate nitrogen, sulfur, lead, and bromine. (XBL 771-220)

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OXIDATIVE DAMAGE BY ENVIRONMENTAL FACTORS: STUDIES ON HUMAN CELLS AND MITOCHONDRIAL MEMBRANES

L. Packer, B. Aggarwal, A. Quintanilha, and R. Mehlhorn

INTRODUCTION

Atmospheric pollutants first interact with biological membranes which separate the intracellular from the extracellular environment. Therefore a detailed understanding of how cellular membranes interact with the major environmental substances of our atmosphere (see list in Table 1), is important in understanding how pollutants act. Some questions that need answers are: How do the different types of pollutants act? What components of membranes are damaged? How does damage occur? How is membrane damage propagated? What type of protective mechanisms can be devised at the level of the membrane, to quench and/or to prevent the spread of pollutant-initiated damage? Finally, how can the damage be repaired?

Table 1. Environmental substances in our atmosphere

Pollutants:
Dust particles, polycyclic hydrocarbons, SO_2, NO, NO_2, CO, CS_2, ozone, free radicals
Ambient Factors:
Irradiation, O_2

We are studying damage processes affecting membranes of several mammalian cell types, and are particularly interested in free radical reactions, including reactions involving molecular oxygen. The occurrence of such reactions may be quite common in cells exposed to environmental stress. Our working hypothesis is that a general mechanism exists for propagating free radical reactions within membranes, and therefore a variety of initiations (Table 1) of free radical reactions, e.g. visible light ionizing radiation, nitrogen dioxide or ozone, will lead to similar subsequent chemical events.

Before an effective strategy can be developed at the membrane organization level of the action of pollutants, it is important to understand first how ambient factors in the environment react, including irradiation and oxygen which in a sense may be considered natural pollutants. There is evidence that the action of many pollutants occurs by free radical-mediated oxidative damage[1,2] and that atmospheric oxygen plays an important role in the damaging process. For this reason, our laboratory has been emphasizing the development of a strategy to understand how visible light and oxygen interact with membranes, primarily using two test systems: the growth and viability of normal human diploid cells in culture and direct experiments on mitochondrial membranes isolated from mammalian cells.

ACCOMPLISHMENTS DURING 1976

Cultured Human Cell Studies

It is known that normal human dipolid cells in culture manifest finite lifespans in vitro.[3] The extent to which lifespan limitation is genetically programmed or environmentally constrained in the culture environment is an important question to resolve. This will help to elucidate why such cells lose their replicative capacity during subculti-

vation in vitro.[4] Last year we reported[5,6] that visible light causes photo-killing of WI-38 human cells, which are oxygen dependent. Photo-killing is prevented by the membrane antioxidant dl-α-tocoherol, vitamin E.

In a previous study[7] we reported that supplementation of the culture medium with dl-α-tocopherol (vitamin E) extended appreciably the lifespan of WI-38 cells growing continuously under 20% O_2 (air). Subsequently these original experiments which took more than a year to complete have not proven to be reproducible. In a re-evaluation of the study, it appears that, when it became necessary to change the serum employed at the 100th population doubling because the original batch was exhausted, the vitamin E supplemented cells went into a senescent stage and phased out. Vitamin E supplementation in these sutdies was found to be effective in preventing lipid oxidative damage, but since subsequent studies have not reproduced the phenomenon, we have tentatively concluded that the environmental factors that affected lifespan were determined by a particular batch of serum. In this case a situation existed where vitamin E supplemented cells growing on a particular batch of serum did not lose their normal replicative capacity in vitro until another, more toxic, batch of serum was employed. Thus no direct evidence for the importance of oxidative environmental damage emerged from these studies.

The effect of oxygen concentration on the growth and lifespan of cultured human cells has also been studied in our laboratory for several years.[1] We have exposed WI-38 and IMR-90 normal human diploid cells to varying oxygen concentrations in the gas phase over the culture medium, and evaluated the effect on growth and lifespan.[8,9] Similar to the finding of other laboratories,[10,11] we found that clonal growth at oxygen concentrations less than 20% (atmospheric concentration) is enhanced. However, we also found that extension of the lifespan in both cell types is also accomplished by long-term cultivation under 10% oxygen (Fig. 1, Table 1). Thus the results of our studies show that the potential long-term growth in culture of normal diploid cells may be appreciably enhanced by more exact control of environmental factors.

Using electron microscopy, J. M. Walton studied the intracellular localization of damage. These studies showed that in four types of cultured mammalian cells exposed to low levels of visible light[12] and in WI-38 cells exposed to high O_2 concentration,[13] major morphological changes are seen soon after exposure in mitochondria.[6] This suggested that further studies using isolated mitochondria as a model system were warranted because, at this place in the cell, oxygen is consumed and pigments are located which absorb light in the visible region.

Mitochondrial Studies

Biochemical studies of mitochondria isolated from mammalian cells were designed to show which substances absorb the light capable of activating damage, how and what is damaged, and how to protect against the damage.[6,14] Thus far, our results indicate that visible light damage is dependent on the presence of O_2 (Stage I), that flavoenzymes of the electron transport chain are inactivited soon after exposure to light (Stage II), that a later stage of the damage involves oxidative damage to membrane lipids (Stage III) and that mitochondrial swelling and polymerization of membrane proteins occurs (Stage IV). Spectral studies have shown that the region of visible light absorption effective in causing damage is mainly where riboflavin absorbs. We suspect that mitochondrial endogenous flavins absorb light and react with oxygen to form activated species of oxygen - either singlet oxygen ($^1O_2$), superoxide ions (O_2^-), or some combination of both species, which initiate free radical damage. The spread of the damage at Stage III can be stopped by the membrane antioxidant vitamin E. This is shown in Fig. 2. Note that the initial damage to the flavoenzymes is not prevented by the membrane antioxidant, vitamin E. Furthermore, mitochondria obtained from rats grown on diets deficient in vitamin E are more easily damaged than those from animals supplemented with vitamin E, which are more resistant to damage.

Our strategy is, therefore, to analyze the temporal sequence of events following exposure of mitochondria to visible light and O_2 and to determine in a stepwise way the stages in initiation and propagation of damage. From such knowledge it may be possible to supply growing animals under different dietary conditions with substances that will optimize the ability of membranes to incorporate within them those chemical factors that quench both the damage and the spread of damage.

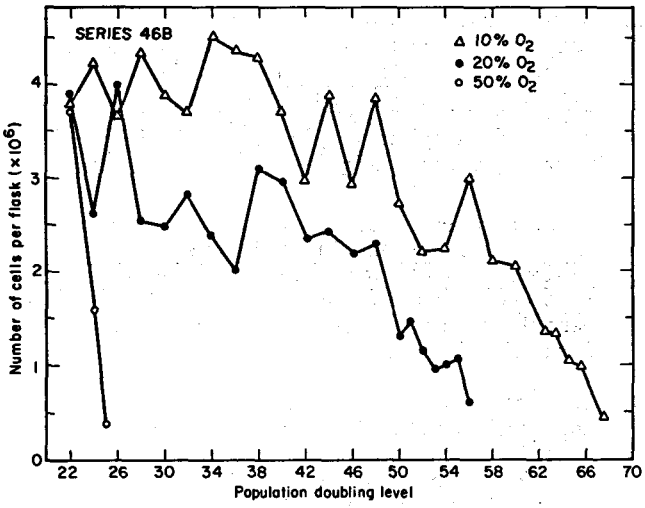

Fig. 1. Effect of Oxygen Concentration on the Lifespan of WI-38 Human Diploid Cells. The parent flask was subcultivated at about 2.5×10^5 cells per flask in duplicate for each oxygen concentration (for details cf. 8,9). Results show that 50% oxygen is very toxic, normal atmospheric O_2 (20%), the control, phased out after 56 population doublings. Note that 10% O_2 cells always grew better throughout the lifespan than the 20% O_2 control cells. (XBL 7610-9356)

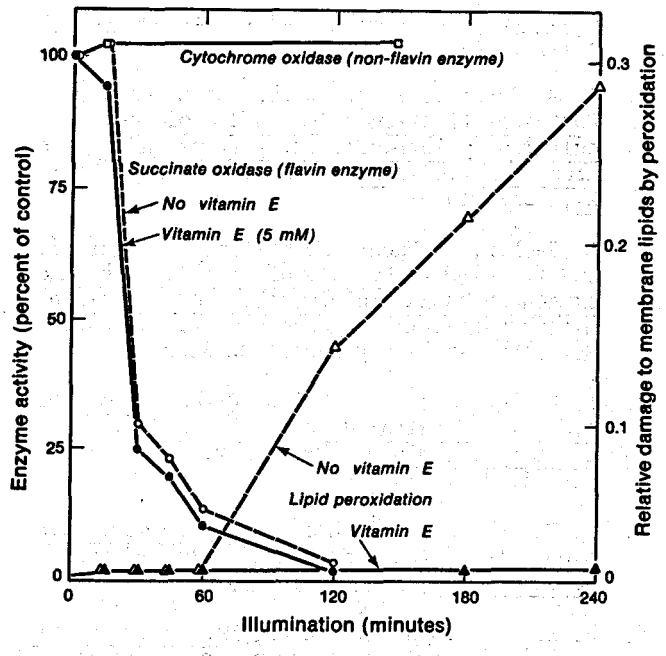

Fig. 2. Visible Light Damage to Mitochondria. Mitochondria were isolated from rat liver and exposed to visible light (> 380) nm) at 10°C in a specially constructed reaction apparatus for the times indicated. They were then assayed for changes in enzyme activity and peroxidation of membrane lipids. Results show that flavoprotein succinate oxidase is progressively inactivated but non-flavin cytochrome oxidase is unaffected. Pretreatment before exposure to visible light with the membrane antioxidant dl-α-tocopherol, vitamin E, protects against the damage of membrane lipids but does not prevent inactivation of flavin enzymes which occurs at an earlier stage. (XBL 7611-4475)

By this same strategy[2] we may also enhance the synthesis of several enzymes known to protect against oxidative damage.

Biophysical studies have involved electron-spin resonance techniques, which afford a means of directly or indirectly monitoring free radical reactions. Our studies so far have taken advantage of the usefulness of spin-labeled hydrophobic molecules to sense the changes in the membrane environment, following and during exposure of mitochondrial membranes to visible light and O_2.

Nitroxide Spin Label Reduction - In one approach the electron transport-dependent reduction of a spin-labeled analogue of the detergent cetyl trimethyl ammonium bromide[15] has been used to monitor damage and protection in the region of the respiratory chain where ubiquinone (a lipid) accepts and donates electrons. It is difficult to look specifically at the ubiquinone region in whole mitochondria in any other way. In a recent report,[16] we showed that this spin-labeled analogue (CAT 16) partitions at the membrane interface and is rapidly reduced, i.e., spin is lost, by coupled electron transport. From the sensitivity of spin-label reduction by respiring mitochondria to various inhibitors of electron transport chain and from analysis of the midpoint potential of the spin label, it was found that the label is probably localized in the ubiquinone region. We found that reducing equivalents of mitochondrial electron transport from this region of the chain were channeled to either membrane interface, probably by the semiquinone free-radical species. We have since been able to establish that ubiquinone is probably the next component along the chain to be inactivated by light (Stage III) after the flavo enzymes (Stage II). The cytochromes seem to be the most resistive enzymes to damage and remain relatively unaffected under conditions where the membrane integrity, or selective permeability, is lost (Stage IV).

Nitroxide Spin Label Destruction - Studies of free radical chemistry are hampered by the fact that reactive free radicals are usually too short lived to accumulate in sufficient concentrations to be observed. Recently, we have employed free radical "traps" to monitor the accumulation of free radicals produced during illumination of mitochondria.[17] We have found that the relatively stable nitroxide radicals, available in many chemical forms because of their usefulness, can be used to trap certain free radicals produced by flavin photo-oxidation. The nitroxides trap certain reactive free radicals by forming stable diamagnetic complexes. Thus, the accumulation of free radicals in a membrane system can be monitored conveniently by following the loss of paramagnetism of nitroxide traps in an EPR spectrometer.

Using the nitroxide free radical assay we found that illumination of mitochondrial membranes by blue light (in the range 400-480 nm) leads to loss of the spin signal of a variety of spin labels. Attempts to recover the spin signal by chemical oxidation revealed that the observed nitroxide signal reduction was irreversibly lost,

Table 2. Effect of oxygen concentration on the lifespan of human diploid cells

	Population Doublings[a]		
	20% O_2	10% O_2	% Increase
WI-38			
Series 32	47	65	38%
Series 46A	57.5	67.5	17%
Series 46B	56.5	67.5	19%
Series 46B	57.5	62.5[b]	9%
IMR-90			
Series 5	39	47	21%
Series 6	38	50	32%

[a]Started at PDL 20 or 22; values derived from averaging duplicate cell counts

[b]Transferred from 20% O_2 to 10% O_2 at PDL 52.5

probably due to reaction with secondary free radicals produced by flavin photoactivation. Furthermore, this spin destruction phenomenon could only be observed after the membranes had been "aged" for a few hours at 25°C under illumination.

A comparison of spin destruction data with enzyme inactivation studies has shown that the former phenomenon is observed prior to the onset of any detectable loss of respiratory activity. This suggests that the nitroxide traps detect a very early stage of the damage (Stage I) and may be acting to intercept radicals near the site of damage initiation, and that much of the enzyme inactivation occurs in subsequent free radical reactions.

FUTURE STUDIES

Further studies will attempt to detail more accurately the temporal sequence of events involved in the various steps of damage and to concentrate more on protection and repair mechanisms. Some of the questions that need to be resolved are: (a) the degree to which O_2^- and/or singlet oxygen, $^1O_2$, are involved in the intiation of damage. These studies will involve the action of superoxide dismutase, and other known quenchers of these activated oxygen species; (b) to improve the design of stress experiments so that we can identify more precisely the stages in damage; (c) to study the involvement of respiration in the generation of the activated oxygen species; (d) to exploit further the techniques of spin reduction and spin destruction, using selected nitroxide spin-labeled molecules to determine the structural localization of damaging capacity (power); (e) to study the extent to which structural modification of the membrane is responsible for functional changes; and (f) finally, to consider how it would be possible both chemically and biochemically, to repair or prevent some of the damages.

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WATER CONSERVATION WITH IN SITU OIL SHALE DEVELOPMENT

J. Thomas, G. Amy, P. Fox, B. Hall, P. Russell

INTRODUCTION

The primary objectives of this project are (1) to identify and assess water-related impacts associated with in situ oil shale development and (2) to develop control measures to mitigate adverse impacts. A secondary objective is to provide part of the data base required for an overall comparison of the environmental impacts resulting from "in situ" and "above ground" methods of retorting oil shale. These objectives are being accomplished by analyzing existing data available in the literature and by conducting basic research in certain areas where data is unavailable. Areas of basic research include (1) minor element release during in situ retorting, (2) leaching of contaminants from in place spent shale, (3) toxicity of retort water to aquatic biota, and (4) treatability of retort water by biological unit processes.

This project is one of many projects that are currently assessing the environmental impacts associated with development of national energy resources such as coal, petroleum, oil shale, etc. Since future energy development will eventually involve a trade-off between economic benefits and adverse environmental impacts, it is anticipated that these projects will provide a detailed data base for making future decisions on energy development.

The project, jointly funded by the Energy Research and Development Administration (ERDA) and the Department of the Interior, was initiated in June, 1976 and will be completed in August, 1977.

ACCOMPLISHMENTS DURING 1976

Work accomplished during 1976 included (1) definition of a study area and study approach, (2) completion of a comprehensive literature survey, (3) organization of a project library, (4) completion of several field trips to the tri-state oil shale region of Colorado, Utah, and Wyoming, (5) compilation of baseline data on the water resources of the oil shale region, (6) description of state-of-the-art technologies available for in situ processing of oil shale, (7) completion of a preliminary qualitative assessment of anticipated water-related impacts associated with in situ oil shale development, and (8) identification of areas where basic research is needed.

The project study area has been defined to be the Upper Colorado River Basin which contains the richest deposits of oil shale in the United State. The study approach consists of defining a "unit processing facility" and locating it conceptually in a number of locales throughout the study area, selected to bracket the probable range of water-related impacts.

A preliminary, qualitative assessment of anticipated water-related impacts associated with in situ oil shale development has revealed that the following categories of impacts will likely occur:

1) Decrease in available water supply;

2) Degradation of water supply;

3) Localized hydrologic changes.

PLANNED ACTIVITIES FOR 1977

Planned activities for the next calendar year include (1) completion of a detailed, quantitative assessment of water-related impacts, (2) development of control measures to mitigate the effects of adverse impacts, and (3) completion of laboratory work and data anlysis required in the aforementioned areas of basic research.

Work to be completed in the various areas of basic research is summarized below:

1) Leaching of Organics. After an in situ retort is abandoned, ground-waters may migrate through the retort chamber and pick up both organic and inorganic contaminants. The contaminants that may be leached and their levels will be determined experimentally by conducting continuous flow, packed-bed column studies. A mathematical/chemical model of the leaching process will be developed.

2) Minor Element Release. The raw oil shale from which oil is extracted is enriched in many of the minor elements. To determine the partitioning of these minor elements during retorting, mass balance studies will be carried out around a bench-scale in situ retort and larger pilot scale retorts. This study will (1) identify the range of minor element concentrations in the oil shale and oil shale products, (2) determine the effect of experimental methods on the measurement of minor elements in oil shale products and (3) determine the effect of retorting variables on the partitioning of minor elements.

3) Bioassay Studies. Retort water from in situ retorting may, under some circumstances (i.e. spills or intentional releases), be discharged to surface waters. To assess the levels of retort water than can be tolerated by the fresh water streams in the study area, continuous flow bioassay studies will be conducted. A laboratory-scale flume system will be designed to simulate as closely as possible field conditions. Using this apparatus, the effect of different dilutions of retort water on algae will be determined by monitoring chlorophyll levels, ATP, photosynthesis, respiration and community structure.

4) Treatability Studies. Retort water generated during in situ retorting will be upgraded in quality before it can be discharged to the environment or reused. Biological treatment together with other unit processes is one of the options. The treatability of retort water by conventional biological treatment processes will be assessed by using the kinetic model of this process and developing kinetic constants using continuous flow stirred tank and plug flow reactors.

THE LAKE COUNTY PROJECT

O. Weres and L. Vollintine

INTRODUCTION

The Lake County Project is an ERDA funded project under the DBER-Integrated Assessment Program. Its purpose has been to study the environmental impacts of the Geysers geothermal development and to project the environmental and socio-economic impacts of future geothermal development at the Geysers and in immediately adjacent Southern Lake County. The main emphasis of our work has been to collect information and conduct studies which are of use to local and state government, industry, and the Lake County public.

RESULTS

Two reports released in mid-FY 1976 were discussed in the proceeding Annual Report.

Two massive reports are now nearing completion and will be released in April and May 1977.

The first[1] is entitled "Resource, Technology, and Environment at the Geysers," and totals approximately 300 pages. It may fairly be described as a short book about the Geysers which describes the development in great detail with an emphasis on its environmental impacts and the technology available to mitigate them. Some attention is also given to the Larderello geothermal development in Tuscany which is also based on the use of native steam. (The chapter which deals with the reservoirs is, in fact, more about Larderello than about the Geysers, and its preparation was supported by an ERDA-DGE supported reservoir study program.)

The chapters which deal with the reservoirs and hydrogen sulfide allotement technology are state-of-the-art reviews and contain significant new theoretical results.

The second report[2] is entitled "The Lake County Economy: Potential Socio-economic Impacts of Geothermal Development," and is approximately 200 pages long. It contains a massive compilation of the socio-economic data about Lake County, along with first order projections of future socio-economic impacts of geothermal development.

Both reports are expected to be extensively used by anyone and everyone involved in the geothermal development or regulation in that area, as well as the interested public.

FUTURE WORK

This project has now passed to the direction C. W. Churchman, who is applying systems-analytic techniques to study how planning decisions which concern geothermal development are made in Lake County. O. Weres is presently engaged in DGE sponsored work, and L. Vollintine is employed by the Lake County Planning Department.

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THE METHYL MERCURY CONTENT OF BENTHIC ORGANISMS FROM CENTRAL SAN FRANCISCO BAY

A. S. Newton and M. A. Wong

This project concerns the analysis for the methyl mercury content of various benthic organisms collected from Central San Francisco Bay during a study[1] of dredge-spoiling effects on trace element availability. Samples were collected by divers,[1] and all species, except Ampelisca milleri and Stylatula elongata, were purged for three days in continuously aerated water which had been collected at the same site. The pelecypods were shucked and the soft tissues saved. Tissues of clams, mus-

sels, and worms were digested for 8 hours in 0.012 M tetra methyl ammonium hydroxide. The samples were then freeze-dried, and the resulting dried tissue ground to a powder for analysis. At least ten individual animals were composited into a single sample.

Methyl mercury was determined on selected samples from this collection. Since the method used for methyl mercury requires about 1 g of sample, for some species of polychaetes, several original samples of each species were composited further in order to get sufficient sample for the methyl mercury analysis. Where possible, three determinations were made on each such composited sample. Methyl mercury was determined by a simplified procedure.[2] The sample was weighed into a 15 ml centrifuge cone, moistened with 3 N HCl and mulched. Then 5 ml of nanograde benzene were added and the mixture allowed to stand for 3 to 5 hours with occasional stirring. The sample was centrifuged and the benzene solution removed for analysis. Methyl mercury in the benzene solution was determined by gas chromatography using a packed column (2% Carbowax 20M TPA plus 2% PMPE (5 ring) on 60-80 mesh Chromosorb G, AW HMDS) at 150°C. The detector was a microwave excited argon plasma detector.[3] A monochromater isolated the 253.7 nm Hg resonace line which was measured with a quartz photomultipler. The sensitivity of this apparatus for methyl mercuric chloride standards in benzene is in the range of 200 to 500 chart divisions/ng of Hg with a noise level of about 1 chart division. The apparatus was calibrated every day.

The results are shown in Table 1. In contrast to the results found for most fish (in which all the mercury is present as methyl mercury[2,4]), the methyl mercury content of benthic organisms from San Francisco Bay is only a fraction of the total mercury.

The fraction of mercury present as methyl mercury is quite low in the polychaetes. Samples of malanidae collected near the EBMUD sewer outfall showed high total mercury but little methyl mercury. Either the worms do not concentrate methyl mercury or there is little if any present in their food.

Nemertea, however, showed the presence of moderate amounts of methyl mercury in a low concentration total mercury. Euchuiroids showed the presence of relatively high concentrations of total mercury, none of which was methyl mercury.

The amphipod, A. milleri, showed no detectable methyl mercury. The decapod, Callianassa sp., the ghost shrimp, showed both high total mercury and significant methyl mercury contamination. The sea pen, Stylatula elongata, was low in total mercury content, but a significant fraction of the mercury present was methyl mercury.

The methyl mercury content of all molluscs represents a significant fraction of the total mercury, with about 25% of the mercury in mollusca, regardless of species (Siliqua patula excepted), being present as methyl mercury.

It does not appear that the benthic organisms of central San Francisco Bay are seriously contaminated with mercury. Of the contamination which does exist, a fraction up to 25 to 40% is in the form of methyl mercury.

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Table 1. Total mercury and methyl mercury in benthic organisms from central San Francisco Bay.[a]

Organism[b]	Collection site[c]	ppm Total Mercury[d]	ppm Methyl Mercury[e]	Methyl Mercury % of Total Mercury
Annelida				
Pectinaria californiensis	CS	0.142	0.021	14%
Pectinaria californiensis	SS	0.150	0.015	10
Glycera americana	EB	0.099	n.d.[e]	0
Glycera robusta	EB	0.075	n.d.	0
Glycera robusta	SS	0.109	0.014	12
Glycera sp.	FL	0.060	n.d.	0

Table 1. (Continued)

Organism[b]	Collection site	ppm Total Mercury	ppm Methyl Mercury	Methyl Mercury % of Total Mercury
Annelida (cont)				
Glycera sp.	EB	0.098	n.d.	0
Glycera sp.	FL	0.89	0.020	2
Asychia elongata[f]	EB	2.00	n.d.	0
Asychia sp.	EB	0.90	n.d.	0
Malanidae sp.	EB	3.21	0.026	1
Cirriformia sp.	FL	0.231	0.007	3
	FL	0.213	0.011	5
	FL	0.140	0.021	15
	FL	0.259	0.014	5
Nemertea				
Unidentified sp.[f]	EB	0.086	0.094	109
Unidentified sp.	SS	0.072	0.025	35
Baseodiscidae sp.	SS	0.076	0.032	42
Echiura				
Unidentified sp.[f]	SS	0.482	n.d.	0
Listriolobus sp.	SS	0.392	n.d.	0
Arthropoda				
Ampelisca milleri	EB	0.184	n.d.	0
	EB	0.188	n.d.	0
Callianassa sp.[f]	SS	0.628	0.306	59[e]
		0.431	0.133	30
Cnidaria				
Stylatula elongata	SS	0.094	0.032	34
	SS	0.134	0.026	19
	SS	0.079	0.021	26
Molusca				
Tritonia diomedia	SS	0.215	0.077	36
	SS	0.126	0.048	38
	SS	0.189	0.038	20
	SS	0.244	0.071	29
Polinices sp.	SS	0.85	0.273	32

Table 1. (Continued)

Organism[b]	Collection site	ppm Total Mercury	ppm Methyl Mercury	Methyl Mercury % of Total Mercury
Molusca (cont)				
Mytilus edulis	BP	0.225	0.062	27
	BP	0.226	0.051	23
	BP	0.222	0.049	22
	FL	0.628	0.071	11
	EB	0.365	0.061	16
	TB[§]	0.257	0.067	36
Crassostrea gigas	TB[§]	0.268	0.098	36
Macoma nasuta	SS	0.468	0.131	27
	SS	0.240	0.049	20
	SS	0.347	0.055	15
Macoma inquinata[f]	EB	0.720	0.095	13
Clinocardium nuttali[f]	FL	0.445	0.122	27
Tresus nuttali	EB	0.276	0.044	16
Solen sicarius[f]	SS	0.230	0.045	19
Lyonsia californica	EB	0.655	0.077	11
Mya arenarea[f]	FL	0.272	0.072	26
Tapes japonica	OE	0.770	0.149	19
	OE	1.026	0.206	20
	FL	0.390	0.128	32
	EB	0.266	0.115	41
Siliqua patula[f]	SS	0.245	n.d.	0
Protothaca staminea	EB	0.353	0.090	25

[a]The organisms were collected in the period October 1974 to February 1975 as part of a study of the effects of dredge-spoiling.

[b]Identification of the organisms was made by John Chapman.

[c]The collection sites were as follows: SS - an experimental site near Buoy 6 in San Francisco Bay. It was approximately 1 mile due east of Angle Island. EB - a site south of the end of the East Bay Municipal Utility District sewer outfall. BP - the outer end of the Berkeley Pier. FL - an experimental site near the Western Pacific Railroad dock, at the entrance to the Oakland Estuary. OE - a site in the Oakland Estuary above the Posey Tube. TB - a site near Marconi Cove in Tomales Bay.

[d]The concentrations of total mercury and methyl mercury are ppm mercury in the dried soft tissues of the animals.

[e]n.d. means that no methyl mercury was detected and the methyl mercury content is < 0.005 ppm.

[f]A single analysis of an undersized sample is presented. No further sample material was available.

[§]Samples from Tomales Bay, assumed to be a clean area, are shown for comparison purposes.

Energy Analysis Program

INTRODUCTION

Historically, the emergence of a new technology has hinged on trial-and-error tests of practicability and profitability. These tests are still sufficient for many technological developments, such as transistors. For others, most notably energy development, they are necessary but no longer sufficient conditions. The ramifications of energy growth and supply technologies permeate in significant ways the whole of society, including its environment, economics, behavior, and the shifting (usually diminishing) resources available to it.

The ubiquitous impacts of growing energy consumption and the means by which it is supplied have become so explicit in the past decade that there now exists a common consensus that the nation must proceed with great prudence in mapping its energy future. Consequently, at the same time that new technologies, and a few old ones such as wind and wood, are explored and tested, the U.S. Energy Research and Development Administration (ERDA) along with a legion of institutes and state and other federal agencies, are also assessing the broader consequences of energy technologies and growth. At Lawrence Berkeley Laboratory these efforts are largely centered in the Energy Analysis Program.

Each of the ERDA National Laboratories is assigned a region of the country for which it is to assess the impacts of alternative choices of energy futures. California, LBL's assigned region, represents about 10% of the nation's population, energy consumption, and gross national product.

In concept, the scope of the "regional energy studies" is comprehensive; it calls for integrated assessments of the environmental, economic, health, resource, and social consequences of, and constraints on, varied choices of technologies, fuels, and growth rates. The objective of these exercises is to develop and display for decision makers the future costs, risks, benefits, and tradeoffs of alternatives. In practice, the enormous complexity of energy-related impacts and constraints compels assessments to focus on issues and problems believed to be particularly significant for developing policies that will shape energy futures.

As part of its energy analysis program, LBL, along with other National Laboratories, is engaged in a two-year National Coal Utilization Assessment. At present, California has no coal and burns none; but undoubtedly it will in the future. Many questions concerning coal utilization need to be answered. Under what conditions and where can coal or its derivatives be burned? What will be the environmental effects and health costs? What are the probable economic impacts, the resource requirements, and the legal and institutional problems?

Other segments of the regional studies program at LBL address similar sets of questions concerning the institution of conservation measures, development of solar and geothermal energy, and the expected flood of Alaskan and OCS oil and LNG imports. Not the least of the tasks is to characterize the California energy structure, its economic ramifications, and social and environmental features that may constrain energy development.

Whereas ERDA's integrated assessments constitute a continuing program, short-term studies are frequently conducted by the Energy Analysis Group in response to urgent needs for information bearing on pending decisions. Such studies include various aspects of nuclear energy and a variety of energy scenarios to test the sensitivity of California's energy industry and economy to specific modifications.

Disciplines represented in the Energy Analysis Program staff include physics, biophysics, economics, engineering, water resource systems analysis, and computer sciences. Professional staff is assisted by graduate students from the University of California Berkeley campus; their contrbutions have been indispensable. When resources permit or when problems seem to defy resolution, we have enjoyed the collaboration of outstanding authorities from the Berkeley faculty, for whose aid the Analysis Program is deeply indebted.

NATIONAL COAL UTILIZATION STUDY

Energy Analysis Program Staff

INTRODUCTION

This project is sponsored by the Energy Research and Development Administration, Administrator for Environment and Safety (AES). It is being conducted jointly at six National Laboratories. Each Laboratory has been assigned to study a region of the country; the region assigned to LBL is California. The purposes of the project are:

1) To provide AES with an assessment of environmental, economic, social, health, and natural resource impacts resulting from coal utilization in California;

2) To identify and analyze mitigation strategies to deal with potential problems;

3) To provide this information to regional

agencies and to other administrators within ERDA in a manner directly applicable to the decisions that will be made.

The project started in October 1976 and is expected to continue through fiscal year 1978.

ACCOMPLISHMENTS DURING 1976

The implementation of this study would proceed along the sequence shown in Fig. 1. The first step is to construct several scenarios detailing a broad range of coal supply options. These scenarios would identify the type and number of facilities, such as power plants, refineries, mines, etc., that would have to be constructed. The next step would be to locate these facilities. The locations of plants would be dictated by environmental, seismic, resource availability, and other similar constraints. The impacts arising due to facilities at these sites would then be analyzed. This analysis would lead to formulation of strategies to mitigate the adverse impacts. A new set of scenarios and siting policies would be formulated after a review of the impacts and mitigation strategies. These would be analyzed during the following fiscal year.

National and regional scenarios identifying four possible energy supply options were formulated during this year. These scenarios were constructed by Argonne and Brookhaven National Laboratories. Scenarios for the Pacific Region included contributions from Pacific Northwest and Lawrence Berkeley Laboratories. While these scenarios are not forecasts, they do set out alternatives in order to display their relative impacts. The four scenarios are:

1) simple extrapolation of recent trends
2) expanded use of coal-derived electrical energy
3) expanded use of coal-derived synthetic oil and synthetic gas
4) combined high coal-derived electrical and high synfuels (combines scenarios 2 and 3).

Each of these scenarios establishes supply quantities of coal, oil, natural gas, synfuels, and different types of electric generating capacity for 1985, 2000, and 2020.

PLANNED ACTIVITIES FOR 1977

The scenarios developed this year will be disaggregated to our region of interest (California). A siting pattern based on these scenarios will be developed (in conjunction with the California Energy Resources Conservation and Development Commission) and the resulting impacts and mitigation strategies will be identified.

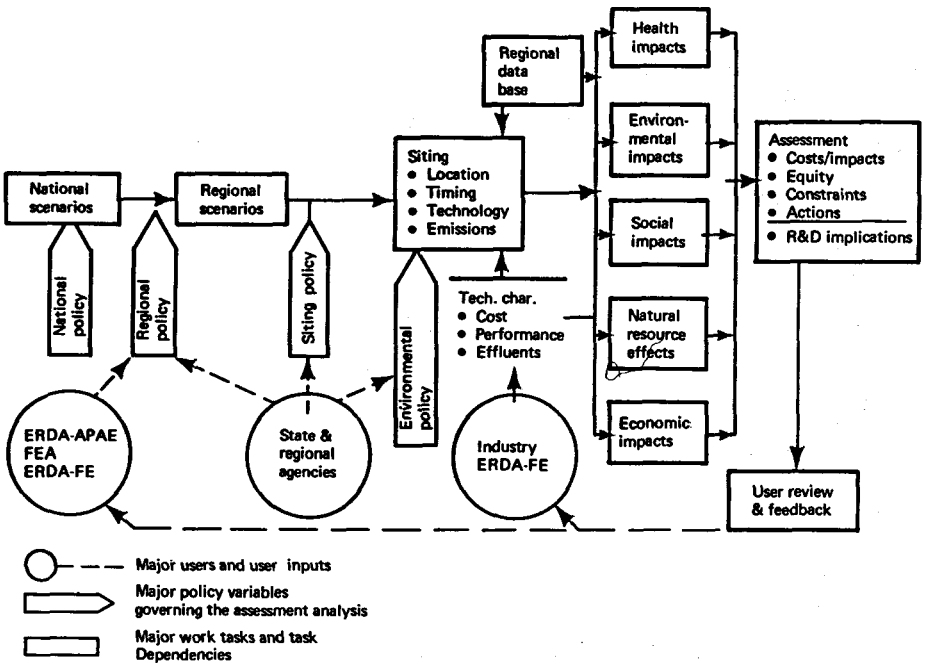

Fig. 1. Study approach. (XBL 773-641)

IMPACT MULTIPLIERS FOR THE MINERAL INDUSTRIES AT THE NATIONAL, STATE, AND LOCAL LEVEL*

F. Andres, A. Levinson, E. Lofting†

This project was initiated on July 1, 1975, and was undertaken jointly with the Dry Lands Research Institute, University of California, Riverside, under a grant from the Bureau of Mines.

The impact of changes in the level of expenditures on total income can be estimated by the use of multipliers. The original Keynesian income multiplier developed in macroeconomic theory is highly aggregated and fails to distinguish among the sectors in which the initial expenditure changes originate. Input-output models enable us to derive sets of multipliers which are disaggregated. Thus multipliers for individual industries can be computed. This recognizes that the total impact on income, output, and employment will vary depending upon which sector experiences the initial expenditure change.

One can also develop various types of input-output multipliers depending upon the degree of closure of the input-output model, i.e., the allocation of sectors between the endogenous matrix and final demand. By including employee compensation and personal consumption expenditures in the endogenous matrix, one takes into account the repercussionary effects of secondary rounds of consumer spending, in addition to the direct and indirect interindustry effects.

In the past, input-output multipliers have usually been used on highly aggregated input-output tables (usually less than 80 sectors). When the official national input-output tables are used, they are at least seven years out of date. While the regional input-output tables used in developing regional multipliers are usually derived from the national input-output tables, they are sometimes developed independently through surveys. While these surveys make it possible to produce a more timely input-output table, the small sample size usually limits the accuracy of the table.

We have attempted to surmount these difficulties by 1) using the official 1967, 367-sector national input-output table; 2) updating the 1967 input-output table to 1972 using the RAS method; and 3) deriving the regional input-output tables from the national table by assuming that the regional technical coefficients were the same as the national coefficients. In addition, the Bureau of Mines for whom the study was conducted, required greater detail on the energy and mining sectors. These industries were therefore disaggregated to 44 sectors which expanded the input-output table to 404 sectors. This level of disaggregation was maintained in applying the methodology to test regions.

While the primary purpose of the study was to develop a methodology for computing the 1972 national and regional Type I and Type II multipliers for employment and income, it was also necessary to demonstrate the method's applicability to the state and county levels as well as to the national level. For this purpose we selected the State of California and Los Angeles County, both representing highly developed and diversified economies for which good data are available. Of the 404 sectors in the model, California is represented by 372 producing sectors including 24 of the 44 new sectors added to the table for energy and mining. Los Angeles County contains 346 producing sectors, including 12 of the new sectors.

The United States is largely a closed economy. The economy of California is less self-sufficient than that of the United States but more so than that of Los Angeles County. Consequently, among the three regions, the largest values would be anticipated for national income and employment multipliers, with intermediate values for California, and the smallest values for Los Angeles County.

Both the input-output tables and the multipliers that have been developed can be used by other projects at the Laboratory that require an assessment of the economic impact of energy projects in the United States, California, and Los Angeles County. If multipliers on tables of other regions of the country are needed, these can be readily obtained using the methodology developed by this project.

The methodology was developed and most of the data were collected during 1975. All of the work required under the contract was completed during 1976. This consisted of collecting the rest of the data, writing the computer programs, producing the updated input-output tables, and computing the multipliers. The results largely conformed to our expectations. Those sectors with large multipliers tended to be capital intensive and had a large linkage to other sectors. The sectors with small multipliers tended to be labor intensive. A comparison of the multipliers from the three regions showed that in general the larger the region the larger the multiplier, an effect that is due to larger leakages from smaller regions.

The only surprise was the ratio of the Type I to Type II income multipliers for the United States. The ratio of 2:84 was the highest value we have seen. Since our results were not based directly on an official input-output table, we checked them by computing the income multipliers using the official 367-sector 1967 input-output table. Using these

multipliers we obtained a ratio of 2:92 which is close to the value obtained from the 1972 multipliers. This tended to confirm the reliability of our results.

The 44 mining sectors in the 1967 404-sector input-output table were obtained by updating the flows for the 44 1963 mining sectors. The Bureau of Mines is in the process of awarding the Laboratory a contract to take 1967 data for the mining sectors which they have provided, to produce a new 1967 404-sector input-output table.

FOOTNOTES

*A joint project conducted with the Dry Lands Research Institute, University of California, Riverside.

†Currently associated with the Dry Lands Research Institute.

MANPOWER CONSTRAINTS ON ENERGY PLANT CONSTRUCTION AND OPERATION*

P. Benenson and T. Simonson†

INTRODUCTION

The original objective of this work was to estimate whether or not there is sufficient manpower in all occupations to construct and operate the energy plants implied by current energy consumption projections. This task required assembly and/or coupling of a series of models and data bases. These are:

(1) A two-region input-output model of the U.S. to capture the interrelatedness of the U.S. economy;

(2) A linear programming model that approximates producer behavior and resource allocation subject to resource constraints;

(3) An occupation-by-industry matrix of the U.S. economy;

(4) A manpower mobility constraint model that simulates occupational changes constrained by occupation similarity, occupational supply, and historical mobility.

We have chosen to model the entire U.S. economy even though our focus is on California. We include the rest of the U.S. because the labor market is to some extent a national one in which there is substantial geographic mobility. By using a two-region model with national, not regional, occupational supply constraints, we account for geographical labor mobility. The work thus far can be broken down into three stages. In the first stage, we assembled the basic components of the model (items 1, 2 and 3 above) and evaluated the feasibility of the results; this work was reported fully in "Analysis of Manpower Constraints on Energy Plant Construction and Operation, "UCID-3760, June 30, 1975. In the second stage, we implemented a series of refinements to the basic model to make it more realistic; these are discussed in the 1975 Energy and Environment Division Annual Report. During this past year, the work has been to develop the manpower mobility constraint model. Also, the scope of the study is being broadened. Earlier work was focused on the relationship between en production and labor; we are now emphasizing a comparison between this relationship and that of energy conservation and labor. Both these developments will be discussed below.

ACCOMPLISHMENTS DURING 1976

Manpower Mobility Constraint Model

The objective of this work is to accurately model manpower constraints on economic activity by taking into account mobility of labor between occupations. This model is designed to be linked with the two-region input-output model that we used in our earlier work which is coupled to an industry-by-occupation matrix that generates manpower requirements by specific occupation and industry for each level of economic activity. We imposed estimates of the supply of labor in each occupation and the industrial capacity in each industry as constraints on a linear programming model which maximizes gross national product.

Prior to developing the constraint model, we investigated previous research on labor mobility and the use of input-output models in manpower problems. Several instances were found in which input-output models were used to derive manpower *needs*, but no work was found in which the *supply* of manpower was taken into account as well. There has been extensive research on labor mobility, but several factors made it difficult to use in operating a model. The classification of occupations was very aggregated, and the classification systems were not the same in all the studies. Also, most work used was economic factors to affect mobility, which are not determined in the input-output framework, e.g., unemployment rates and wage rates.

The only tabulation we found useful was contained in a report from the Center for Advanced Computation, University of Illinois.[1] This tabulation, based on Census data, shows the number of people who changed occupations between 1965 and 1970. The tabulation is broken down into 304 occupational categories that are consistent with the occupational classification used in our input-output model to derive manpower requirements. The tabulation distinguishes moves in each direction between occupations. The period covered was one of particularly high mobility, and thus gives a historical view of the capacity of the occupational structure for mobility.

Our model of mobility is structural; there is a pattern to the way people move through the occupational structure that we expect to persist through time, and this pattern is reflected by our data on mobility during the past ten years. The supplies of labor in each occupation in 1980 are not independent point estimates, but rather are fluctuating ranges that are mutually dependent, linked by movement between occupations. Thus, an increase in the supply of labor in one occupation implies decreases in others. We constrain the mobility between each pair of occupations not to exceed the observed degree of mobility in the period 1965-1970.

The supply of labor in each occupation in 1980 is determined by the number in that occupation in 1975, less those leaving that occupation and/or the labor force by 1980, plus those entering from outside the labor force and from other occupations. With these more flexible labor supply constraints, the linear program is solved for the pattern of occupational changes required to achieve the occupational structure of the labor force implied by the chosen pattern of final consumption. The program solution is obtained subject to upper bound constraints on the changes between each set of occupations and the total number of persons in the labor force.

In order to implement this model, we have accumulated data from several sources and put them in a mutually consistent form. Estimates of the 1975 labor force by occupation have been computed from the Bureau of the Census Decennial Census and Current Population Survey data presently at LBL. From the Center for Advanced Computation, we acquired data (derived from Census) on net occupational changes in the period 1965-1970. To compute the employment requirements, we used the matrix of persons employed by industry and occupation that was constructed at LBL.

A computer test run at the nine occupation level of aggregation is being prepared. Final corrections to the data are being made to render the data consistent with the input-output model; we also are modifying the linear program to accommodate the new constraint model.

This model of mobility and the resulting manpower constraints should not be interpreted in the same way as natural resource constraints; clearly an attempt to forecast the decisions people make among occupations must be uncertain at best. Thus, we cannot predict an absolute ceiling for each occupation beyond which any labor requirement could be considered infeasible. However, the new occupational constraints can serve as a benchmark that represents a relatively high degree of mobility. If the occupational constraints are binding, then we have some indication, relative to our recent historical experience, of the degree of mobility required to achieve the occupational pattern given in the solution. The model can also be used as an indicator of the interrelations among occupations; it shows the potential tradeoffs between expansion of some occupations and contraction of others, with their attendant impacts on production in various sectors.

Related Studies

Several other avenues of work are in progress at LBL that relate to the manpower constraint model. First, a national and California input-output table have been updated from 1967 to 1972. These form the two regions of the input-output model to be used in subsequent scenario analysis. Formerly, a multiregion input-output model based on 1963 data was used. Second, a study of energy flows between California and the rest of the U.S. is being conducted. When completed, the output of this work will form the link between California and national I-O tables. Third, work has begun on estimating the income and employment impacts of energy conservation measures. This entails data acquisition regarding the material and manpower requirements for specific conservation measures, the associated energy and power plant capacity savings, and estimates of the rate of conservation implementation. This work is discussed in more detail in the report "Analysis of the California Energy Industry," LBL-5928, January 1977.

DIRECTION FOR FURTHER WORK

We plan to broaden the scope of this study to include a comparison with the manpower impacts from energy conservation. Work has already begun in this direction in the California Energy Industry study. There are several reasons for pursuing this direction. First, the issue is timely. Second, it is linked to the larger question of the relationship between energy use and GNP. Third, more accurate estimates of the direct impacts are possible relative to our ability to estimate occupational supply. The latter are extremely difficult to estimate because of the general uncertainty regarding the size of the labor force and the degree of occupational mobility if economic or other incentives become strong enough. The scope of our investigation will be determined in consultation with state government agencies and will be based jointly upon their priorities and the feasibility of data acquisition.

FOOTNOTES AND REFERENCE

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†Department of Economics, University of California, Berkeley.

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IMPACT AND ASSESSMENT OF GROWTH AND CHANGE IN SOCIAL SYSTEMS FROM ENERGY PROJECTS: A SYSTEMS APPROACH

C. W. Churchman and H. G. Nelson

INTRODUCTION

Geothermal energy, despite the potential to provide only a small portion of the total energy needs for California, is growing in importance, and increasing attention is being directed towards these locations of major "Known Geothermal Resource Areas (KGRA's)." One such area is located in Lake County of north central California. This mostly rural county has a permanent population of about 24,000 people, which in the summer more than doubles as tourists come to enjoy the natural amenities offered by the area. One of the major attractions is a large, picturesque lake called Clear Lake, around which most of the recreational activities take place. Other recreational features include outdoor activities that take advantage of the large blocks of public lands included within the County boundaries.

Three groups of people make up the major portion of the permanent population in Lake County. The first group includes those working in jobs related to the extensive recreation industry. The second major group is involved with the agricultural industry, which consists mainly of pear and walnut crops. The third group consists of retired people attracted to the County by its low cost of living and its rural setting.

Adjacent to Lake County's western boundary is an area known as "The Geysers" which has been actively using the geothermal resource to produce electrical energy since the 1950's. Here at this boundary region with The Geysers area, Lake County expects to have its first geothermal power plant. Presently there exists a full field development able to provide steam to a proposed utility power plant; and a great deal of activity related to other potential geothermal developments is taking place throughout the County.

The opportunities as well as the dangers involved in such a large-scale resource development are appreciated by residents and governmental agencies, and are the major reasons why the Energy Research and Development Administration (ERDA) is funding an impact and assessment study, to be done by the Lawrence Berkeley Laboratory (LBL).

ACCOMPLISHMENTS DURING 1976

The impact and assessment study dealing with the potential geothermal development in Lake County, California, has been divided into two phases. The first phase, just completed, deals with a variety of subjects leading to an overall picture of the physical and demographic characteristics of the County. It includes an introduction to the development process prior to producing electricity from a geothermal resource, starting with exploration and leasing policies and continuing through power plant operation, especially as it relates to fiscal impacts upon the County. Also included is a site-specific study of the geothermal resource as found in Lake County and the related technical aspects of the state-of-the-art technology in extraction and use of the resource for generating electrical energy. Information is discussed dealing with the impact of different chemicals associated with the geothermal resource.

The Lake County demographic information and the geothermal resource information will be published as separate LBL reports. Two related LBL reports dealing with public opinion questionnaires have already been published. One concerns a questionnaire sent to people within the Cobb Mountain area of the County, which faces imminent geothermal development pressure.[1] The second report discusses the same questionnaire sent to a random sample of the registered voters of the entire County.[2] The purpose of the questionnaires was to discern attitudes and perceptions relating to the geothermal energy development.

PLANNED ACTIVITIES FOR 1977

The second phase of the study will deal with humanistic concerns, using the "systems approach" assessment method.[3,4] Growth and change in social systems brought about by the intentional energy development policies of agencies such as ERDA promise opportunities for residents of the County and for energy users residing elsewhere; but the County residents are concerned over the potentially negative side effects that have historically plagued similar rural communities faced with intense development from outside forces.[5-8] Such potential costs and benefits are not always measurable on economic scales. Therefore, the second part of the study will model the community and related interest groups as a system and will use the system method to address important issues that are difficult to deal with using only economic models.

The study will provide information on values and perceptions of Lake County residents and individuals from the interest groups involved in the geothermal resource development. The members of these groups will be divided into three separate roles, which may overlap: (1) the clients or people who should be served by policies relating to the geothermal resource, (2) the decision-makers or those who by their control of resources can make changes in the components of a system, and (3) the planners or those who conceptualize a change and assess its value.

Data will be collected by a variety of methods. Questionnaires, workshops, and interviews will be used as active methods of data gathering. Unobtrusive measures will be used to provide complementary information, not accessible through the active methods. As the study progresses and an understanding of the problem increases, more appropriate methods will be used. The same approach is true for data sources. With the systems method, data are collected sequentially, beginning with a broad

sweep and then concentrating on the most relevant sources.

In order to accomplish the goals of this phase of the study, a variety of tasks must be completed; the results will be in three forms:

(1) There will be the introduction and development of the systems approach which can be used as a model by those persons involved in future problem-solving attempts in Lake County and other communities with similar developmental changes;

(2) There will be information and data collected for a report dealing with humanistic values;

(3) There will be the observations, discussions, future tasks, and, where warranted, conclusions (drawn from the perspective of planners with explicit world views).

While working on these tasks, information will be collected to answer nine basic questions of humanistic assessment of social change:

(1) Who should be the client?

(2) What should be the goal of the system?

(3) What should be the measurement of performance for the system?

(4) Who should be the decision-makers?

(5) What components of the system should the decision-makers control?

(6) What should be considered as the environment of the system?

(7) Who should be the planners of change in the system?

(8) How should plans be implemented?

(9) What should be the design of the control of the implemented plan?

The results of this study will consist of information (sometimes conflicting information) on each of these nine questions. In many cases the information will be in the form of a dialectic process. By explicitly stating the differing views on issues and by exploiting these differences, those who will be using this information for judgments and policy decisions will have a much higher probability for making proper decisions. In other cases, the information will be concerned with areas of agreement and will be considered as base line information. It is expected that this information will prove valuable both to the citizens of Lake County and to the planning organizations.

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RESIDUALS FROM CALIFORNIA POWER PLANTS

H. Ruderman and R. Sextro

INTRODUCTION

We have made estimates of pollutants and other residuals associated with power plants supplying electricity to California. The calculations were based on three scenarios for power plant construction and operation that were supplied by the Energy Assessment Division of the California Energy Resources Conservation and Development Commission (CERCDC). The first scenario is based on the utilities' schedule for new generating capacity, which was submitted to CERCDC in May 1976. The other two scenarios, low demand – new technology (LD/NT) and high demand – new technology (HD/NT) were developed by the Energy Assessment Division staff of CERCDC to examine alternatives to the utilities' plans.

The residuals were calculated for each of eleven years from 1975 to 1985 and for the twentieth year, 1995. They were classified into emissions to air and water, solid wastes, land use, occupational health and safety, radiological emissions, and radioactive material in irradiated fuel rods. Geographically, they were disaggregated by air basin, hydrological basin, utility service area,

and in- and out-of-state. These data, in the form of computer printouts, were submitted to the Energy Assessment Division for their use in analyzing the potential environmental impacts of the utilities' resource plans. Some of these results were incorporated in the staff-proposed draft of the Electricity Forecasting and Planning Report.[1] In addition, a report containing the methodology and assumptions used in performing these calculations was submitted to CERCDC.[2]

SCENARIOS

The "Business as Usual" scenario is based on the statewide supply forecast submitted by the electric utilities to CERCDC. The high demand – new technology scenario (HD/NT) couples the utilities' forecast[1] of electricity demand to a supply mix developed by CERCDC calling for rapid implementation of advanced technologies. This results in more electricity generation by coal, geothermal, wind, solar, and waste energy facilities and less by oil and nuclear than the BAU case (see Table 1). The low demand – new technology scenario (LD/NT) is based on CERCDC estimates of the impacts of energy conservation on the growth in demand for electricity. This scenario shows decreased reliance on coal, nuclear, and geothermal sources as compared with the HD/NT scenario. The assumptions that went into constructing these scenarios is discussed in Chapter VII of Ref. 1.

METHODOLOGY AND DATA

The calculation of residuals is based on the concept of a nominal facility which is a hypothetical power plant with a generating capacity, capacity factor, and efficiency typical of existing or planned power plants of that type. Each nominal facility burns fuel with certain assumed characteristics such as energy, ash, or sulfur content. A method of cooling and pollution abatement equipment for the plant are also assumed. In general, we have used the nominal facility sizes from the Energy Supply Planning Model developed by the Bechtel Corporation.[3]

Using these assumptions we calculate the amount of fuel consumed (energy input) for each nominal facility expressed in Btu's per year and in physical units (barrels or tons). The pollutants emitted to air and water, the amount of solid and radioactive waste produced, and the occupational health and safety impacts are all assumed to be proportional to the annual energy input to the facility. The only exception is land use which is taken to be proportional to the plant size (generating capacity). The primary sources used for data on pollutants and other residuals associated with power plants are two reports by Teknekron, Inc.,[4,5] and the MERES data base,[6] from which additional data on occupational health and safety were obtained. The data from these sources were then scaled by the energy input for each facility, resulting in the residuals associated with each nominal facility.

Next, a generating facility data file was constructed using data submitted to CERCDC by the California electric utilities. These submissions contained a year-by-year and facility-by-facility listing of generating capacity additions (including present capacity) or retirements planned up to 1985, and for the twentieth year, 1995. Wherever possible, each facility was identified by name, location, fuel type, and cooling method. Plant location was specified by county, air and hydrological basin, and Bureau of Economic Analysis (BEA) region. Fuel consumption was estimated by the utilities for each power plant type within an air basin. The capacity factor, by plant type and air basin, used in the model was adjusted so that fuel requirements

Table 1. Scenarios for residuals calculation (generating capacity in MWe).

	1975	1980			1985			1995		
	All	BAU	LD/NT	HD/NT	BAU	LD/NT	HD/NT	BAU	LD/NT	HD/NT
Nuclear (in)[a]	1379	3657	3657	3657	7907	5857	7457	34657	6817	10344
Nuclear (out)[a]	--	--	--	--	381	--	381	571	--	381
Oil	21361	22005	22026	22005	21252	21496	21496	17630	15941	15387
Coal (in)[a]	--	--	--	--	800	--	800	2880	--	5600
Coal (out)[a]	2276	2433	2433	2433	4033	2433	4948	4483	2433	6808
Combined cycle	24	1096	1096	1166	1456	1096	2462	3424	1072	3842
Gas turbines	1083	2314	2314	2314	4339	2314	3739	6210	2083	3475
Geothermal	502	1178	1178	1178	1978	1286	2048	3458	11646	12844
Advanced Tech.	--	26	--	--	224	2400	250	680	4745	7600
Total	26625	32709	32704	32753	42370	36882	43581	73993	44737	66281

Source: CERCDC Energy Assessment Division.

[a]In or out of state.

[b]Includes fuel cells, solar, wind, and waste generation.

for each fuel type within an air basin matched the utility estimates. For hydro, geothermal, and advanced technology facilities, the utilities' estimates for capacity factors were used.

The yearly changes in plant capacity and capacity factor for each facility were converted into an annual schedule of the number of nominal facilities of a particular type operating during that year. The number of nominal facilities of a given type that are operating is equal to the energy input to the actual facility for that year divided by the annual energy input to a nominal facility of the same type. The amount of any residual produced during one year by a given facility or group of facilities is equal to the annual production of that residual by a nominal facility of the corresponding type multiplied by the number of nominal facilities of that type operating during the year.

RESULTS

Since the purpose of this task is to provide the Commission staff with data for their assessment of the environmental impacts of the utilities' plans or alternative plans, we have done little analysis of our results. In this section we present some selected results as an example of what can be done using our methodology and data. All the results shown are for the San Francisco Bay Area for the years 1975-1985 and for 1995.

In Fig. 1 we present the utilities' estimate of electricity generated in the Bay Area by plant type. Presently all generation is from oil-fired plants. The utilities' plans call for additional capacity in the form of gas turbine and combined cycle plants coming on-line about 1980 and a coal-fired plant in 1983. The oil-fired plants are expected to be run at a higher capacity factor during this period. After 1985 the older oil-fired plants are phased out and the gas turbines run at a lower capacity factor. The HD/NT scenario is very similar, whereas the LD/NT scenario shows no coal or combined cycle plants being built and only half of the new gas turbines.

The estimated amounts of particulates, oxides of nitrogen, and sulfur oxides that would be emitted by power plants in the Bay Area under the BAU scenario are plotted in Fig. 2. These show that there may be more than a factor of two increase in particulates and NO_X by 1985. The proposed coal-fired plant is a major contributor to this increase. Its effect on SO_X emissions is relatively smaller

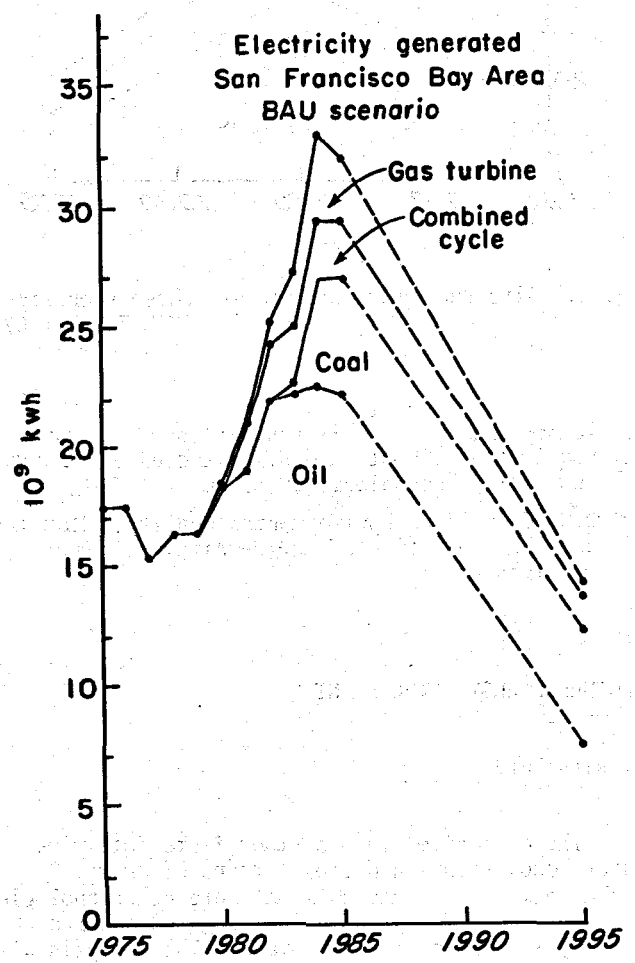

Fig. 1. Utilities' estimate of electricity generated in the Bay Area by plant type. (XBL 7612-11109)

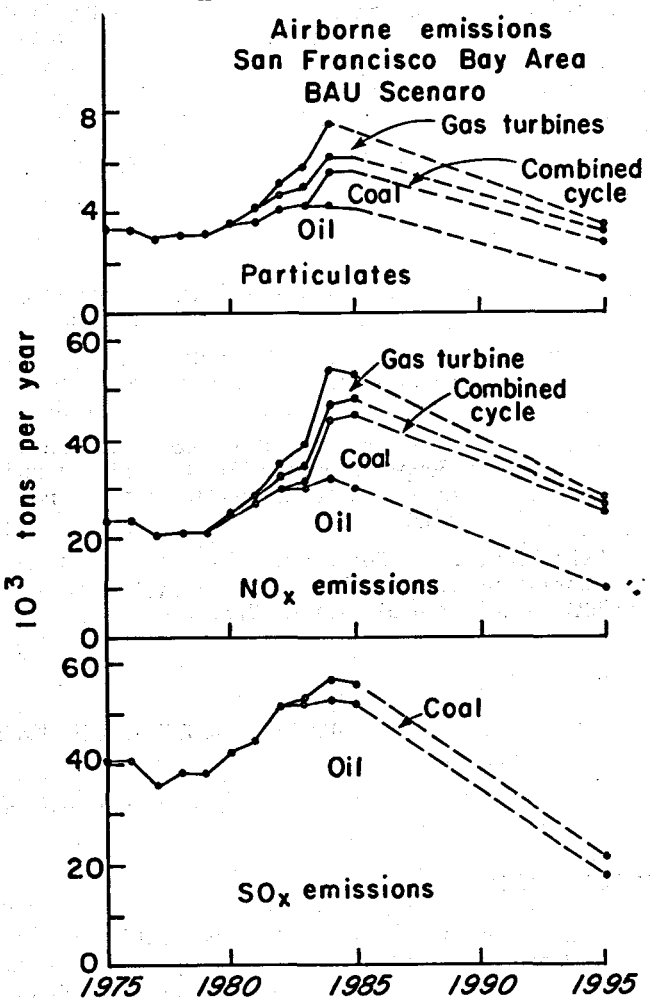

Fig. 2. Estimated amounts of particulates and oxides emitted by Bay Area power plants under the business-as-usual scenario. (XBL 7612-11110)

as it is expected to burn low sulfur coal (1% sulfur content) and will use scrubbers. The gas turbine and combined cycle plants, which burn distillate, make a negligible contribution to the SO_X emissions. The levels of air pollutant emission decrease by 1995 with the phase out of oil-fired power plants.

In Fig. 3 these same three airborne emissions are shown for all three scenarios on a five-year basis to 1985 and then for 1995. The LD/NT scenario shows a significantly lower level of emissions than the other two scenarios. The decline from 1975 to 1970 is primarily due to running existing plants at lower capacity factor because of lower demand in this scenario. After 1980 there are additional savings since no new coal-fired or combined cycle plants are built. The HD/NT and BAU scenarios are nearly the same. By 1995, however, the HD/NT scenario shows slightly lower emissions. In this scenario the power plants are running at a lower capacity factor, and more electricity is being supplied from outside the region.

Our results are a first step in evaluating the environmental impacts of a given electricity supply mix. They could serve as input to a pollutant dispersion model which would calculate the concentration of these substances in the air and water, and their deposition on the ground. It would then be necessary to trace the paths in the food web by which they are distributed to the species in the local ecosystem. Finally, the effects on human health and the ecosystem should be estimated from the population exposed to these pollutant levels. So far no reliable methodology has been found to carry out these calculations.

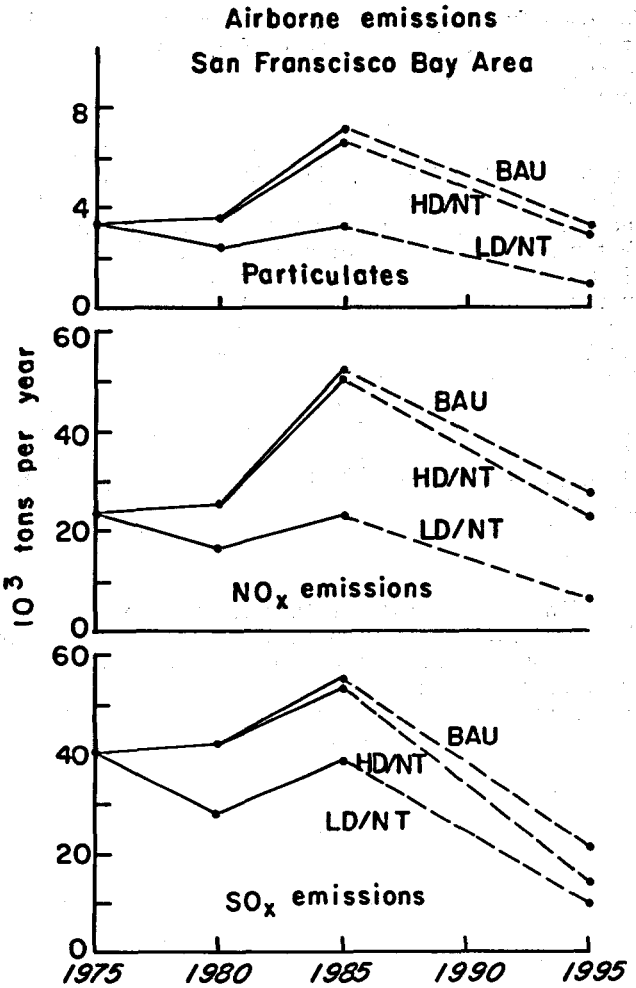

Fig. 3. Airborne emissions for all three scenarios. (XBL 7612-11107)

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SURVEY OF WATER REQUIREMENTS FOR FUTURE ENERGY DEVELOPMENT

J. Sathaye and R. L. Ritschard

INTRODUCTION

This project is part of the cooperative Federal Water Resources Council (WRC) – Energy Research and Development Administration (ERDA) program to conduct a Water-for-Energy Assessment under the provisions of Section 13 of the Federal Non-nuclear Energy Research and Development Act of 1974.

The objective of this study is to determine water requirements and implications of energy technologies, with emphasis on emerging technologies for certain WRC regions and aggregated subareas (ASA's) in California and Nevada. The analysis will be incorporated into WRC's Water-for-Energy Program and other WRC and ERDA programs, and will enable consideration of new technologies within the 1975 National Assessment.

The project has been divided into two phases. The first phase, which commenced in August 1976 and was completed in November 1976, provided projections and demands for energy and water resources as perceived by regional and state entities responsible for or involved in energy planning.

Phase II begins in January 1977 and includes the collection of data and an analysis of the impact on water resources arising from development of various energy technologies by 1975, 1985, and 2000. The current and projected energy use by fuel type, including electrical demand, will be defined by ERDA and FEA scenarios. The specific fuel supply activities to be considered are extraction of fossil fuels, processing and conversion of fossil and nuclear fuels, including electric power generation, and new technologies such as coal gasification, coal liquefaction, biomass conversion, geothermal, and waste utilization.

This project relates directly to the water resources analysis portion of the National Coal Utilization Assessment that is currently a major activity of the Energy Analysis Program. The overall objective of both these studies is to determine the effects of energy-related activities on the quantity and quality of water resources and how these effects might constrain the utilization of energy resources in California and the West.

ACCOMPLISHMENTS DURING 1976

The Phase I portion of the project was completed in November 1976. It resulted in a draft report[1] which was submitted to WRC and is currently being reviewed by various WRC committees, WRC staff, and the Regional Sponsors. A final report will be prepared incorporating the comments made by the reviewers.

The information used in the Phase I effort was obtained from a variety of regional and state sources including representatives of State energy offices, public service commissions, water resources offices, and planning agencies. This information will be used as well in the water resources analysis portion of the National Coal Utilization Assessment.

The following observations regarding the water-energy picture in California were made:

(1) Energy development in California could require a significant amount of fresh water for power plant cooling by 1995;

(2) Major impacts of this increased water-requirements level would be felt in some hydrologic basins;

(3) Several measures are available to mitigate the potential adverse impacts on water resources, among which are the use of wet/dry or dry cooling towers, water conservation, use of agricultural and municipal waste water, and development of groundwater sources.

Future increases in water availability for the development of energy technologies in Nevada will probably come from pumping groundwater. Several hydrographic areas have been identified by the State where groundwater exists in sufficient quantity to support an expansion of electric generation capacity. The focus in Nevada's energy and water future seems to be in the import-export areas. Nevada is currently a net electrical energy exporter and could continue to expand that role. Large exports of electrical energy, however, could have a substantial effect on Nevada's total energy market, the State's economy, and its environment.

PLANNED ACTIVITIES FOR 1977

The following activities are planned for next year:

(1) Disaggregate current and projected (1985 and 2000) fuel supply as appropriate to WRC region and to ASA's based on ERDA and FEA scenarios. California's supply technology siting will be based on the long-range plans (to 1995) of the Conservation and Development Commission and the California utilities;

(2) Determine unit water requirements for non-nuclear energy technologies which are likely to contribute significantly to national energy supply by the year 2000;

(3) Calculate aggregate water requirements for 1975, 1985, and 2000 by WRC region and by selected ASA's for each fuel supply technology, including nuclear;

(4) Identify the possible implications on water and related land resources associated with ERDA and FEA scenarios.

A draft of the final report will be provided to WRC at the end of April 1977, with a final report one month later.

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ANALYSIS OF CALIFORNIA ENERGY INDUSTRY

J. A. Sathaye, H. Ruderman, R. Sextro, P. Benenson,
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INTRODUCTION

The California energy supply system forms an integral part of the State's economy. It provides an important input for production of most commodities and services, and competes with other economic sectors for capital and manpower. In this study, we focus on the capital and manpower which would be required under alternative paths of energy development. In particular, we

(1) Describe quantitatively the California energy industry and its relationship to the California and the U.S. economies,

(2) Provide the analytic capability for determining the direct and indirect employment and income impacts resulting from a given energy future for California,

(3) Demonstrate and test the methodology with scenarios that embody varying combinations of conventional energy technologies, new energy technologies, and energy conservation measures.

The methodology developed in this project is generally applicable to any set of California energy futures up to the year 1995. It is planned to use this methodology for other projects such as the ERDA National Coal Utilization Assessment and the Regional Studies Program. California scenarios formulated as part of these projects will be analyzed using these models. The project started in May 1976 and was completed at the end of December 1976.

The Present California Energy Industry

At present, natural gas, petroleum fuels, and electricity form the major part of energy supply to California. Natural gas and crude oil production peaked in the latter part of the 1960's and has declined steadily since 1968. On the other hand, sales of electricity have exceeded in-state production since 1970.

The present energy industry accounts for about 1.4% of nonagricultural employment and about 3.5% of the Gross State Product. In terms of labor intensity (employees per million dollars output), the energy sectors are among the lowest twenty percent of all economic sectors; therefore, large changes in output from those sectors are required before significant changes in level of employment are felt.

Future Energy Supply Systems: An Assessment Methodology

In order to quantify the employment and income impacts of future energy systems, we have developed an energy supply model for California and linked it to an input-output (I-O) model of the California economy. This energy supply model simulates the construction and operation of energy resource extraction, transportation, and conversion facilities. It calculates capital and operating requirements, including materials and fuel for these facilities. The indirect manpower and income effects are then estimated by transforming these requirements into inputs to the I-O model. In the I-O model the interdependence among sectors is explicitly accounted for, so that the impact of changes in the production of any given sector can be traced to all other sectors. The impacts calculated by these models include fuel requirements, capital and manpower needs for the construction of new energy facilities, the indirect manpower required for the supply of construction materials, and some of the costs and manpower associated with operation and maintenance of these facilities.

Three alternative energy scenarios were analyzed to demonstrate this methodology. While these scenarios are not forecasts on our part, they do set out three energy futures which display conventional technologies, alternative supply technologies, and conservation measures.

In the first scenario, the schedule for adding new electricity generating capacity was acquired from utility submissions to the California Energy Resources Conservation and Development Commission (CERCDC). The supply and demand schedule for oil and gas in this scenario is based on published forecasts.[1-3] The second scenario includes a shift in emphasis to new electricity supply technologies, active solar heating of residential buildings, and a decreased availability of natural gas for California. The new technologies are geothermal units, wind turbines, solar-thermal systems, and waste-fired power plants.

The third scenario emphasizes use of three conservation measures: delamping in commercial buildings, retrofit ceiling insulation in residential buildings, and construction of passive solar houses. These measures lead to a reduction in energy consumption and to a reduction in new gas and electricity supply facilities. The third scenario was formulated by removing these facilities from the first scenario, and decreasing the energy flows appropriately.

Energy consumption in the three scenarios grows annually at a rate of 2.6%, 2.0%, and 2.4%. The 20-year cumulative energy requirements for the three scenarios are shown in Fig. 1. In terms of cumulative resource use, the consumption of nonrenewable resources (natural gas, coal, oil, uranium, and geothermal heat) is 11% lower in the second scenario, as compared with the 151×10^{15} Btu consumed in the first scenario. The major differences are a 66% decline in nuclear fuel requirements and a 31% drop in natural gas supply. A comparison of the first and third scenarios shows the effect of conservation measures. These measures account for a 4% decrease

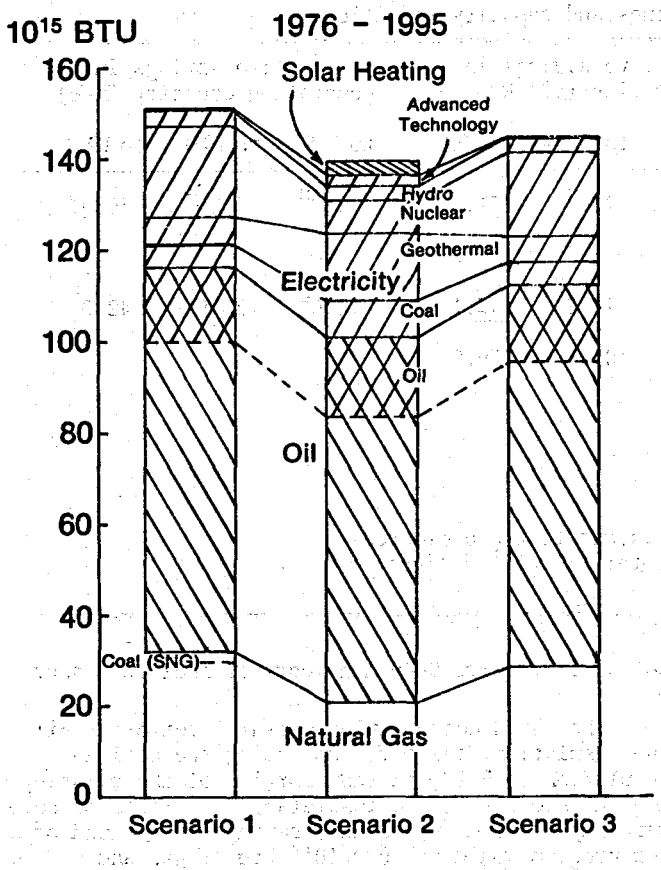

Fig. 1. Total primary energy use in California. (XBL 771-7198)

in nonrenewable resource requirements from those called for in the first scenario. This decrease is due to a 6% savings in natural gas, a 42% drop in coal requirements, and an 8% decline in nuclear fuel requirements.

The capital and manpower requirements are summarized in Table 1. The capital requirements for the three scenarios over the 15-year period, 1976-1990, amount to $48 billion, $55 billion, and $43 billion, respectively. A significant portion of the capital in the second scenario is expended on active solar heating devices. In terms of the overall State economy, the capital requirement for the construction of new energy facilities averaged over 15 years ranges from 11% to 15% of $25 billion, the 1974 value of Gross Private Capital Formation in California.

The average annual manpower required by each of the three scenarios was calculated to be 144,300 man-years, 183,600 man-years, and 137,600 man-years. The difference between the first and second scenarios is 39,000 man-years, or less than 0.5% of the 1974 labor force of 9.5 million. When compared, however, with the average number of new nonagricultural jobs that have been created annually in California (about 210,000 per year), these additional jobs make a large contribution to employment growth. Our results show that one can formulate an energy scenario that is more labor intensive than another. However, this does not imply that energy policy can or should be used to make employment policy.

IMPACTS OF ALTERNATIVE INVESTMENTS

We examined the tradeoffs between the three

TABLE 1. Summary of construction and operation requirements.

		—Capital (10^6 1974 $)—		—— Manpower (Man-years) ——				
		Construction	Operation	Construction	Operation	Indirect	Total	Average annual
Scenario 1	1976-80	10,131	7,073	101,900	259,800	189,000	550,700	110,000
	1981-85	22,544	7,906	203,400	274,500	374,600	852,500	170,500
	1986-90	15,239	9,116	177,900	300,000	282,800	760,700	152,140
	Total	47,914	24,095	483,200	834,300	846,400	2,163,900	144,300
Scenario 2	1976-80	19,051	7,470	258,500	298,300	330,700	887,500	177,500
	1981-85	17,712	9,466	224,200	382,700	298,800	905,700	181,100
	1986-90	18,141	10,962	208,000	450,100	302,700	960,800	192,160
	Total	54,904	27,898	690,700	1,131,100	932,200	2,754,000	183,600
Scenario 3	1976-80	9,423	6,948	94,800	258,300	180,600	533,700	106,740
	1981-85	18,283	7,616	172,800	267,800	337,600	778,200	155,640
	1986-90	15,097	8,763	177,000	290,700	284,200	751,900	150,380
	Total	42,803	23,327	444,600	816,800	802,400	2,063,800	137,600

Table 2. Estimates of energy savings and capacity reduction.

	Cumulative savings in natural gas (10^{12} Btu)			Cumulative savings in electricity (10^9 Kwh)			Cumulative savings in generating capacity (MWe)		
	to 1981	to 1986	to 1991	to 1981	to 1986	to 1991	to 1981	to 1986	to 1991
Delamping	0	0	0	26.2	78.7	131.3	3080[a]	3080[a]	3080[a]
Retrofit insulation[c]	248	745	1242	1.1	3.3	5.5	0	0	0
Passive solar housing	39	155	349	4.8	19.2	43.1	1400[b]	2800[b]	4200[b]
Total	287	900	1591	32.1	101.2	179.9			

[a]Base load

[b]Peak load

[c]These programs, taken together, save natural gas equivalent to the projected output from two synthetic natural gas (SNG) plants (total 141×10^9 ft^3/yr).

energy conservation programs and some of the energy facility construction programs that are rendered unnecessary by energy conservation. Table 2 shows estimates of energy savings and capacity reduction due to the conservation programs. The delamping program involves reducing the lighting level in commercial buildings by replacing a portion of the existing fluorescent tubes with nonluminous Phantom™ tubes. We assumed this program would require no additional expenses. At the completion of the 5-year delamping program, there would be an annual electricity savings of 10.5×10^9 kWh. Over a 15-year period (1976-90), the program would save 131×10^9 kWh. It would result in reduced demand for 3080 MWe of base load capacity. This would remove the need for two 1100 MWe nuclear power plants and one 800 MWe coal-fired power plant. These power plants would have required $1.2 billion (1974 dollars) of capital outlays and 39,000 man-years of direct and indirect labor.

For the passive solar housing program, we postulate a change in building codes for new residential construction. The code change increases the requirements for insulation and glazing to maximize solar heat gain during the winter and to minimize it during the summer. In addition, we assume the buildings are constructed with the appropriate physical orientation and thermal mass. We assume, based on available data and engineering estimates, that these changes would reduce the cooling and heating load of the house by 60%. The annual natural gas savings would amount to 28×10^6 Btu or 4600 kWh for electrically heated homes. Savings in air conditioning would be 1600 kWh per year. All new housing units (estimated to average 205,000 units per year) are assumed to meet the revised code which would result in incremental annual savings of 3.1×10^{12} Btu of gas and 380×10^6 kWh of electricity. The capacity savings would amount to 4200 MWe by 1991. These capacity savings would result in reduced demand for $510 million (1974 dollars) of capital outlays and 13,500 man-years of direct and indirect labor. The passive solar program would require no additional direct expenses, but would require 9000 man-years of indirect labor.

The third conservation measure, retrofit ceiling insulation, calls for upgrading the ceiling insulation to R-19, in that portion of the existing housing stock that are insulatable. If this measure were implemented, the annual savings by the end of the program would be 100×10^{12} Btu of gas and 440×10^6 kWh of electricity. The gas savings accumulated by the passive solar housing and retrofit ceiling insulation programs would negate the need for two synthetic natural gas (SNG) plants. These two plants would need $1.5 billion (1974 dollars) and 56,000 man-years of direct and indirect labor for construction. The retrofit insulation program would call for $760 million (1974 dollars) and 23,000 man-years of direct and indirect labor.

The three measures would obviate 3080 MWe of baseload capacity (two 1100 MWe nuclear plants and one 800 MWe coal plant), 4200 MWe of peaking capacity, and two SNG facilities. Together, these measures would reduce the demand for capital by $3.2 billion and the demand for labor by 109,000 man-years. The three measures on the other hand would need $760 million and 32,000 man-years of labor.

Several important limitations of this study should be kept in mind. First, there are limitations in terms of both accuracy and availability of data. The uncertainties in facilities construction data range from ±10 to ±50%. Data on new technologies and energy conservation measures are even less reliable. Secondly, we have assumed linearity in both energy supply processes and in economic structural relationships. These assumptions do not take into account economy-of-scale considerations or improvements in technologies that may take place over time. Finally, the temporal, geographic, and system boundaries imposed in this study precluded a broader analysis of the impacts. Such an analysis could alter the magnitude of some of the results.

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