Basic Research Needs in Seven Energy-Related Technologies

- *Conservation*
- *Conversion, Transmission & Storage*
- *Environmental*
- *Fission*
- *Fossil*
- *Geothermal*
- *Solar*

Published July 1980

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U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences

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BASIC RESEARCH NEEDS
IN
SEVEN ENERGY-RELATED TECHNOLOGIES

- o CONSERVATION
- o CONVERSION, TRANSMISSION & STORAGE
- o ENVIRONMENTAL
- o FISSION
- o FOSSIL
- o GEOTHERMAL
- o SOLAR

STUDIES PERFORMED FOR THE DEPARTMENT OF ENERGY
OFFICE OF BASIC ENERGY SCIENCES

JULY, 1980

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FOREWORD

The reports contained in this document outline research needs in the various energy technologies and have been extremely useful in developing the agency R&D plans. The Director of Energy Research has the responsibility to advise the Secretary of Energy on the physical research programs and to monitor the R&D with respect to any undesirable duplication or gaps in these programs. This document has already played an important role in the research planning within DOE. I have asked the respective laboratories to expand the content to include the applied research and exploratory development research needs. This information is being incorporated in the DOE technology base assessment. The technology base assessment covers basic research, applied research and exploratory development; it provides essential information as to the needs for research required for the orderly development of our energy technologies. I encourage the readers of this document to provide us with their suggestions so that we can make continued improvement in subsequent studies.

Edward A. Frieman
Director of Energy Research

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INTRODUCTION

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Any administrator of basic research at a mission-oriented agency, such as the Department of Energy (DOE), is constantly confronted with the questions: Which scientific disciplines are most relevant to the agency's mission? Within those disciplines, which specialized areas deserve particular emphasis? What should be the relative priorities assigned to research activities in the various areas?

Those are not abstract questions. Every year they translate into decisions involving millions of dollars in research funds, decisions with serious, long term implications.

How are the choices made? After all the reports from all the advisory committees and panels of experts have been received and studied, the decisions are invariably made by single individuals, each using his best judgment based on the best information available.

It was with the thought of providing the decision makers in basic energy research with an input which they may find helpful in establishing research priorities that the present study was undertaken. It was felt that for an energy science administrator, it is most important to know how do *active researchers in various energy-related technologies* perceive the needs for basic research support in their various areas of endeavor. The emphasis is worth noting: The perspective of this study is not that of a technology program manager, informed as it may be; nor is it the perspective of a basic scientist, insightful and inspiring, as it may be. It is, to repeat, the perspective of an *active technologist*.

The present volume comprises seven studies, performed by seven groups at seven national laboratories. The laboratories were selected because of their assigned lead roles in research pertaining to the respective technologies.

The researchers who undertook the studies were requested to solicit views of other workers in the fields. Thus, each study should reflect, in some measure, not only the views of its authors, but also those of others, especially workers at industry and universities. Furthermore, the authors were requested to indicate, if possible, the relative priorities of the

various research areas discussed. Some did not do it: they found such judgments too arbitrary. Those who did, invariably stressed the subjective and uncertain nature of "prioritization."

As a first exercise of this type, the study is far from being all-encompassing. Not all technologies are included. The depth of analysis and the degree of detail vary from report to report, as does the number of contributors. Certainly future studies will improve on those and other aspects of the present assessments.*

By now it should be clear that the views expressed, opinions voiced and priorities assigned in these studies do not necessarily reflect the positions of the Department of Energy. Still, they appear to represent the thinking of a good size sample of the technology development community and therefore are certainly worthy of close attention.

In the course of the study, well over one hundred -- perhaps closer to two hundred -- individuals contributed to the reports by submitting their inputs, reviewing and revising the drafts, etc. Some contributions are acknowledged in the reports, but there were many more. On behalf of all of us at the Office of Basic Energy Sciences, I want to thank all the individuals: authors, contributors, reviewers and others, involved in the preparation of the reports, for the effort they put in to make the study a meaningful and useful endeavor. I know it already had an impact on DOE research planning. I hope it will have more in the future.

* The reader is encouraged to send, to the attention of this writer, any comments on issues related to the present report, including the issue of priorities.

BASIC RESEARCH NEEDS

IN

ENERGY CONSERVATION

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October 1, 1979

I. WHAT IS ENERGY CONSERVATION?

While energy conservation has come to have many political, social, and environmental connotations, the most important reason to find ways to use energy more efficiently is that, on the average, it now costs considerably less to save a unit of energy than to produce one from new supply (1-3). To the extent that presently non-quantified social and environmental costs (externalities) are also included in the accounting, the impetus to use energy efficiently would be even greater. Energy conservation is thus the economically efficient societal response to the rising cost of energy relative to other resources. The overall goal of conservation is to enable society to accommodate future demands for goods and services with minimum total costs, including energy and resources.

Under the general rubric of energy conservation we include the following societal responses:

1. Responses by which existing energy-using equipment and processes are gradually replaced with more-energy-efficient ones. To bring about this replacement, other resources of lower cost are substituted for energy. The substitutes include capital, labor, materials, information and, above all, human ingenuity. Development of new equipment and processes requires time -- in some instances only a few years, in others decades or more -- and is subject as well to a variety of non-economic constraints. This class of responses does not involve change either in short-term consumer behavior or in the long-term level or mix of consumer amenities and activities (i.e., no life-style change).
2. Responses that involve short-term changes in consumer behavior towards important energy-intensive activities. These changes are induced primarily by higher energy prices. The consumer continues to use existing capital equipment in the short term, but reduces the amount of use, in the judgement that this is less costly than investment in new, more efficient equipment. Examples are: reduced use of hot water, less driving, lower settings of

thermostats in winter and higher settings in summer.

3. Responses that involve long-term structural changes in the economy that produce a less-energy-intensive mix of consumer activities. Such changes may either come about as a result of energy conservation or themselves be a cause of energy conservation. They would be brought about, in the first case, by relative energy price increases and government regulations; in the second case, by changing social values affecting consumers' tastes and preferences in consumption, location, and occupation (4).

The combined impact of these responses to higher prices and government policy will be a lower growth rate of energy use than would otherwise be the case. But, how much lower? An assessment of a wide range of energy futures made by the National Academy of Sciences CONAES study indicates that a serious national energy conservation program, implemented gradually and consistently over the next two to three decades, could reduce energy consumption by 2010 (in relation to gross national product) to about 60% of what it would be in a "business as usual" future (1-3). For example, in the case where 3% average annual GNP growth is assumed, total U.S. energy use in 2010 was projected to be around 115 quads for a high-conservation scenario, in contrast with around 190 quads for a "business as usual" demand scenario for 2010. This corresponds to a potential "saving" of 75 quads, which is equivalent to the total present U.S. energy consumption.

The energy supply analyses done by CONAES show a similar differential: in a "business-as-usual" future, the U.S. domestic energy supply system will probably produce only about 75 quads* in 2010, whereas a national program committed to enhanced supply production could deliver around 150 quads (5).

Thus, the potential overall impact of a vigorous energy conservation program is similar to that of a vigorous energy supply program. Since neither energy supply nor energy conservation goals are likely to be fully met, the nation needs both elements as partners in its energy program. Indeed, energy conservation should be considered as the equivalent

*primary resource input equivalent

of an energy supply system: every quad saved by use of a more efficient technology or practice is equivalent to a quad that does not have to be supplied by an existing or new supply technology. And conservation has the advantage that it generally involves lower environmental costs than supply systems and renders the economy more resilient to supply interruptions.

II. GOVERNMENT RESEARCH IN ENERGY CONSERVATION

In this section, we develop these themes:

1. The role of research in energy conservation.
2. The role of government in conservation research.
3. The role of basic research in conservation.

Why energy conservation research? If we accept the strictly economic definition of energy conservation as a rational response to higher costs of energy, should not the market place alone be able to handle the inevitable adjustments? In a "perfect" economic market, energy prices would reflect the true total costs to society of supplying and using energy. Consumers would have perfect information about those costs, and would spontaneously adjust the nature and magnitude of their purchases to the lowest total cost for each amenity desired. The commercial sector would include energy costs as one of the relevant factors of production, and would make appropriate investments in R&D to bring about cost-effective increases in efficiency of energy converting-and-using equipment and processes. The time involved in bringing about these adjustments would be socially optimum.

In fact, none of these situations obtains. The energy market is far from ideal; its natural workings are inconsistent with U.S. national security; and the economic adjustments take too long. Domestic and international political forces have produced an energy market with a price structure very different from what it would be if it had been determined entirely by economics. Although the price structure is changing, future trends in regulation and in foreign supplier policies are uncertain. Social and environmental costs are not fully included in energy prices as they would be in an ideal market, and there is great uncertainty as to how they can be evaluated and internalized. Consumers generally do not have adequate information on energy costs and cost trends, and do not know how to relate these to decisions on purchases. Balancing increasing domestic demand in the face of diminishing domestic supply by ever-growing dependence on imports may be workable from a market standpoint,

(at least in the short term), but it is not consistent with U.S. national security, both because the extent of imports contributes directly to inflation, and because most of the imports originate from politically unstable regions of the world. Therefore, acceleration of energy conservation has an important national security value. Finally, experience has demonstrated that the energy-conservation response of private-sector institutions is excessively slow because of the many uncertainties of the energy market. This inertia is a matter for public concern because of the very long lead times required to develop and deploy long-term energy supply systems and because of the formidable problems faced by the available short-term supply alternatives to oil and gas.

Research in energy conservation is necessary to help mitigate all of these market shortcomings, to catalyze the taking hold of conservation. Technical research can accelerate the introduction of innovative ideas and technological options as substitutes for energy use. Environmental research can help ensure that proposed conservation measures adequately protect public health and safety, and can assess the level of environmental benignity of conservation solutions in comparison with equivalent energy supply alternatives. Social research can provide the framework for developing institutional mechanisms to accelerate the implementation of energy conservation practices and technologies.

Energy conservation research can thus contribute in essential ways to slowing the growth in energy consumption, and providing valuable time needed for solving the many problems accompanying the development of long-term sustainable energy systems. An important specific benefit of conservation research is to reduce uncertainties in our estimates of future energy demand, or, stated another way, to increase our confidence in assessments of the implications for future energy prices and energy demand of today's trends and decisions. To the extent that these uncertainties can be reduced, planning for the development and allocation of alternative energy supply resources and technologies can be done in a more economically efficient way.

Why government research? As the cost of energy rises, more and more investments in increasing the productivity of energy use will become profitable. Where there is a clear potential for nearterm payback from investments in improved efficiency of products or processes, private industry can usually be expected to sponsor the requisite applied research, as well as subsequent development and commercialization efforts. This is especially true where unique skills or manufacturing facilities are possessed by particular firms. Normally, government should not compete with industry in doing short-term, low-risk applied research. The principal role of government research should be to keep informed on the state of the art. If it appears that a stimulus is needed for industry to move as quickly as is warranted by societal need or commercial opportunity, government should sponsor the needed research, in collaboration with industry if possible. Examples where DOE laboratories are playing a key role in applied research, working collaboratively with industry, are in the development of heat pumps and energy-efficient windows and lighting.

A class of research problems intermediate in character between short-range applied research and fundamental research pertains to problems which, although related to specific technological goals, either do not show sufficiently high probability of early economic return to industry or have an inherent time horizon beyond that normally considered by industry. The responsibility for such applied research usually falls to government; nonetheless, the work is best carried out in close coordination with industry in order to facilitate the transfer of results when the work reaches a stage appropriate for industrial interest. Activities of this kind constitute the major missions of the various DOE technology divisions; in conservation, they are conducted under the auspices of the Assistant Secretary for Conservation and Solar Applications.

Why basic research? Fundamental long-term research in many sciences has traditionally been supported by government simply because it is in the nations's interest to do basic science and such studies are beyond the reach of most private capital. Opportunities abound in energy conservation for rich rewards in the long term, yet basic conservation research has had a slow start because of the widespread, yet erroneous, impression

that most conservation goals are short range. In fact, a dedicated and continuously supported public program of basic research in energy conservation could have a major positive impact on the nation's long term energy future by facilitating the emergence of a high-efficiency, low-energy use society which will be much easier to supply from the high-cost energy technologies of the future than would be a society extrapolated from today's low-efficiency, high energy use.

J. H. Gibbons has stated well the ultimate challenge to energy conservation: "To what extent can man substitute ingenuity for resource consumption?" (6). Basic research in energy conservation is largely addressed to this question. The following are major goals:

1. Obtain a sufficient foundation of physical, chemical, and biological knowledge to make possible the economic development of future energy-efficient conversion and end-use technologies. Learn how to accomplish tasks that require energy, in entirely new ways rather than by incremental improvements to existing ways. Most of today's uses of energy are far from the limits of efficiency imposed by physical laws; basic research should aim to "constantly roll back the limit to efficiency that is compatible with a given energy price." (6)
2. Gain a greater fundamental understanding of how energy is used in this and other societies, in order to reduce uncertainty in assessments of future energy demand and to facilitate the transition to an energy-efficient society. Greater knowledge is needed of how energy use responds to price signals from the market and non-economic signals from government and social groups, and of how these responses affect social equity, civil freedoms, environment and health, national security, and the levels and time-scales of energy-supply development.

The second goal bears some elaboration. Traditionally, energy research and policy has made little use of the social sciences and, conversely, little social science research has been done on problems related to energy. It is clear, however, that there are fundamental unknowns about the human dimensions of the energy problem: impacts of energy use on people, and impacts of how people live on energy use.

Past research efforts have been too few and usually done in an ad-hoc fashion in support of or opposition to particular policies or technologies. Such investigations should be elevated to the level of basic research into the interaction of energy and society.

The following sections are devoted to a discussion of areas in energy conservation where basic research is needed. This presentation makes no pretense to be exhaustive nor even completely uniform; some topics are described in much more detail than others. What it does do is provide important examples in each identified category of research need. It was beyond the scope of this initial effort to review or provide commentary on ongoing programs of the Office of Basic Energy Sciences, relevant to energy conservation, or to set priorities for the support of further research. These tasks should be done.

III. RESEARCH NEEDS: PHYSICAL AND ENVIRONMENTAL SCIENCES

The expected increasing price of energy in the coming decades will in principle provide many economic opportunities for increasing the efficiency of energy use. Great uncertainty exists throughout the economy, however, in the levels of efficiency that are technically achievable at given energy prices. It is extremely important that these uncertainties be reduced by research, so that short-term energy supply production targets can be set at realistic levels, and better assessments made of our probable long-term energy requirements.

The major goals of the basic research described in this section are increasing the technical efficiency and environmental benignity of energy production and use. These long-range studies would explore the fundamental causes of energy inefficiency and the achievable limits to energy efficiency; the complex coupling between energy efficiency and pollutant formation; the matching of energy quality and technological scale with characteristics and requirements of energy use; the substitution of new ideas for existing technologies. The research needs run the gamut of disciplines and potential applications.

A. Industrial Processes

Research is needed in a number of areas, some of major scope. Optimal changes to improve industrial productivity are often multi-purpose, so certain areas not specifically focused on energy may well have the greatest impact on energy. Many long-existing areas of study have been relatively neglected in modern research. For example, fundamental research on basic materials processing (such as paper and steel) and exploration of new basic materials processes are needed. Basic mechanical studies should be carried out on friction and lubrication, control of fluid flow, and (at the microscopic level) fundamentals of separation of materials by processes such as osmosis or adsorption. Heat transfer should be more deeply examined, e.g., at surfaces, in boiling, and in two-phase flow. Studies of sensors are needed, to facilitate application of automatic control systems.

The processes for coal conversion to synthetic fuels currently under development themselves consume an appreciable fraction of the energy content of the coal used (7). In the process industries generally, up to 50% of energy consumption has been estimated to result from inadequate process control (8). Study of process efficiency is therefore important from an energy conservation standpoint. In particular, studies are needed of catalytic mechanisms relating to less severe and more selective reaction conditions for coal liquefaction and gasification. Less severe conditions mean lower temperatures and more energy-efficient processing. For in-situ conversion processes, studies should be made of fluid flow in porous media of low void fraction. Control and dynamic interactions of complex, highly integrated process systems should be studied, in order to devise ways of achieving favorable process dynamic interactions in such systems. Also, more extensive use of heat exchange and other energy-integration methods in processes can be facilitated by more effective control.

For direct coal use to be able to develop in an economically and environmentally acceptable manner, flue-gas desulfurization processes must be improved. Many processes have been proposed but assessment, utilization and improvement of most is held back by lack of knowledge of fundamental chemistry or mass transport mechanisms (9). In the chemical and food-processing industries, at least 80% of energy consumption takes place in separation processes. There is need for energy-efficient alternatives to presently used vaporization methods (distillation, evaporation, drying), which are particularly energy intensive yet widely used because of their simplicity (10,11). Efficiencies of material contacting devices need to be better understood and improved. In particular, gas-to-gas heat exchangers are very inefficient. Vapor-liquid contacting devices are poorly understood and consequently often over-designed and energy inefficient (8,10).

Several percent of the total U.S. energy consumption is attributable to electrochemical processes, offering a major opportunity for energy conservation by efficiency improvements. These processes are used for preparation of metals and chemicals, and for the storage of energy. Electrochemical processes have the potential for considerably higher energy efficiency, but this potential has not been achieved in spite of

the long history of economically significant industrial applications. A major reason for this is the complex nature of transport phenomena in ionic media as they relate to the charge transfer processes at electrode surfaces. Although there have been rigorous methods introduced recently in the analysis of the processes, further research is required to improve their efficiency. Electrode geometry, surface potential, boundary-layer control, and non-aqueous ionizing media should be investigated, and corrosion-resistant materials developed for use in electrochemical cells. This research could have major impacts on the efficiency with which important industrial electrolytic processes can be carried out and in the development of very efficient batteries for energy storage purposes.

B. Combustion Systems

In order to develop and evaluate conservation strategies involving fossil-fueled combustion systems, both their costs and their environmental impacts should be considered. Before the recent sensitivity to environmental concerns, combustion systems were reasonably well optimized for minimum fuel and capital costs. Today, in the face of escalating fuel costs, this optimization must accomplish simultaneously higher fuel efficiency and increased control of combustion-generated pollutants. Nitrogen and sulfur compounds, particulates in various size ranges and unburned fuel must all be controlled ultimately, and further regulations may be expected for presently uncontrolled pollutants. This problem involves complex and poorly understood chemical and fluid mechanical phenomena. The special demands on combustion-system design posed by this complexity cannot be addressed by standard engineering methods, but only through a deeper understanding of the basic chemistry and mechanisms of combustion.

The example of the diesel engine illustrates the problem. The diesel is one of the most efficient internal combustion engines and also meets present emission standards for mandated pollutants -- CO, HC, and NO_x. However, under normal operating conditions diesels produce carbonaceous soot particles with an emission rate approximately 30 times

that of equivalent internal combustion spark engines (12). Thus there is uncertainty about the desirability of increasing the diesel mix in mobile traffic, even though such a policy would be reasonable from conservation considerations alone. Further research is essential to characterize the particle emissions of diesel engines as a function of combustion parameters in well-controlled laboratory conditions, and to work out strategies for mitigating these effects. For the characterization of particle emissions, combustion nuclei and gases, in-situ-on-line monitors need to be developed and a wide range of analytical techniques brought to bear on the problem.

Another focus of combustion research should be on coal, which is likely to become increasingly utilized. Better understanding of the chemical and physical phenomena involved in coal combustion, gasification and liquefaction is needed, and problems of safety should be given increased attention. In particular, research is needed on the chemistry of coal combustion reactions, including the rates and mechanisms of reactions leading to release of heat and generation of pollutants. Both gas-phase and surface reactions need study. The coupling of combustion heat release and pollutant chemistry to turbulent fluid mechanisms should be investigated. Studies of flammability, flame spread, and toxic-gas generation should be included. To facilitate identification of chemical species in the investigations of high-temperature kinetics and turbulent fluid mechanics, a variety of new diagnostic instrumentation is required.

C. Energy Storage, Conversion, and Transmission

As the prices of fossil fuels continue to rise, advanced energy conversion processes designed to conserve fuel and to use the thermal values from waste streams will become economic. The three main paths to high thermal efficiency in advanced energy conversion are:

1. higher topping-cycle temperatures;
2. development of combined cycles using several different cycles, each operating at its best temperature range;
3. development of highly efficient fuel cells.

An example of the first and second paths is combined-cycle power plants using gas-turbine and steam-turbine components. An efficient magneto-hydro-dynamic (MHD) power plant will also be a combined-cycle plant. An example of the third path is fuel-cell development for megawatt-size efficient power plants. Many important basic research problems are connected with these developments, including the development of materials of appropriate properties and costs, and the study of environmental impacts associated with obtaining and using these new systems.

In fact, materials problems are of central importance in almost all energy technologies. Materials that would permit conventional fossil or nuclear fueled boilers to operate at even slightly higher temperatures -- hence efficiencies -- could have dramatic economic consequences; inner wall materials problems may be among the most serious to be encountered in progress central in the development of solar energy technologies. Costs and reliability are among the major issues. There are many areas for important basic research in metals, ceramics, refractory and resistant materials, corrosion, high-temperature performance and in thin films of particular importance in solar work. Basic solid-state research, including studies of both crystalline and amorphous semi-conductors, is very important for the development of advanced energy conversion systems.

Research should aim at developing conversion processes that best match future fuel supplies, for example, the substitution of electrochemical or photochemical processes for current thermal chemical processes, so that more appropriate and efficient use can be made of electricity and solar energy than simply as heat sources.

Progress in the technology and economics of long-distance transmission of electric power may alleviate the problem of power-plant siting by increasing the distance between plant and consumer, and possibly by co-locating several plants to concentrate the safety problem and introduce economies of fuel handling or reprocessing.

The possible wide application of hydrogen as a carrier and secondary source of energy in the future requires solution of many fundamental chemical problems relating to its storage, transmission, and use. Basic electrochemical and thermochemical studies are also required to build

a foundation for development of improved batteries.

One example of an important basic research area is investigation of the use of underground aquifers as a low-cost method of storing a large amount of thermal energy, to compensate for the time mismatch between periods of energy input and power demand in large energy systems (13). Early work in numerical modeling demonstrated the feasibility of the concept. Although several DOE demonstration projects are planned, important basic research is necessary to understand the physical and chemical processes involved and to study various possibilities associated with the concept. In particular, equilibrium and kinetic data are needed for geochemical reactions at higher temperatures. Physical processes that may affect storage efficiency need to be studied; these include thermal dispersion due to aquifer inhomogeneity and thermal front tilting from buoyancy flow. Studies need to be made of optimal aquifer characteristics and storage periods and cycles. Major work must be done to improve modeling capability in incorporating ground surface temperature and rainfall conditions; this is relevant to proposals for use of shallow aquifers, which have the advantage of lower cost but the disadvantage of being more affected by surface conditions.

D. Buildings

With proper building design or retrofit, it is possible to save at least half of the energy needed to heat and cool a typical building. Since the buildings sector consumes 36% of total U.S. energy consumption, the potential savings from conservation in buildings is substantial. To achieve this potential, better understanding is needed of the factors contributing to energy use, including design components (e.g., windows, envelope, insulation) and construction factors (e.g., air infiltration). The principles of energy- and optically efficient lighting are poorly known. Improved theoretical methods for modeling energy use in buildings are required as a prerequisite to the design of enforceable building performance standards.

The development of more efficient heat pumps, including designs with thermal activation for use with solar systems, is very important

to increasing the energy efficiency of buildings. Better concepts for hot and cold storage systems are also needed. Research is needed to increase the energy efficiency of total communities, including studies of community heating and cooling systems.

Improvements in energy-efficiency of buildings by technical innovations in energy conservation are intimately related to the use of both active and passive solar energy concepts and designs. It is very important that research, development, and demonstration programs in energy conservation and solar energy for buildings all be closely integrated.

One example that illustrates this close connection is research into control of solar heat through windows. Existing methods include mechanical shutters, blinds, drapes, and shades, as well as non-operable devices such as reflective coatings and heat absorbing glass. The latter sacrifice operability but are easier to retrofit, having no moving parts and requiring no special hardware. However, such non-operable devices cannot take full advantage of situations where solar gains are desirable for only part of the year or where increased visible transmission would be desirable during overcast periods. A cost-effective optical shutter with a variable solar transmission ranging from transparent to opaque-reflecting would be a very desirable complement to existing mechanical sun-control options. It is estimated that the energy savings from such a device would justify an added investment cost of \$10/ft².

Research and development of reversible optically active materials is taking place today in diverse fields, and many physical mechanisms are being explored, including photothermochromic and electrochromic materials, liquid crystals, colloidal suspensions, absorption edge shifts, solid state phase transformation, and electrolytic precipitation of metals (14). There are serious problems with most available techniques, and none that are promising can be produced at the fast rate, high volume and low cost required for widespread use, especially for retrofits. Basic research is essential in order to develop and produce a cost-effective device with the proper characteristics.

One promising basic research area is the study of photochromic light absorbing glass of the type used successfully for sunglasses. The mechanism involved is light scattering from silver particles formed by photochemical decomposition of silver halide crystallites. The presence of metal particles indicates the potential to make a device that becomes reflecting rather than absorbing, to avoid reradiation of heat to the interior. Research is necessary to understand better the scattering reflection process. Another problem is incomplete darkening in sunlight due to strong absorption at the peak activation wavelength of 0.35 microns, thus confining the effect to a thin surface layer. If a deposition method can be devised to apply a thin film of photochromic material to glass or plastic, direct transmission could be reduced and less silver halide required..

E. Transportation

Basic research in the transportation sector is needed to obtain knowledge required for development of extremely energy-efficient engines, vehicles, and transportation systems. Included should be fundamental properties of fluids that might be used in advanced engine cycles. As stated above, basic research in many aspects of the chemistry of combustion could lead to design of more efficient and less polluting engines, especially in the case of diesel engines. Engine efficiency can also be markedly improved by the design of "smart" control systems that use advanced microelectronics. Vehicle efficiency can be increased by studies of air drag at operating speeds.

One facet of the potentially great impact of telecommunications is its ability to help moderate transportation energy demand by substituting for travel and by improving the efficiency of transportation energy consumption. In regard to substitution, quantitative data are sparse and the element of causality complex (15). It cannot be ignored that previous growth periods of travel, transportation, and congestion occurred during the burgeoning of telephone and telegraph. In regard to efficiency, the potential impact is less complex, as telecommunications will be able to improve vehicle flow to optimize speed and reduce stop-and-go cycles, indirect routing, and unnecessary repositioning of empty

vehicles. Much more study is needed to examine quantitatively these important potential energy-conserving ramifications of telecommunications.

F. Thermodynamics and Systems Studies

The present U.S. energy system is far from optimized in regard to matching of the type, thermodynamic quality, and unit scale of energy supply with end-use function. For example, about one-third of U.S. electricity supply is used for heating and cooling, functions that do not require energy of such high thermodynamic quality. Both economic efficiency and energy conservation would suggest that energy should be supplied only in the quality needed for the task at hand (16). Competing goals, such as convenience, often work in the opposite direction (e.g., use of electricity for residential heat) and these should be considered in any analysis. Today there does not exist a compendium of energy end-uses, analyzed according to these characteristics. Research is necessary to obtain such correlations and analyses of the energy end-use spectrum.

Basic thermodynamic theory is a subject that can contribute importantly to gaining an understanding of how well real processes can perform when they operate at real, non-zero rates. Thermodynamics research can clarify how closely maximum efficiencies can be approached, and has a great bearing on the future design of engines.

G. Environmental Impacts of Energy Conservation Strategies

Two important avenues to improving the energy efficiency of buildings have been use of more insulation and tightening of building envelopes to reduce air infiltration. These conservation measures could have significant negative impacts on human health. There is, however, little information today regarding either the level of risk involved or practical measures that could be taken to reduce that risk. Basic research is needed in both areas (17, 18).

Indoor air pollution results from emanations of chemical compounds and radiation from building materials, as well as from indoor activities

such as cooking or heating with open gas flames. The level of pollutants was probably negligibly low as long as high ventilation rates were being maintained, but has become of concern since lower rates of air exchange are now being recommended or used as energy conservation measures. Research is needed as background to the development of energy efficient yet environmentally clean mechanical ventilation systems. Materials studies are needed to develop and evaluate suitable heat exchanger media in heat recovery devices that transfer both sensible and latent heat, yet impede transfer of pollutants across the heat exchanger media.

Basic research is also needed to understand the mechanisms of pollutant release from insulation materials and to develop ways to reduce such releases. Urea-formaldehyde is the most common resin used in wood products; research is needed on release of free formaldehyde (and other organics) from particleboard and plywood, and on specific additives to reduce the formaldehyde release. Other bonding techniques currently being considered by the industry (for example, nitric acid under pressure) also need to be studied in terms of chemical characteristics and potential side effects of the pollutants released from the materials employed. Studies should be conducted on emanation mechanisms of radon gas and other contaminants from various building materials (e.g., concrete and brick), as well as from soil and water. An understanding of the health risks of fiberglass insulation is also needed.

IV. RESEARCH NEEDS: SOCIAL AND ECONOMIC SCIENCES

A wide variety of basic research challenges in the social and economic sciences complement those in the physical and engineering sciences. The research agenda described in this section is aimed at increasing our fundamental knowledge of energy use in this and other energy-consuming societies, furthering our understanding of how and why people make the choices they do regarding energy, and facilitating the transition to a more energy-efficient and resource-conserving society. A central problem in energy conservation is the types and magnitudes of impacts on individuals and on society as a whole from measures to reduce the growth in energy consumption. To what extent can energy use be reduced without significant adverse impact on the well-being of individuals and society? Conversely, to what extent can energy conservation activities strengthen the economy? These and similar questions are subject to much controversy, largely because of a lack of information grounded on experience and fundamental studies. The suggested studies do not fit naturally into the present organizational structure of the Basic Energy Sciences Office of D.O.E. Because of their importance, that structure should be broadened to accommodate them.

The following are examples of some important social and economic research needs:

A. Energy Use Data Bases and Systems Studies

It is essential to collect and analyze data on actual energy consumption, highly disaggregated by individual end-uses (e.g., space heating, commercial lighting, automobile use, process heat) to determine current energy efficiency in each sector and to assess how people have actually responded to price changes and energy conservation measures over the last decade. In order to obtain maximum benefits from experience in energy conservation, it is important to obtain comparative data across different regions and countries, and to take into account relevant structural and lifestyle differences among them

as factors influencing total demand. Investigation of the details of energy use in other countries can reveal much about the link between energy demand, conservation, and lifestyle (19, 20). Investigations of time series of energy use across national boundaries (21,22) can give valuable information about fundamental relationships between energy use and the economy, especially in societies where energy prices are higher or lower than in the United States, or where incomes are higher or lower than in the United States. Other countries -- or even different regions within this country -- might serve as useful "laboratories" for the exploration of consequences of changes in lifestyle, energy prices, or energy-related policies.

It is very important for energy policy makers to understand "where we stand" with regard to the impacts and consequences of past energy price levels or increases and existing conservation legislation. Research of the kind described will provide the data bases and analyses to give that information; and should be considered of the highest priority.

B. Energy Use and Evolutionary Social Trends

Some recent studies have suggested that spontaneous changes in patterns of consumption, location, and occupation among Americans may drastically reduce future growth in energy consumption (23). Up to now, such studies have been very preliminary; however, the importance of the questions they raise for future energy planning suggests that they be pursued in depth. In particular, a variety of assumptions about future life styles should be investigated, and, insofar as possible, quantitative assessments made of the impacts on energy use likely to come about from the specified assumptions.

C. Barriers to Energy Conservation

Increasing the efficiency of energy use requires not only improvements in technologies but also changes in the behavior of institutions and individuals. Often it is possible to identify factors that inhibit specific changes. Examples of such barriers include laws and codes

(e.g., obsolete building codes), social norms (e.g., traditional prestige of owning a large car), mismatches between costs and benefits (e.g., master metering in apartment buildings) and poor information (e.g., lack of efficiency labeling, inability to do life-cycle costing). In these cases, strategies can be initiated for overcoming such barriers in regard to specific technologies. However, a fundamental understanding is lacking both of the problem and the proper governmental role in solving it.

- Methods need to be developed for identifying and understanding the basic factors impeding the transition to higher energy efficiency. An example is the identification of individuals and groups who would be most affected by specific conservation measures or who must take action to implement them, assessment of the nature of these impacts and involvements, and investigation of methods by which the interests of such participants can be included in the policy formation and implementation process. Examples of relevant questions are: how are habits regarding use of appliances, automobiles, and other energy-consuming devices formed and changed; how can consumers be motivated and educated to consider life-cycle costs rather than only first costs of purchases; how have consumers actually responded to the changing energy situation of 1973, in terms of identified motivations and specific energy-conserving actions.

The proper relative roles of government and the private sector in implementing energy conservation is an important and controversial question. The government's massive support of R&D helps to overcome economic barriers, but does not ensure implementation. There is considerable uncertainty and disagreement about the efficacy and necessity of government energy-efficiency regulation, such as energy-performance standards for vehicles and appliances, and stricter building performance standards and building codes. Other possible government roles are providing information for consumers, businesses, and communities (e.g., energy extension services). All need study.

D. Socio-economic Impacts of Conservation

Capital, materials, and labor are required for implementation of energy conservation measures that involve change-over to more energy-efficient capital stock. This causes an increase in economic activity. As energy consumption is subsequently moderated by these measures, requirements for energy resources and attendant materials and labor may decrease. These first order effects lead to multistage expansions and contractions throughout the economy, including perhaps effects on interest rates and the availability of financial resources for further investment. The net impacts are likely to vary among conservation measures as well as from broad policies or programs. An understanding of these impacts can assist in the design of economically efficient policies.

For the most part, energy conservation has fewer undesirable environmental and health impacts than supply strategies to provide equivalent energy. At some level of application, however, conservation would give rise to indirect socioeconomic and political effects, mostly through economic adversity, that would predominate over the direct benefits. Current technical and economic analyses suggest that this point is a long way from where we are now, possibly at an E/GNP ratio of 1/3 to 1/2 of present values (1). Because of the extreme importance of this issue, continuing study of the fundamental relationships between energy consumption and economic activity is important. Basic studies in energy/economy modeling are required, and in this connection studies should be pursued of fundamentally important economic parameters such as the long-term price elasticity, substitutabilities of energy demand, and the impacts of energy supplies and prices on productivity.

There is considerable uncertainty about the distributional and equity impacts of energy conservation measures. For example, any measures that directly or indirectly raise energy prices will differentially affect poor people. Distribution should not be used as an excuse to forego conservation, but it must be analyzed so that it can be dealt with by simultaneous compensatory measures.

E. Long-Term Energy Demand

Gaining an understanding of long-term energy demand -- the practical and economic limits to the physical efficiency of energy and materials use -- is an important and neglected element of the energy problem. Basic research is needed that would lead to improving energy-use efficiency in fundamental ways, that would examine the social effects of substituting one means to supply consumer amenities by others, that would look at the relationship of long-term world energy needs to U.S. supply and demand and to the global situation. Fundamental information is needed about possibilities for geographical rearrangement of man's activities, recycling of materials, enhanced product repair and reuse, and the development of extremely energy-efficient structures and products.

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TECHNOLOGY CROSSCUT REVIEW
OF
BASIC RESEARCH RELATED TO THE TECHNOLOGIES
OF
ENERGY CONVERSION, TRANSMISSION & STORAGE

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INTRODUCTION

This paper is a brief review of needed areas of basic research underlying many of the technologies of energy conversion, storage, and transmission. It is a segment of a more general technology crosscut review of basic research related to energy technology carried out by the various national laboratories for the Office of Basic Energy Sciences of the Department of Energy.

At the outset, we wish to emphasize the value to future technological development of basic research that is undertaken not primarily for its relationship to problems encountered in the development of specific technologies, but which is chosen for its potential contribution to more general understanding of various areas of science. In large measure, this is due to our lack of ability to predict the detailed nature of the technologies of the future, which suggests that a wide variety in scientific "capital" is needed for these future developments, and because ideas for the most novel of these technologies will spring from a better understanding of fundamental phenomena. Therefore, a vigorous and balanced program of fundamental research chosen solely for its scientific merits is essential to provide the foundations for the development of future technologies, the outlines of which can be perceived only indistinctly at present.

In the shorter term, there are areas of basic research which can be beneficial to the solution of problems in technologies currently being developed. In the main body of this paper, we briefly discuss such areas of research related to various technologies of energy conversion, storage, and transmission. In the identification of these research areas we have attempted to strike a balance between categories that are neither too general nor too specific. Some important technologies of energy conversion, photochemical energy conversion and the use of turbines to generate electricity for example, have

not been discussed in this paper because they are contained in sections of the review prepared by other national laboratories. We have focussed our attention primarily on problems related to the development of particular technologies and have given only slight attention to research related to the safety of these technologies. Some discussion of such problems is contained in the section of the review concerned with environmental questions. We have included all technological problems that we and our contributors and consultants have considered to be important, but we have avoided assigning relative priorities. We believe that precipitously setting priorities is undesirable and that a proper assignment of relative priority requires considerably more study and a broader consensus that can be obtained within the constraints of time and manpower which exist for this review.

Our sources of information about various technologies and important problems which have arisen in their development have been: published research papers, review articles, and workshop proceedings, together with personal communications, both oral and written, with a number of experts from various national laboratories, universities, and private industry, as well as consultation with some members of the technology divisions of the Department of Energy.

The main body of this report is organized in three sections, discussing research needs in: A. Conversion, Storage, and Transmission of Energy by Primarily Chemical Means; B. Conversion, Storage, and Transmission of Energy by Primarily Electromagnetic Means; and, C. Storage of Thermal and Mechanical Energy. By this method of organization, we discuss together a number of technologies with many common problems. For example, conversion of chemical to electrical energy by fuel cells, conversion of electrical energy to chemical energy by electrolysis cells, energy storage by batteries, and energy

transmission by "chemical heat pipes" have many related problems in chemical reaction kinetics and catalysis. At the end of each section we have a series of general needs in basic research reiterated by flagging to the technologies being discussed.

Consideration of the areas of basic research identified in the various sections reveals the recurrence of several broad areas of basic research. We have also identified some areas in which the support of research is, at present, rather weak. We discuss these topics in a final section which includes a matrix connecting these broad areas of recurring themes in basic research to the particular sections of the paper. Finally, we conclude with an Appendix listing a number of people who have provided us with information and discussion of these topics.

CONVERSION, STORAGE, AND TRANSMISSION OF ENERGY BY PRIMARILY CHEMICAL MEANS

In this section we briefly discuss needed topics in basic research related to energy conversion by fuel cells and electrolysis cells, to energy storage by batteries, to energy storage and transmission by thermochemical methods and by the use of hydrogen and other gaseous fuels.

Electrochemical Systems

Electrochemical systems such as batteries, fuel cells, and electrolysis cells have many common features. Their essential components are electrodes, at which chemical reactions featuring electron transfer take place, separated by an electrolyte which transmits selected ions but not electrons. We shall discuss fuel cells (and, by implication, electrolysis cells) first; many of the fundamental problems of batteries are essentially related.

Of the two electrodes in fuel cells, the behavior of the "air" electrode, at which gaseous oxygen is reduced to ions, is most poorly understood and presents the best opportunity to achieve improvements. This electrode is inefficient, the detailed mechanism of oxygen reduction is poorly understood, and the need for new electrocatalytic materials to replace platinum as the catalyst at this electrode, or in the electrolyte, is of paramount importance. Fundamental studies of the mechanism of oxygen reduction on a variety of well-characterized electrode surfaces in contact with different types of electrolyte (e.g., aqueous and organic solutions, fused salts, solid oxides, etc.) would be of great value. Of particular interest are studies on catalysts other than Pt, such as electronically conducting oxides, organometallic compounds, alloys, etc. The behavior of the "fuel electrode," especially when the fuel is hydrogen, is better understood. However, mechanistic studies will still be of value, and a detailed understanding of how electrocatalysts are poisoned by CO, H₂S, etc. in impure fuels is still needed.

Many of the problems occurring in connection with electrode reactions in "advanced" battery systems, especially those utilizing the reduction of O_2 , Br_2 , Cl_2 , etc., are similar to those described above for fuel cells and areas of needed basic research are the same. In addition, studies of the physical and electronic properties of non-metallic electrode materials, such as FeS , $NiOOH$, etc., and unconventional electrode materials (e.g., intercalation compounds; alkali metal solutions in tungsten bronzes, etc.) and the relationship of these properties to electrochemical behavior would be of value, as would detailed studies of electrode reaction mechanisms and kinetics in well-characterized model systems related to concepts for advanced batteries.

The importance of using well-characterized electrode surfaces and electrolytes in such studies must be strongly emphasized, since lack of such characterization has been the origin of much ambiguity in the past. The aim of such research should be the elucidation of reaction and charge transfer mechanisms, kinetic behavior, etc., and their relationship to atomic and electronic structure of the interface, and in some cases, three-phase interfaces. Improved methods for studying and improvements in the theoretical framework for describing the structure and properties of electrode-electrolyte interfaces are greatly needed; new developments in ellipsometry, the use of EXAFS, Raman spectroscopy, infra-red reflectance, etc., for this purpose should be encouraged. Studies of interfacial phenomena combining modern electrochemical techniques such as voltammetry with such structural and spectroscopic characterization are greatly needed.

At present, fundamental studies of heterogeneous and homogeneous catalysis are being pursued vigorously. Theoretical studies should be conducted to elucidate the relationship of the results of such research to problems in electrocatalysis.

The morphological stability of electrodes and catalysts is an important constraint in electrochemical systems; for example, there are currently problems associated with sintering of dispersed platinum catalysts and with the dendritic growth of zinc electrodes. Studies of the nature of the interaction between dispersed microcrystals and their supporting substrate are desired, both with regard to the stability of the dispersion and with regard to the effect of such interaction on the catalytic properties themselves. Studies of the nature, on a microscopic scale, of electrocrystallization and dissolution are needed. (Only very recently have modern electron microscopical techniques been applied very fruitfully to this problem in lead-acid batteries, rather late in the two-hundred year history of this system.)

Fundamental studies of structure and other factors which influence rates of mass transport, degree of ion selectivity, and related properties of electrolytes are needed. Of special interest are non-aqueous electrolytes, molten salt systems, and solid electrolytes. Solid electrolytes have many attractive features, among them compactness and stability. If a stable solid electrolyte could be discovered which is capable of transporting either protons or oxygen ions with high mobility in the temperature range 200-400°C, where an optimum balance exists between thermodynamic factors, such as cell voltage, and the kinetics of electrode reactions, the design and use of fuel cells would be revolutionized. Similarly, suitable proton, lithium, and sodium ion conductors would make great impact on the development of batteries. Solid electrolytes suitable for use at temperatures of 1000°C are needed for the production of hydrogen in high-temperature water electrolysis cells, and a wide variety of fundamental studies of the electrical, mechanical, and chemical properties of electrolytes is needed to support such development. There are currently many basic studies of crystalline "superionic" conductors, which hold great promise

for this high temperature application, and extension of this type of research to cover mass transport in polymer membranes and inorganic ion-exchange membranes would also be valuable.

The task of designing and efficiently testing electrochemical systems would be greatly assisted by the existence of analytical models describing various electrochemical processes. The development of such models requires both adequate theories of the processes and the expression of these theories in a sufficiently simple and flexible form to permit their efficient use in models of complex systems. Continued research in the theory of electrochemical processes is needed to attain this goal.

Finally, the problems of corrosion, materials incompatibility due to solid state reactions, and mechanical instability which arise in the harsh environments encountered in electrochemical (and thermochemical) systems are not trivial; their solution is often the critical factor in bringing a system to technological maturity. Fundamental study of these topics, particularly at high temperatures, is needed, yet such studies are often considered as something of an afterthought. For example, there is comparatively very little basic research on the mechanical properties of superionic conductors, although fracture and creep of the beta-alumina electrolyte is an important factor limiting the lifetime of the sodium-sulfur battery; the mechanical properties of polymer membranes also should be studied.

General Needs

- o The fundamental nature of electrode processes should be studied using a variety of well-characterized electrode surfaces and electrolytes, with particular emphasis on characterizing interfacial phenomena.
- o The relationship between the mass and charge transport properties of

both solids and liquids and their atomic and electronic structure should continue to be studied by a wide variety of techniques.

- o Development of theoretical descriptions of electrochemical phenomena should proceed in tandem with experimental studies, as should the development of instrumental techniques.
- o Mechanisms of catalysis and of catalyst degradation and poisoning should be studied.
- o The physical and mechanical properties of materials exposed to harsh environments, the mechanisms by which these are degraded by environmental interactions, and the relationships of these properties to structure and composition should be established.

Thermochemical Systems

Schemes for the thermochemical storage and transmission of energy involve carrying out a chemical reaction at high temperature, then "turning off" the reaction by removing the catalyst, cooling the system, or separating the products, etc. The deactivated products are then stored or transmitted elsewhere (i.e., acting as a "chemical heat pipe") to be recombined, with the evolution of heat, at a different time or place. There are many reversible chemical reactions in the solid, liquid, and gas phases which are potentially useful for such applications. Some examples of reversible reactions are thermal decomposition reactions (e.g., $\text{CaO}/\text{Ca}(\text{OH})_2$), solution/dissolution reactions (e.g., dilute H_2SO_4 /concentrated H_2SO_4) and catalyzed reactions (e.g., SO_3/SO_2). An example of another type of thermochemical storage is afforded by various chemical cycles proposed to use reactor heat to dissociate water into hydrogen and oxygen. Fundamental studies of factors influencing the mechanisms, kinetics, and reversibility of interesting systems would be of value. Heterogenous catalysis plays a critical role in this technology; a continuing

vigorous program of basic studies on this subject will be of great value. Studies of the factors which influence ion selectivity and atomic mobility in ion-exchange and semi-permeable polymer membranes will contribute to the solution of the problems of efficiently separating the reaction products.

General Needs

- o Fundamental studies of the factors that influence the kinetics and thermodynamics of candidate thermochemical processes are needed, particularly heterogenous catalysis.
- o Detailed studies should be performed to determine the relationships between the composition and structure of membranes, particularly polymeric membranes, and of factors which influence their selectivity and permeability.

Storage and Transmission of Hydrogen and Other Gaseous Fuels

Because of the wide variety in the means of its production, its versatile and non-polluting character as a fuel, and because it is easily stored and transported, hydrogen has been widely promoted as an energy carrier. Transmission of hydrogen gas is thought to be preferable to electric power transmission for distances greater than 500 miles, and it is a convenient secondary source of energy (the concept of the "hydrogen economy"). There are a number of topics in basic research which are needed to support the development of this technology; several of these topics are also relevant to the storage and transmission of gaseous (at room temperature and atmospheric pressure) hydrocarbon fuels, such as natural gas and related fuels.

Such fuels, and hydrogen as well, can be and have been stored and transmitted as gases and liquids. Although this is a rather mature technology, there remain some nagging problems, one of the most important being the catastrophic fracture of pipelines and storage containers. Although

there is a long history of study and much empirical lore exists on two of the primary areas of difficulty--stress-corrosion phenomena and hydrogen attack and embrittlement--the fundamental nature of these processes is still far from clear. Basic research, theoretical as well as experimental, on well-characterized and not-too-complex systems, using modern microanalytical techniques, would be of great value in seeking solutions in a more efficient manner than the rather "Edisonian" approach employed at present.

It is thought that the mode of storage for hydrogen to be used in large-scale energy systems will be, as it is today for natural gas, in natural geologic formations or man-made caverns. Successful application of such natural reservoirs requires more knowledge of the flow characteristics of hydrogen and other gases, as well as of gas-liquid mixtures, in general within rock structures and other porous systems. Furthermore, studies of the fundamental aspects of the mechanical behavior of minerals and rocks will help to improve the methods of creating and modifying underground caverns for use as storage reservoirs.

One of the attractive features of the use of hydrogen as a fuel, especially in applications to transportation, is the possibility of storing it in a very densely-packed state in the form of a reversibly formed and decomposed hydride. (The density of hydrogen packing in most metal hydrides exceeds that of liquid hydrogen and, in some cases, that of solid hydrogen.) The ideal hydride for such applications would have a high retentive capacity for hydrogen, a relatively low temperature of dissociation, preferably less than 100°C, have a low heat of formation, exhibit a minimum amount of hysteresis in the pressure-composition-temperature relations, have good kinetics of absorption and emission with good resistance to poisoning by impurities, and, of course, be light in weight and inexpensive. Obviously the ideal hydride has not been

found. Some basic research which can contribute to achieving this ideal is as follows. A vigorous program of studies elucidating the relation of atomic and electronic structure to hydride formation and to equilibrium pressure-composition-temperature relations in a variety of systems is needed. Theoretical research on an upper limits to the density of hydrogen packing in intermetallic compounds would be helpful. Since reaction rates are often the limiting factors, the kinetics must be characterized and understood. Fundamental studies are greatly needed to clarify the relationship between both the surface and bulk characteristics, such as electronic structure, defect structure, surface segregation and inhomogeneity, presence of impurities, etc., and the kinetics of hydrogen uptake and release. As usual, the need to use well-characterized systems is of utmost importance. There is also great need for improved techniques for the study of surfaces in "real" as well as in ultra-high vacuum conditions. In addition to continuing such studies on metallic systems, extension of fundamental studies to less "traditional" hydrides such as inorganic salts, zeolites, etc. is to be encouraged, and fundamental studies of the behavior of hydrogen in glass are important to support the development of glass microspheres as a hydrogen storage and transport medium.

General Needs

- o A better understanding of the fundamental nature of stress-corrosion phenomena and hydrogen attack and embrittlement of metals is needed.
- o The detailed relationships between the thermodynamics and kinetics of metal hydride formation and decomposition, on the one hand, and properties such as the atomic and electronic structure of the metal (and hydride), its defect structure, impurities, etc. are still not well understood. More experimental and theoretical work, particularly in well characterized systems, is needed.

- o Basic studies of the fluid mechanics of gases and gas-liquid mixtures are needed, particularly of flow in porous media.

CONVERSION, STORAGE, AND TRANSMISSION OF ENERGY BY PRIMARILY ELECTROMAGNETIC MEANS

In this section, we will briefly discuss topics in basic research related to the conversion to electrical energy by magnetohydrodynamic and thermionic methods and to the transmission and storage of electrical energy.

Magnetohydrodynamic (MHD) and Thermionic Energy Conversion

In its essence, MHD conversion consists of creating a high-velocity plasma and directing it between electrodes in a strong magnetic field. Its principle, discovered by Faraday, is that when a conductor moves across a magnetic field a voltage is induced in it which produces an electric current. (The current emphasis in MHD development for civilian applications is on the coal-fired open-cycle converter to serve in a topping cycle for a conventional steam generating plant; we will not consider here the problems associated with coal combustion and related matters, only problems related to the MHD channel itself.) Let us consider each of these elements in turn.

There yet remain problems in understanding the behavior of the high-velocity partially-ionized gas stream containing solid and liquid droplets of slag (which result from the mineral content of the coal). Basic research in gas dynamics, particularly in regimes of two-phase flow, and in low-energy plasma physics to clarify and characterize such areas as the structure of the boundary layer, turbulence, deposition of solid and liquid particles on walls,

plasma stability, and arc formation will be of value. The development of better "non-intrusive" diagnostic methods for the study of these topics is also necessary.

It is easy to appreciate that the combination of high temperatures, exposure to high-velocity gases containing reactive species and particulate matter, and electrochemical effects presents a severe assault on the integrity of the electrode and insulator materials which make up the electrode system. A marked improvement in the lifetime of these materials is of the utmost importance in making this technology a commercial reality. Basic studies of the high-temperature mechanical properties, of mass and charge transport, and of the mechanisms of corrosion, erosion, and dielectric breakdown of both insulating and electronically conducting ceramic materials are needed. (This is also true, to a lesser degree, for metals and alloys suitable for high-temperature service.) Basic studies of mechanical and mass transport properties of electronically conducting ceramic materials have been scarce and have been neglected relative to studies of electrical properties. Investigation of the physical and microstructural factors which affect electron and ion transfer across the solid/plasma interface would be of value.

It is highly desirable to use superconducting magnets to generate the high magnetic field necessary to MHD conversion (although conventional and hybrid magnet systems will play a role). Basic research on a wide variety of properties of superconducting materials with high critical temperatures and magnetic fields is essential to improving the technology of such magnets.

The process of electron transfer across a solid/plasma interface is central to the operation of thermionic conversion devices. (These devices are, like MHD, intended for use in topping cycles.) The heart of such a device contains electrodes at different temperatures embedded in an ionized vapor

containing cesium or other alkali metals. Basic studies are needed of structural and electronic factors which influence electron and ion emission and reflectivity from crystal surfaces, with attention to the detailed mechanism whereby adsorbed alkali metals, oxygen, and other adsorbants affect this process. In the past, the phenomenology of thermionic devices has been described in terms of equilibrium concepts such as work functions, the Richardson-Dushman equation describing thermal emission of electrons, etc. The degree to which such equilibrium concepts can be applied fruitfully to decidedly non-equilibrium circumstances, such as current densities of circa 10 Amps cm^{-2} , requires both theoretical and experimental research. Finally, while the operating environment of thermionic devices is not so severe as that encountered in MHD converters, corrosion and material degradation by solid state reactions often place severe constraints on operating conditions. Basic research in these topics can help in the rational solution of the problems.

General Needs

- o Basic research in low-energy plasma physics and gas dynamics is needed.
- o Understanding of the high temperature mechanical and physical properties of both insulating and electronically conducting ceramics is needed, as well as studies of the mechanisms of their corrosion, erosion, and dielectric breakdown.
- o A better understanding of the physical and microstructural factors that affect electron and ion emission and transport across the plasma/solid interface is essential.
- o Basic research must be done on a wide variety of superconductors.

Transmission and Storage of Electrical Energy

For the purposes of this discussion, an electrical power transmission

system can be considered to be made up of a transmission line, which consists essentially of a number of parallel metallic conductors insulated from each other and from the environment by a dielectric medium, together with associated transformers for increasing or decreasing the voltage, switches and circuit breakers for interrupting the flow of energy, and a system of surge arresters, capacitors, etc., for smoothing and shaping the energy flow characteristics. If the transmission line carries direct current (DC), inverters are required to convert this to alternating current (AC). The areas of basic research required in support of the technology of such a system are dictated by some of the trends expected in future development: toward more compact and less environmentally obtrusive equipment (e.g., underground transmission lines, etc.).

The use of dielectric insulation is pervasive in electric power transmission systems, and as operating voltages increase and systems become more compact, problems of dielectric loss and breakdown become increasingly severe. Basic research into the fundamental aspects of dielectric loss and breakdown in a variety of liquid, solid, and gaseous dielectrics, as well as elementary composite systems (e.g., oil or liquid helium impregnated polymers), is of great importance. There is a wealth of empirical lore and "rules of thumb" available on these topics but a fundamental underpinning is needed; existing theories are inadequate for making quantitative predictions. Research is needed to clarify the mechanism of the nucleation and propagation of plasma "streamers" during breakdown; the influence of the atomic and electronic structure, microstructure, purity, and other such characteristics of the dielectric need to be explored systematically, as well as the influence of the structure of the dielectric/conductor interface. Suspended particles of conducting materials are thought to play an important role, but the details are

obscure at present. The dielectric breakdown of solid insulators across wet and degraded surfaces ("flashover") is an important practical problem for which very little knowledge of the detailed characteristics of the process exists. The influence of fluid motion in liquid dielectrics and of the interplay of thermal, mechanical, and electrical stress in the dielectric loss and breakdown in solid dielectrics needs systematic study. Finally, such studies must include the effect of non-uniform and time varying electric fields, subjects which are generally not included in basic investigations in this area, but which are the rule rather than the exception in practical applications. Research is required to provide the basic insights into the relation between composition, structure, and physical properties needed to "tailor-make") dielectric solids and liquids with appropriate combinations of properties, e.g., high dielectric strength combined with good thermal conductivity; this is particularly true in the area of polymeric solids and organic fluids (where substitutes for toxic dielectrics such as PCB's are greatly needed).

Basic research into the dynamics of high-pressure plasmas under the conditions of arc formation in dielectric gases and in metal vapors could make a significant contribution to the technology of circuit breakers and switches. Studies are needed of the mechanisms of corona discharge and of the generation by such discharges of electromagnetic and acoustic noise.

Fundamental study of magnetic materials, particularly of new low-loss materials (e.g., metallic glasses, etc), are needed for support of transformer technology. Materials with highly non-linear voltage-current characteristics, such as silicon carbide, zinc oxide, etc, are important for application in surge arresters; fundamental studies of the electronic transport properties of such materials are needed. Increased use of DC transmission requires

inverters to provide AC current; at present, thyristors based on single crystal silicon technology are used as inverters, and they suffer significant energy loss in the conducting state. Basic study of the process of current rectification at high power densities by solid state methods is needed to help solve this problem.

A vigorous program of study of materials for use as electrical conductors is still necessary. Basic studies of the properties of novel materials, such as intercalation compounds, conducting polymers, etc., which might if perfected provide some radical saving in weight or cost, are of interest. Superconducting power transmission lines show great promise, and their technology requires support from basic research on a wide range of physical and mechanical properties of superconductors with high critical temperatures, current densities, and magnetic fields.

Electromagnetic energy can be stored in electric fields, for example in charged capacitors, and in magnetic fields, for example in superconducting inductors. The principal problems of capacitors arise from dielectric breakdown, which we have discussed in detail above. The areas of research on superconductors for use in inductors for energy storage are the same as those for transmission lines discussed above; however, large stresses are produced in these inductors and special emphasis needs to be placed on the study of the mechanical properties of materials at cryogenic temperatures. In present designs, the inductors are contained in tunnels in rock formations to support the stress; basic research in rock mechanics and the mechanical properties of non-metals will help to improve the efficiency of this process.

General Needs

- o A detailed understanding of the phenomena of dielectric loss and breakdown in a variety of materials and subject to a wide range of

environments is clearly needed.

- o Basic research is called for in the area of the electrical conductivity of non-conventional conductor materials, e.g., intercalation compounds, conducting polymers, novel organometallics, etc.
- o A strong program in superconductivity is needed, with emphasis on superconductors with high critical temperatures, current densities, magnetic fields.
- o Basic research into the mechanical properties of structural materials, electrical conductors, and insulators is needed.

STORAGE OF THERMAL AND MECHANICAL ENERGY

Thermal Systems

In addition to the storage of thermal energy by thermochemical means (discussed in an earlier section), heat can be stored in heated bodies as the energy of atomic motion (sensible heat) and subsequently be extracted by cooling, or it can be stored as the energy expended to change atomic or molecular arrangements during phase changes (latent heat), and be extracted by subsequent reversal of the phase change. Of these two, sensible or latent heat, the latter has the higher intrinsic storage capacity and also requires the larger amount of basic research. Some topics which can contribute to advancing this technology are: studies of the relationship of microscopic structure and nature of chemical bonding to the physical properties (e.g., mass and heat transport properties, hydrodynamic characteristics, etc.) of fluids, especially complex fluids such as molten salts with polyatomic ions, salt hydrates,

and organic polymers; theories of melting in these materials, together with studies of the nucleation mechanism in freezing; determination of physical and chemical factors which favor large enthalpy changes and small volume changes on freezing; determination of those physical and chemical factors which determine the topology of phase diagrams in molten salt mixtures (e.g., under what circumstances are there eutectics and congruent melting?); fundamental studies of corrosive reactions between molten salts and prototypical materials of construction.

General Needs

- o Systematic studies of the relationships among composition and structure, on the one hand, and the thermodynamic and kinetic behavior of phase transitions, on the other, are needed. Of particular interest is the solid-liquid transition.
- o The corrosive behavior of molten salts, prime candidates for phase-change materials, on materials of constructions must be studied.
- o Basic studies of hydrodynamic mass and heat transfer properties of fluids, and solid-fluid mixtures are needed. Of particular importance are complex fluids and the relationship of their properties to structure.

Mechanical Systems

Mechanical energy can be stored as either kinetic energy or as potential energy; we consider here one example of each: energy storage using rotating flywheels and energy storage using compressed gases.

The needs in basic research related to flywheel storage are principally mechanical in nature. Research is needed on the fundamentals of mechanical properties, especially the mechanics of fracture and fatigue and their relation to structure and other physical properties, particularly in the area of

high-strength synthetic polymers, amorphous materials, and composites. Basic research to further the development of methods of non-destructive evaluation, particularly of composite materials, is required. Basic studies in tribology and the physics of lubrication will contribute to improvements in bearing systems.

Facilities for storing energy by pumping compressed air into underground caverns and other geological formations are being developed. Basic research in the fluid mechanics of two-phase flow, flow in porous media, and studies of the mechanism of entrainment of gas bubbles in flowing liquids is desirable to support this technology. Scaling relations are needed to translate the results of laboratory scale experiments to a scale appropriate to full-sized storage reservoirs; the fundamental bases for such scaling are poorly developed at present. Basic research is needed on the thermal and mechanical behavior of rock and geological formations.

General Needs

- o Studies of the relationships of mechanical properties, especially the mechanics of fracture and fatigue, to structure and other physical properties are needed for a wide variety of materials.
- o Improved methods of non-destructive testing and evaluation are needed.
- o Basic research in fluid mechanics is desirable.
- o Verified scaling relations are needed to go from laboratory scale experiments to field applications.

BASIC RESEARCH THEMES RECURRING IN THE TECHNOLOGIES
OF ENERGY CONVERSION, STORAGE, AND TRANSMISSION
AND SOME GAPS IN COVERAGE

Consideration of the various basic research topics identified in the sections of the paper devoted to the various technologies reveals the recurrence of several broad areas, or "recurring themes", in basic research appropriate to many different technologies. In Figure 1 we have listed these recurring themes and indicated the various areas of technology (grouped as in the sections of this paper) to which they are particularly germane. Many topics within these areas of basic research are currently being supported by the Office of Basic Energy Sciences, and we have not attempted to survey the current support coverage on any systematic way. However, in the course of this study we have noted several topics which are currently receiving comparatively little support and which are important to the technologies which are the subject of this paper. Among these are: 1) magnetohydrodynamics and low-energy plasma physics, 2) the chemistry and physics of organic substances, and 3) the physical and mechanical properties of polymeric solids.

FIGURE 1. BASIC RESEARCH THEMES RECURRING IN THE TECHNOLOGIES
OF ENERGY CONVERSION, STORAGE, AND TRANSMISSION

	Electrochemical Systems	Thermochemical Systems	Storage and Transmission of H ₂ and Gaseous Fuels	MHD and Thermionic Energy Conversion	Transmission and Storage of Electrical Energy	Thermal Storage Systems	Mechanical Storage Systems
Atomic & Electronic Structure	X	X	X	X	X	X	X
Physics of plasmas, electric discharge, & MHD	X			X	X		
Mechanical & Thermal Properties of Matter	X	X	X	X	X	X	X
Phase Equilibria & Transitions	X	X	X			X	
Electron & Mass Transport in Matter	X	X	X	X	X	X	
Superconductivity				X	X		
Chemical Kinetics & Catalysis	X	X	X	X			
Surfaces & Interfaces	X	X	X	X	X	X	
Corrosion & Environ- mental Interactions	X	X	X	X	X	X	X

APPENDIX

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ASSESSMENT OF BASIC ENERGY RESEARCH NEEDS IN SUPPORT OF
THE ENVIRONMENTAL CONTROL TECHNOLOGY PROGRAMS OF
THE OFFICE OF THE ENVIRONMENT

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I. INTRODUCTION

This document is a preliminary draft of an assessment of basic research needs relating to environmental concerns associated with energy research, development and demonstration.

We have made extensive use of information gathered in the Environmental Development Plans recently issued by DOE (Publications DOE/EDP-001 and succeeding documents).

The assessment has been organized by energy resources (fossil energy, nuclear fission energy, solar energy, geothermal energy, and magnetic fusion energy), with a separate chapter on energy conservation.

Within chapters, the research needs have been organized by research categories rather than by traditional environmental concern areas such as air quality and water quality. The research categories used are the following:

- A. Characterization, Measurement and Monitoring: environmental surveys; pollutant characterization, detection, measurement, and screening; instrumentation development; and ambient and point-source monitoring activities.
- B. Physical and Chemical Effects: movement, transformation and dispersion of pollutants in the physical environment; identification of effects of energy activities on physical and chemical aspects of the environment (atmospheric, hydrologic, meteorologic, terrestrial, aquatic processes).
- C. Environmental Control Technology: development of alternative processes and systems to mitigate the environmental health and safety impacts that might result from emissions, effluents, and discharges of various energy systems; disposal technology; reclamation techniques.
- D. Socioeconomic Effects: social, economic, political, institutional and critical resource impacts of energy technology development.
- E. Ecological, Health, and Safety Considerations: characterization of base-line conditions; toxicity of hazardous pollutants to humans, other organisms, and ecosystems; metabolism and biological fate of pollutants; sinks and pathways of pollutants in the environment; processes of repair, recovery, protection and amelioration of adverse health effects; safety standards; etc.

In this report, only research categories A through D are included; information developed for category E has been omitted because it does not appear to be of direct interest to BES.

The listed research needs include many others that appear to be of no direct interest to BES. They are included for the purpose of placing in perspective the research needs in which BES might be interested. Possible BES roles are briefly described where appropriate, and the BES divisions that could be involved are listed in the columns to the right (BER = Biological Energy Research, CS = Chemical Sciences, EMGS = Engineering, Mathematical and Geo-Sciences, MS = Material Sciences). A rough estimate of importance is also included (1 = most important, 3 = least important). For many of the research areas shown, the primary responsibility will rest

with EV, but BES can play a significant role by assisting in developing the basic science, the experimental methods, and the hardware required by EV for discharging their responsibilities.

One recurring theme is the characterization of pollutants released by energy technologies and monitoring for these pollutants. In these situations there is a compelling need to identify the chemical species involved, not just the chemical elements, and it is the development of techniques for gathering samples and characterizing the chemical species that is implied. The needs include proper sampling, analytical, and monitoring techniques for purposes of chemical speciation.

In some cases, BES divisions that have no readily apparent contribution to make to a particular research need may well have a role to play. For example, a need for better characterization may appear to be of interest mainly to Chemical Sciences, but a useful nuclear technique might be developed by Nuclear Sciences. Thus, the fact that a division is not listed as having a role for some research need should not be taken to mean that it should ignore that need.

II. FOSSIL ENERGY

The Fossil Energy program of DOE concerns itself with the nation's coal, oil and gas reserves. The primary emphasis is on the solid fuels (coal and lignite), since they apparently constitute a far larger resource than the fluid fuels. Important components of the program are:

1. New technologies for direct combustion of coal: atmospheric fluidized bed combustion, pressurized fluidized bed combustion, and the use of coal/oil mixtures.
2. Magnetohydrodynamics (MHD), including open-cycle MHD, closed-cycle plasma MHD, and closed-cycle liquid metal MHD.
3. Advanced power systems such as open cycle gas turbine for combined cycle use, closed cycle gas turbine, and alkali metal vapor turbine.
4. Coal gasification above ground, for production of both high- and low-BTU gases.
5. Underground (in-situ) coal gasification.
6. Coal liquefaction through direct hydrogenation, solvent extraction, pyrolysis and indirect liquefaction.
7. Extraction, beneficiation and transportation of coal.
8. Enhanced gas recovery directed at new sources such as Devonian shales, tight sandstones, non-surface coalbeds, and geopressed Gulf Coast aquifers.
9. Oil shale development.
10. Enhanced oil recovery.

The major environmental concerns associated with these fossil fuel technologies are: (1) air pollution, including combustion gases and particulate matter from the combustive processes and a variety of toxic gases and particulates from the conversion processes; (2) water pollution by heat, process effluents, solid waste leachates, and (in the case of

underground coal conversion and oil shale processing) possible aquifer disturbances; (3) land use and soil contamination from disposal of wastes, including ash, slag, fly ash, sludges, spent catalysts (from coal gasification and liquefaction) and drilling and mining wastes (from oil shale); (4) health and safety hazards from exposure to toxic substances and the potential for industrial accidents; (5) significant socioeconomic effects in remote areas in which large new conversion facilities might be located.

Important research areas identified include:

	BER	CS	EMGS	MS
<u>A. Characterization, Measurement and Monitoring</u>				
1. Accumulate baseline, operational, and post-operational air and water quality data from MHD and coal liquefaction facilities and characterize and monitor their emissions and effluents. BES role: conduct basic research to assist in development of instrumentation, analytical methods, monitoring equipment.		1		
2. Characterize the leachate associated with solid wastes from direct combustion, MHD, coal liquefaction, and oil shale systems. BES Role: develop analytical methods for characterization.		1		
3. Sample, analyze and characterize the air emissions from advanced power systems and develop methods for on-line monitoring. BES role: conduct basic research to assist in development of instrumentation, analytical methods, monitoring equipment.		2		
4. Develop instrumentation for (and conduct) experimental monitoring of subsidence associated with underground coal conversion.				
5. Analyze the chemical and physical stability of MHD slag and fly ash and the implications for treatment and disposal. BES role: analysis of stability; development of processes to extract useful materials.		2		2
6. Determine the extent and nature of groundwater contamination at and near underground coal conversion facilities. BES role: conduct basic research useful in leading to reliable, inexpensive equipment and techniques for sampling and analysis.		1	1	
7. Characterize and quantify the chemical constituents of liquid and solid wastes and those released to the atmosphere as a result of coal conversion processes. BES role: develop analytic methods for characterization.		1		

8. Develop individual dose monitoring systems for evaluating exposure to hazardous systems such as polynuclear aromatic hydrocarbons at coal conversion facilities. BES role: conduct basic research to assist development of such systems.

B. Physical and Chemical Effects

1. Perform geological evaluations and analyses to predict the effects that oil shale mining and retorting will have on local water. BES role: basic research applicable to development of instrumentation; perform geological evaluations and analyses; use results to predict effects.	1	1
2. Quantify the degree and extent of impacts related to aquifer disruption from underground coal conversion and oil shale plants. BES role: basic research applicable to development of instrumentation; perform geological evaluations and analyses; use results to predict effects.	1	1
3. Characterize the transport and transformation of air emissions and water effluents from the various fossil energy technologies. BES role: develop and validate models.	1	
4. Determine the mechanisms of transport and fate of pollutants from solid waste leachates associated with several of the technologies.		
5. Develop better analytical models to predict air emissions into the environment from coal combustion and conversion facilities. BES role: develop models to predict sources of emissions.	1	
6. Improve atmospheric transport and dispersion models for these facilities.		
7. Improve predictive models of in-situ subsidence and compare with field data at existing underground coal conversion facilities. BES role: develop and validate models.		1
8. Model the environmental transport transformation and fate of pollutants released to surface and subsurface waters by coal conversion facilities and their residence time in the soil/water environment. BES role: develop and validate models for transport, transformation and fate.		1
9. Develop models to predict future global concentrations and climatic effects of carbon dioxide produced by fossil fuel combustion.	1	

	BER	CS	EMGS	MS
<u>C. Environmental Control Technology</u>				
1. Assess particulate matter and nitrogen oxides control technologies for MHD power plants.				
2. Analyze alternative means (including uses of residuals) of solid waste management for direct combustion and MHD facilities. BES role: develop alternative processing methods and uses.		2		2
3. Develop economic and environmentally acceptable seed recovery subsystems for MHD power plants. BES role: develop recovery subsystems.		2		2
4. Evaluate the effectiveness of air pollution controls and identify those pollutants having unsatisfactory controls, particularly for advanced power systems and underground coal conversion.				
5. Develop techniques for reestablishment of key microbiological processes in soil, and determine the recovery time for reclaimed landscapes, at oil shale facilities.				
6. Develop capability for response to major accidental releases at coal conversion facilities.				
7. Develop chemical approaches to reducing carbon dioxide emissions from coal combustion.			1	
8. Develop control technologies for pollutants from combustion of liquid hydrocarbons. BES role: basic research on chemistry of incompletely oxidized hydrocarbons and nitrogen and sulfur oxides.			1	
<u>D. Socioeconomic Effects</u>				
1. Study changes in population and community needs where large facilities are constructed, particularly in remote areas currently having limited infrastructures.				
2. Quantify consumptive water use in coal conversion and oil shale facilities and determine the effects on the quality and availability of surface and groundwater supplies.				
3. Develop water conservation plans for MHD, coal conversion, and oil shale facilities.				

III. NUCLEAR ENERGY

The nuclear fission program is a large one dealing primarily with several technologies that have been under development for many years and cannot really be called new technologies. Environmental and safety concerns have been addressed for many years by DOE and predecessor agencies; they are well-known and the subject of active investigation.

The issues discussed below are associated with several selected sub-programs that involve new or rapidly developing technologies, namely:

1. Advanced Isotope Separation: the recovery of uranium-235 from the depleted uranium tails generated by diffusion and centrifuge enrichment plants, in order to reenrich them to normal feed assay of 0.7% uranium-235. Research is being carried out on two laser methods (molecular and atomic vapor) and a non-laser plasma method (ion cyclotron resonance).
2. Uranium Enrichment: the improvement of existing gaseous diffusion plants and the development of new gas centrifuge processes for uranium enrichment.
3. Decontamination and Decommissioning: the disposition of older nuclear facilities of various types which are no longer useful or needed for nuclear purposes.
4. Space Applications: developing and fabricating nuclear power supplies for use in space, including radioisotope sources and compact fission reactors.

The environmental concerns of these programs center around the radio-nuclides that are used or produced by the nuclear technologies and that can affect the safety of nuclear workers or the quality of air, water, and land. A special socioeconomic concern of the nuclear energy program is the safeguarding of nuclear materials.

Important research needs in the nuclear energy program are:

	BER	CS	EMGS	MS
<u>A. Characterization, Measurement and Monitoring</u>				
1. Improve instrumentation for characterization and measurement of radioactivity. BES role: basic research applicable to development of better instrumentation.		1		1
2. Evaluate adequacy of instrumentation for special decommission and decontamination problems, such as the detection of alpha emitters in soil. BES role: conduct basic research applicable to development of improved instrumentation.		2		2
3. Evaluate adequacy of monitoring instruments for measuring magnetic field intensity and other field characteristics, and for dosage (of special interest to Advanced Isotope Separation program). BES role: evaluate instrumentation; develop or improve if necessary.			2	2
4. Characterize magnetic fields and measure exposure at facilities.				
5. Identify all chemicals used in isotope enrichment process or produced as reaction products.				

B. Physical and Chemical Effects

1. Evaluate the environmental behavior and effects of pollutant releases from enrichment plants, particularly new types.
2. Improve knowledge and models for the fate of radioactive contaminants released to the environment, with special emphasis on plutonium-238 (from Space Applications). BES role: develop and validate models for transformations and fate. 2

C. Environmental Control Technology

1. Develop methods to assure the availability of decontamination and decommissioning waste receiving sites, improve waste volume reduction technology, and establish procedures and criteria for recycling valuable components of older nuclear facilities. BES role: improve waste volume reduction technology. 2 2 2

D. Socioeconomic Effects

1. Evaluate the possibilities for advanced isotope separation to increase the threat of nuclear weapons proliferation and develop safeguards against the proliferation of this technology. BES role: evaluation of proliferation threats; development of safeguards. 1
2. Determine the best balance between the degree of cleanup, the cost, and the degree of risk in decontamination and decommissioning of older nuclear facilities.
3. Evaluate the financial impact of new government enrichment facilities on communities.
4. Evaluate the risks and consequences associated with space nuclear system applications.

IV. SOLAR ENERGY

The solar energy program is a very broad one, including the use of solar radiation as a direct source of space and water heating and space cooling, the use of photosynthesis to produce fluid fuels from biomass, and the production of electricity by a variety of technologies. The main subprograms in this area are:

1. Solar Heating and Cooling of Buildings: the use of active and passive solar systems for water heating and space heating and cooling, for buildings of different sizes ranging from single family homes to large office buildings.
2. Agricultural and Industrial Process Heat: the use of flat-plate concentrating, and other collectors to provide process heat for agricultural applications such as grain drying and for a great variety of industrial applications ranging from those requiring low temperature heat to those requiring very high temperatures.

3. Fuels From Biomass: the production of gaseous (for example, methane) and liquid (for example, alcohols) fuels from biological materials, using such processes as anaerobic digestion and fermentation.
4. Solar Thermal Power Systems: the production of electricity using solar radiation gathered using large fields of heliostats; solar total energy systems.
5. Wind Energy Conversion: the use of wind power on large and small scales to generate electricity and for other purposes.
6. Photovoltaics: the direct production of electricity using single-crystal silicon and other photovoltaic devices.
7. Ocean Thermal Energy Conversion: the production of electricity using the temperature differences between the upper and lower layers of the ocean.

The diversity of solar energy research leads to a wide variety of environmental concerns. The major ones are associated with some of the more sophisticated solar technologies. Some of the important concerns are: (1) large land requirements for solar thermal power plants, biomass production, agricultural and industrial solar systems for large-scale applications, and wind systems; (2) potential water pollution from heat transfer fluids, additives, and wastes from several of the solar systems; (3) air emissions and fire hazards associated with the overheating of collectors; (4) socioeconomic concerns regarding zoning, building codes, financing, insurance, access to sunlight, component quality assurance and regulation, and so forth.

Important research needs include:

A. Characterization, Measurement and Monitoring

1. Measure alteration of microclimate resulting from solar thermal power systems.
2. Characterize explosive and flammability properties of fluids and wastes from solar thermal power systems.
3. Survey fluids and additives used in solar thermal power systems which may contaminate potable water.
4. Monitor ambient levels of silicon dust in manufacturing and refining facilities producing photovoltaic cells. BES role: basic research leading to development of monitoring equipment and techniques. 3
5. Identify combustion products resulting from off-gassing, overheating and fires during photovoltaic systems malfunction or accident.
6. Monitor ambient levels of toxic gases from doping in photovoltaic manufacturing facilities. BES role: basic research leading to development of monitoring equipment and techniques. 3 3

BES CS EMCS MS

7. Identify and characterize specific compounds and combustion products resulting from collector overheating and fires.
8. Identify and characterize specific compounds from release of heat transfer fluids; determine their biodegradability.
9. Characterize and monitor air, water and land residuals from biomass conversion facilities.
10. Determine and assess combustion pollutants from biomass fuels.

B. Physical and Chemical Effects

1. Determine pathways of entry and review effects of potable water contamination from solar thermal power systems.
2. Analyze release pathways of system fluids and wastes from solar systems.
3. Develop model to predict micro- and macro-climatological effects of ocean thermal energy conversion operations.
4. Determine nutrient requirements relating to soil depletion and assess amount of residue which can be removed in biomass fuel projects. BES role: develop any basic information needed for this assessment.
5. Analyze entry paths for fluids causing product contamination in agricultural and industrial process heat applications.

1

C. Environmental Control Technology

1. Assess control strategies relating to alteration of microclimate resulting from solar thermal power systems.
2. Develop measures to mitigate impingement and entrainment of biota in ocean thermal energy conversion systems.
3. Develop disposal techniques for residuals from silicon distillation in the manufacture of photovoltaic cells.
4. Determine optimal treatment and disposal of sludge for anaerobic digestion.
5. Develop control and mitigation technology for working fluid release in agricultural and industrial process heat applications.
6. Develop control and mitigation measures for collector overheating and fires.

D. Socioeconomic Effects

1. Determine water and land use requirements, assess availability and effects of competition with food and fiber production and socioeconomic impacts of use of biomass for fuel production.
2. Determine land use requirements and impacts associated with solar thermal power systems.
3. Determine impacts of cogeneration and "time of day" metering on rate schedules, with particular reference to use of photovoltaic cells.

V. GEOTHERMAL ENERGY

The geothermal energy program is directed at the use of three types of geothermal resources:

1. Hydrothermal: convective systems of water and steam which are trapped in fractured rocks or sediments by impermeable surface layers and which are released when tapped by drilling. These are already used in the U.S. for generation of electricity at The Geysers, California.
2. Geopressured: zones of highly porous sands saturated with high-temperature, high-pressure brines, at depths of 6500 feet and more under the Gulf Coast of Texas and Louisiana.
3. Hot dry rock: heat contained in rock without natural circulating fluids that overlays a local heat source (such as a magma chamber). These are widely distributed throughout the U.S.

Major identified environmental concerns associated with geothermal energy development are: (1) air pollution from non-condensed gases (such as H_2S , NH_3 , CO_2 , CH_4 , radon, mercury, and H_3BO_3) in the hydrothermal fluids; (2) effects resulting from cooling tower drift: microclimate alteration and dispersal of dissolved gases and toxic substance; (3) water pollution from dissolved non-condensed gases, toxic trace elements, radionuclides, heat, spent fluids, and dissolved solids; (4) effects on land from subsidence and seismicity; (5) health and safety considerations due to well blowouts and to the corrosive and potentially explosive nature of some of the working fluids.

Important research needs are:

BER
CS
EMGS
MS

A. Characterization, Measurement and Monitoring

1. Gathering of base-line data on the frequency and depth of microseismic activity at possible geothermal sites. BES role: basic research leading to improvement of instrumentation and measuring techniques, such as to obtain better geographical resolution.

1

B. Physical and Chemical Effects

1. Conduct basic geophysical research and develop models in relation to the different geothermal systems and land stability. BES role: conduct the basic geophysical research and develop models. 1
2. Conduct geophysical research on subsidence problems arising from removal of large quantities of fluid from hydrothermal and geopressured reservoirs. (Geopressured reservoirs are usually along the coast, only a few feet above sea level, and subsidence may be particularly serious a problem.) BES role: conduct basic geophysical research and develop appropriate models. 1
3. Conduct geophysical research on seismicity associated with the withdrawal and injection of geothermal fluids. (Injection of fluids is well-known to lead to seismic activity.) BES role: conduct basic geophysical research and develop appropriate models. 1

C. Environmental Control Technology

1. Develop H₂S removal techniques for hydrothermal systems.
2. Develop disposal techniques for brine and spent fluids.

D. Socioeconomic Effects

1. Determine effects on land uses in geothermal zones and nearby communities, due to subsidence, seismicity, air and water pollution, and noise (a significant problem at The Geysers).
2. Critical resource: water and its long-term allocation and availability; many geothermal resources are located in areas of limited water supply.

VI. MAGNETIC FUSION ENERGY

The objective of the magnetic fusion energy program is to develop and demonstrate the use of nuclear fusion energy using magnetic confinement for the production of commercial electrical power. The two principal approaches to fusion reactor design -- tokamak and magnetic mirror -- differ in their magnetic field configurations used to confine the plasma but early reactors of either type are expected to use deuterium-tritium mixtures and have a lithium blanket to generate tritium by the reaction $\text{Li} + n = \alpha + \text{T}$.

The primary environmental concerns are: (1) exposure of reactor personnel and the environment (by air and water) of radionuclides, particularly tritium and neutron-activated materials; (2) presence of large magnetic fields (up to several hundred gauss) in occupied areas of fusion reactors; (3) exposure of reactor personnel (and, in the case of accident, the environment) to potentially hazardous materials such as lithium, lithium compounds, and beryllium.

Research needs include:

	BES	CS	EMGS	MS
<u>A. Characterization, Measuring and Monitoring</u>				
1. The measurement of background exposure to tritium in its significant chemical forms (such as HT and HTO). BES role: basic research to assist development of instrumentation for measurement of these chemical compounds.	2			
2. Development of instrumentation to measure radiation exposure to tritium at less than 1 picocurie/cm ³ (approximately the occupational limit for HTO in air). BES role: basic research to assist development of instrumentation.	2			
<u>B. Physical and Chemical Effects</u>				
1. Evaluation of the physical and chemical behavior of tritium in the reactor environment. BES role: evaluation of tritium behavior in reactor environment.	2		2	
2. Evaluation of the major sources of tritium release to the environment. BES role: evaluation and measurement of natural and artificial sources of tritium.	2			
3. Determination of HT and HTO conversion rates and identification of atmospheric, hydrologic and terrestrial transport and accumulation processes which distinguish between HT and HTO at points proximate to release as well as globally. BES role: basic chemistry of HT and HTO conversion; development of models of transport and accumulation.	1			
<u>C. Environmental Control Technology</u>				
1. Develop tritium control and recovery techniques to reduce the potential for radiation exposure. BES role: develop tritium recovery techniques.	1			
<u>D. Socioeconomic Effects</u>				
1. Siting of fusion reactors.				
2. Critical resources: helium, beryllium, lithium.				

VII. ENERGY CONSERVATION

The energy conservation program is directed at improving the efficiency with which energy is produced, converted, stored, and used, and managing the transition from limited fluid fossil fuels to more abundant sources of energy.

The program consists of six subprograms:

1. Building and Community Systems deals with energy conservation in buildings, community systems, consumer products, and urban waste technology.

2. Conservation Research and Technology deals with generic technology research and development that is primarily directed at improving the efficiency of energy conversion devices and at enabling these devices to use alternative fuels. Its major R & D areas are (a) heat cycles and combustion, (b) waste heat utilization technology, and (c) fuel cells.
3. Electric Energy Systems deals with overhead AC/DC transmission, underground (including superconducting) transmission, electrical power generation, storage applications, and systems development and control.
4. Energy Storage Systems has as its main objective the development of energy storage systems that permit coal, solar and nuclear energy to be substituted for oil and natural gas energy in all end-use sectors (transportation, electric power generation, residential, commercial, and industrial).
5. Industrial Energy Conservation has the objective of reducing the energy consumed per unit production in the industrial and agricultural sectors through improved process efficiency and re-optimization of material flows within and among process streams.
6. Transportation Energy Conservation deals with transportation technologies and operational strategies to significantly reduce energy consumption used for transportation and ultimately eliminate the dependence on petroleum-based fuels. Examples of the technologies are Stirling and gas turbine engines, alcohol and synthetic fuels, electric and hybrid vehicles, hydrogen fuel, and continuously variable transmission.

A wide variety of environmental concerns, not easily summarized, are associated with these programs. Examples are:

- Odor, noise, and aesthetic problems with urban waste plants.
- Possible health and safety concerns from toxic, hazardous, and explosive substances.
- Emissions into the air of toxic gases and particulate matter from the manufacturer or use of some of the conservation technologies.
- Water pollution by exotic compounds and solid waste leachates.
- The use of critical resources such as platinum and other metals as catalysts or alloy constituents in some of the technologies.

The research needs in this area are likely to change more rapidly than in the energy supply programs because of the constant development of new concepts and new goals as the nation's energy program evolves. This is an area in which new research needs will be constantly revealed.

Important research needs identified at present include:

	BER	CS	EMCS	MS
<u>A. Characterization, Measurement and Monitoring</u>				
1. Determine types, levels and sources of indoor pollutants, allergens and pathogens, including trace elements, particularly in buildings with low air infiltration. BES role: conduct basic research useful in developing needed instrumentation and sampling and analytical techniques.		1		1
2. Conduct tests to determine flammabilities and combustion products of new insulation and bonding materials.				
3. Characterize, measure and monitor air emissions and water effluents from urban waste pilot and demonstration plants. BES role: conduct basic research useful in developing instrumentation and characterization, measurement and monitoring techniques.		1		1
4. Characterize, measure and monitor air emissions and water effluents from aluminum remelting operations using coal. BES role: conduct basic research useful in developing instrumentation and characterization, measurement and monitoring techniques.		3		3
5. Characterize and quantify emissions and effluents generated during battery component materials manufacture, such as nickel carbonyl generation from nickel-iron and nickel-zinc battery production. BES role: study the chemistry of the generation of the effluents.		3		
6. Characterize exposure levels to arsine and stibine generated during lead-acid battery overcharging.				
7. Develop information on the thermal stability of heat cycle device working fluids and their decomposition products; develop information on their flammability and explosive potential; establish methods of monitoring air emissions and water effluents from heat cycle devices. BES role: develop basic thermodynamic data and conduct basic research applicable to development of instrumentation and techniques for monitoring.		2	2	2
<u>B. Physical and Chemical Effects</u>				
1. Determine transport and fate of air emissions from alcohol fuels. BES role: develop models for transformation and fate of emissions.		1		
2. Determine transport and fate of Freon-11 and trifluoroethanol emitted to atmosphere. BES role: develop models for transformation and fate of emissions.		2		
3. Determine transport and fate of heat cycle device working fluids emitted to water. BES role: develop models for transformation and fate of emissions.		2	2	

	BER	CS	EMGS	MS
<u>C. Environmental Control Technology</u>				
1. Develop new uses and safe disposal techniques for fly ash and slag waste at facilities that have converted to coal for remelting aluminum. BES role: develop new uses for the wastes.		3		3
2. Identify alternative methods to control noise from corona discharge at high voltage overhead transmission lines. BES involvement in new types of transmission lines is relevant to this concern.				3
3. Establish reliability of building ventilation controls.				
4. Develop control technologies and alternative designs for fuel storage systems which will store highly flammable and potentially explosive alcohol fuels.				
5. Study alternative procedures for handling battery materials in manufacture, recycling and disposal.				
6. Design portable collectors and instruments to control stibine and arsine generated during battery overcharging. BES role: basic research useful in developing collectors and instruments.		3		
7. Establish guidelines for handling, storage, recycling or disposal of heat cycle device working fluids.				
8. Identify materials in waste disposal/recycling chain which may pose environmental problems if they increase dramatically, such as				
a. metal (particularly aluminum) cans, whose inks and coatings may need to be removed before recycling. BES role: review removal methods; develop improved procedures, including handling of wastes.		2		2
b. plastics (polyethylene terephthalate) soft-drink containers. BES role: conduct tests to determine biodegradability and combustion behavior of these containers; identify needs for monitoring emissions.		2		

D. Socioeconomic Effects

1. Conduct a comparative environmental, health and safety analysis of alternative battery technologies that show commercial promise for utility and transportation applications.
2. Conduct assessment study to update electric energy systems studies completed for 500 kilovolt overhead transmission lines to include 1200 kilovolt lines.

Fundamental Research Needs for Fission
Energy Technology Development

An Assessment Prepared by Staff Members of
Argonne National Laboratory

October, 1979

For Submission to Department of Energy
Office of Basic Energy Sciences

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I. INTRODUCTION

In response to a request from DOE Office of Basic Energy Sciences (BES), Argonne National Laboratory has prepared this assessment of the fundamental research needed for development of fission-energy technologies. This assessment has been developed from a broad perspective, representing a critical review of recommendations received from a spectrum of experts at Argonne, other National Laboratories, universities, and nuclear industries*. Following BES guidelines, the recommendations given here are organized by specific fission-energy technology components and are made independent of the current status of program funding.

Such an assessment is complex because of the many important components of fission energy technology which must be considered. Among these are nuclear fuel material exploration, mining and milling, isotopic enrichment, fuel fabrication, reactor design and operation, fuel reprocessing, and nuclear waste isolation. The assessment is also complicated by the many technical, social and political uncertainties currently surrounding the future of fission energy development. Technically we have entered the first generation of nuclear energy production with thermal reactors, uranium enrichment capabilities are well advanced and in place, a new major fuel reprocessing plant is completed (but unlicensed), and progress is being made on developing methods to safely isolate radioactive wastes. Furthermore, a great deal of research and development has been devoted to the next generation of nuclear energy, breeder reactors. Several European countries have even more advanced technologies under development or in place than does this country. In spite of the fact that a sizable nuclear technology is already established, further development is being delayed due to remaining technical issues, the lack of a commitment to a selected fuel cycle strategy, and unfavorable public and government attitudes.

An attempt has been made in this assessment to recommend high priority basic research needs which can make direct contributions to the resolution of major technical issues which now confront the development of nuclear energy - in particular, fission fuel supply, nuclear waste management, reactor operational safety, proliferation of fissile materials and fuel-cycle optimization. A brief discussion of these issues with general recommendations is given in Section II. Specific recommendations for fundamental research are given in Section III. Based upon the input received, the recommended highest priority research needs are italicized throughout this report.

*A listing of contributors is given in the attached Appendix.

II. MAJOR ISSUES CONFRONTING FISSION ENERGY TECHNOLOGY DEVELOPMENT

A. Fission Fuel Supply and Improved Fuel Utilization

The selection of a specific fuel cycle strategy to be adopted is complicated, at present, because of uncertainties of the total world supplies of uranium and thorium, competition for these supplies, and the global distribution of these resources. Relatively large supplies and free trade of uranium would decrease the incentive for development of thermal reactor cycles with improved fuel utilization, breeder reactors and fuel reprocessing. Relatively small or inaccessible supplies would provide a strong incentive for development of these more advanced fuel cycles. *In light of the present uncertainties of fission fuel resources, fundamental research efforts should be directed to providing the scientific foundation for development of advanced nuclear fuel cycles with better fuel utilization as well as developing better methods for uranium and thorium ore exploration, improved efficiencies of mining, milling, enrichment, etc. With this scientific foundation in place, future decisions on fuel cycle strategies can be made more promptly and with increased confidence. Improved thermal reactor cycles can present opportunities for more efficient fuel utilization. Current-generation LWRs could operate with significantly improved resource utilization and reliability if higher fuel burnups and higher fluences on structural materials could be sustained. Alternative thermal reactor concepts like the HWR (CANDU), the HTGR, the SSCR, and the LWBR offer varying degrees of improvements in resource utilization and will require varying degrees of additional research and development. Introduction of fast breeder reactors, with the optimum fuel material utilization also will require significant additional research and development of the reactor technology and of associated fuel reprocessing and refabrication technologies. Only through further research can the feasibility and potential impact of these improved and advanced fuel cycles be accurately assessed. Common to more effective fuel utilization and the development of these alternate reactor concepts is the high priority need for research leading to development of structural materials with increased resistance to degradation at high temperatures and high neutron fluxes and fluences and of fuel elements with improved performance at high burnups.*

B. Nuclear Waste Management

The absence of an established technology for safe long-term disposal of radioactive nuclear wastes has been a major handicap to the development of nuclear energy. As a result of an intensified effort in recent years, a consensus is now emerging from technologists that deep geological nuclear waste repositories can be successfully developed to ensure safe long-term isolation of nuclear wastes.

One of the areas of highest priority for basic research related to nuclear technology is the development of the underlying

scientific foundation for deep geological disposal of nuclear wastes. At present, because of the urgency to proceed rapidly with site selection criteria and design, the major emphasis in nuclear waste management-related research is being expended on studies of an empirical nature. However, many of these empirical studies are of limited value because of the complexities of the phenomena being considered. The number of variables needed to be considered is quite extensive and not all of these variables and their inter-relationships can be studied empirically. Fundamental research paralleling the empirical studies is needed to fully understand the basic mechanisms of processes which can take place in actual repositories as well as to develop needed new experimental methods. Understanding the basic mechanisms involved will greatly add to our confidence in extrapolating the many short-term laboratory and field studies now underway in order to assess the long-term stabilities of actual waste repositories and the consequences of low probability breachings of repositories.

C. Reactor Operation Safety

Recent events, in particular the Three Mile Island Reactor incident, indicate that prevailing views of reactor safety research must be thoroughly reassessed. The future of fission energy rests on the ability to assure the public that nuclear technology is safe. *Research is needed to develop a better understanding of the factors which can lead to reactor malfunctions, to understand the properties of systems under extreme transient conditions, develop more reliable and safe reactor components, and develop improved instrumentation. Research leading to development of materials that can function more reliably and predictively in adverse reactor environments is also a high priority need in reactor safety. Improved technology based on additional research can improve reactor operational safety. There are also a number of non-research areas (outside the scope of this assessment) which should receive serious attention and can contribute to improved reactor safety, e.g., better operator training and certification programs, improved operating procedures, better emergency planning, improved decontamination methods, and improvements in the quality of manufactured components.*

D. Proliferation of Fissile Materials

To enhance guarantees that the technology and material of commercial nuclear power will not be diverted to weapons-related activities, three new dimensions of fission energy technology must be developed. The first is safeguards, encompassing the areas of material accountability and physical protection. Effective safeguards depend both on widespread acceptance of safeguards procedures and on accurate methods

to assay special nuclear materials in a variety of environments. Research to reduce the uncertainties in nuclear material accountability is thus an important element of non-proliferation policy. Institutional arrangements are a second dimension in the non-proliferation area. Here multinational participation in fuel cycle facilities, guarantees of fuel supply, and fuller participation in non-proliferation treaties are needed. Since these activities are more administrative than technical, they will not be considered here. The third dimension is alternatives to current reactor and fuel cycle concepts. These are being studied during the course of the International Nuclear Fuel Cycle Evaluation (INFCE), and several options are emerging. Examples of alternative reactor concepts include thermal reactors using de-natured ^{233}U - ^{238}U fuel and breeders operating partly or wholly on the ^{233}U -Th fuel cycles. Examples of alternative fuel cycle processes include coprocessing of spent fuel with fissile material always diluted by fertile material, and radioactive spiking of materials in various places of the fuel cycles. The scope of research efforts needed to pursue the large number of non-proliferation strategies presently proposed is unmanageable. Therefore, the recommendations of the extensive INFCE evaluations, when finalized, should be used as guidelines to delineate and focus the scope of research activities needed in support of non-proliferation fuel cycle strategies.

E. Fuel Cycle Optimization

Successful development seems reasonably assured for several of the technologies needed in the different nuclear power options. For example, LWRs operating in a once-through mode need only the spent fuel storage technology developed; oxide-fueled breeders are likely candidates to be successfully developed with low technical risks; and Purex reprocessing can probably be successfully adapted to a breeder fuel cycle. For these and other nuclear power options that might be used, development appears to represent a modest extension of current technology. But success in initial development is often separate from the economic optimization that can occur later. This optimization requires a research commitment. This can be illustrated by the following example. The data base of nuclear cross-sections is adequate to design and construct most, if not all, of the alternative reactor concepts now considered. Uncertainties might be characterized generally as small enough to permit reactor design, but often are large enough so that considerable performance penalties are incurred as a result of the need to overcome uncertainty by conservatism in the design. Thus improving the accuracy of a given cross-section may not alter the perception of a concept's feasibility, but such an improvement may lead to tighter design margins, reduced costs and better performance. Some examples of research areas which could contribute to optimization are additional and more accurate

measurements of neutron cross-sections, decay heats, fission neutron properties, and development of improved structural materials.

In summary, the lack of a commitment to develop a specific nuclear fuel cycle strategy at this time coupled with the uncertainties of future alternative energy sources makes the role of fundamental research increasingly more important. Fundamental research programs must, during this period of uncertainty, provide the broadly based scientific foundation needed to assess the relative merits of different proposed fuel cycles accurately and dispassionately. When selection of a fuel cycle strategy is made, we must have much of the needed scientific data base well in hand to permit prompt and effective development of that cycle.

III. RESEARCH RECOMMENDATIONS

In considering the specific recommendations presented in this Section, we have attempted to identify and recommend basic research needs to be pursued by DOE as a whole, and not necessarily solely by the Office of Basic Energy Sciences. Since the demarcation between research labelled "basic" and "applied" is not sharp, a rather liberal interpretation was used throughout this study so as not to eliminate important recommendations arbitrarily. It is also important to note at this time that there are both short-term and long-term fundamental science needs. It is essential to maintain a healthy balance between the two. Basic Energy Sciences is one of the relatively few successful supporters of long-term fundamental research and bears a major responsibility in insuring that fundamental research in this country remains productive and innovative. In addition to responding to short-term objectives, DOE and Basic Energy Sciences must maintain this long-term "National Trust".

A. Fission Fuel Exploration

Much of the scientific foundation needed to search for ore deposits is now available. Short-term developments needed are more in the area of engineering, for example, improving the efficiency, resolution, and portability of radiation detectors. On the most fundamental level, a better understanding is needed of how uranium, thorium, and other valuable mineral ore bodies are formed in order to guide exploration efforts more effectively. Fundamental studies of the mechanisms by which elements migrate and deposit in geological media are needed and will contribute to our understanding of how ore bodies are formed. Furthermore, extensive knowledge of the geochemistry of these ore deposits will facilitate the development of mining and milling techniques.

B. Mining and Milling

In order to provide the uranium resources needed for an expanding nuclear industry, methods must be developed to exploit continually more dilute uranium sources. These future sources will include low-grade ores, uranium by-products from mineral extraction processes (e.g., copper and phosphates), tailings and wastes (e.g., coal flyash), granitic rocks, and possibly sea water.

To exploit many low-grade ore deposits economically, it may be necessary to develop in situ leaching processes. Information on the geohydrology and geochemistry of these deposits will be needed. Basic studies on the dispersion of liquid solutions through porous geological media are needed. The basic chemistry and kinetics of "solution-rock" interactions should be pursued as well as development of more effective leaching techniques. Sizable quantities of uranium exist in oil shale deposits. The development of a coprocessing method for isolating the kerogen material and uranium, although difficult, would be highly desirable for it is not likely that these resources can be exploited economically for a single product.

Additional research is needed on hydrometallurgical processes, extraction processes, complexing chemistry, electrochemistry and precipitation properties of uranium (thorium) from complex mixed solutions to increase the efficiency of current milling procedures. Development of new processes is also needed for extracting uranium from by-products of industrial processes: e.g., tailings from phosphate, uranium, vanadium, copper, and molybdenum mills.

Over a longer time scale, the feasibility of extracting uranium from sea water (in the parts per billion range) should be explored. Because of the extremely large volumes of solutions that must be handled, direct extraction of uranium from sea water at this low concentration will probably only be economically feasible when conducted in conjunction with other metal extraction processes. Development of general methods for removing heavy metals from very dilute aqueous solutions containing higher concentrations of competing ions and the use of chelating complexes should be pursued. Also heavy metal ion concentrating mechanisms such as utilization of marine organisms and organic sediments to scavenge uranium from sea water should be investigated.

Current mining and milling, as well as future in situ leaching technologies, present serious environmental problems. In order to develop methods to minimize the detrimental environmental impacts of these processes we must fully understand how hazardous by-products are transported through the biosphere.

Such studies should include the leaching and water mobilized transport of ^{230}Th and ^{226}Ra and the diffusion of radioactive rare gases such as ^{222}Rn through heterogeneous media.

C. Isotope Enrichment

The existing first generation uranium enrichment facilities based on gaseous diffusion technology, coupled with current diffusion plant expansions and construction of the second generation, gas centrifuge, plants are expected to meet this country's enriched uranium needs for the next decade while new plants based on gas centrifuges or possibly a third generation technology are being developed. Future research on uranium enrichment should emphasize improvement of the performance of the less-energy intensive gas centrifuge technology, basic research which might lead to development of a third generation technology, and investigation of enrichment processes less sensitive to nuclear proliferation.

Materials problems are the major weaknesses in gas centrifuge development. New materials with high strength to density ratios for rotors and materials which are chemically resistant to attack by UF_6 are needed. Also, to optimize gas centrifuge designs, a better theoretical understanding of rotor dynamics and fluid dynamics in strong rotational fields is needed.

Development of any third generation technology should emphasize low total energy consumption and substantially lower total costs for producing enriched uranium than those associated with gaseous diffusion or centrifuge technologies. Currently, the most promising candidates are laser isotopic separation methods based on using atomic and molecular species, plasma separation methods and chemical exchange processes. Molecular laser-based isotope separation processes based on UF_6 require development of new better lasers at $16\text{ }\mu\text{m}$ and ultraviolet lasers. There is also a need to develop volatile compounds of uranium with isotope shifts at more convenient laser wavelengths and with simple photochemistry for isotopic separation. More generally, it is important to improve our understanding of how laser energy absorbed into a specific molecular state is translated into the various available molecular degrees of freedom and of the photochemistry which takes place in cases of multiple photon absorption. Current atomic vapor laser isotope separation processes require development of better containment materials for molten uranium, (e.g., solubility, thermodynamic, and reaction rate measurements are needed for molten uranium with potential containment materials such as refractory metals, metal carbides, oxides, and sulfides) as well as detailed spectroscopic studies of actinide element vapors. Plasma separation processes which utilize electromagnetic separation of ion plasmas also require additional

research on containment materials for molten uranium as well as uranium-uranium ion collision cross section measurements and an improved theoretical model of the motion of ions in high-density charged-neutralized plasmas in rf electric and magnetic fields. A number of processes are under development which exhibit an isotope separation effect based upon a difference in equilibrium or kinetic behavior in solutions, e.g., isotopic preference in redox and aqueous-organic extraction systems. Current uranium isotopic separation processes based on such chemical exchange reactions require a better understanding of the solution and coordination chemistry of uranium, of synthesis and testing of new extraction ligands, and more information on kinetics and equilibrium isotopic effects in homogeneous and heterogeneous systems. Modern theoretical chemistry has made considerable advances in recent years and a renewed theoretical activity should be applied to isotopic separations to guide the experimental programs.

D. Reactor Materials Research

More efficient nuclear fuel utilization (which implies higher neutron fluences, more complete fuel burn ups, and longer core residence times) and the increased emphasis on reactor safety requires the development of fuel cladding and structural materials with improved performance at high temperature and greater resistance to damage by radiation and corrosion. Significant advances in fuel fabrication technology are also needed.

The degradation of mechanical properties of materials, particularly the embrittlement of pressure vessel steels and of fuel claddings, comprises the major problem arising from irradiation effects in existing thermal reactors. A strong research effort should be maintained to study these degradation mechanisms and to develop materials more resistant to degradation by radiation. Embrittlement limits the lifetime of reactors, requires their operation under less than optimal conditions, and demands expensive monitoring. All of these factors lead to a considerable economic penalty. At present there is an inadequate understanding of the basic mechanisms by which irradiation raises the temperature below which metals fail by brittle fracture. Research is needed to guide the development of materials that are more resistant to embrittlement and to determine the validity of current test programs designed to monitor the degradation of reactor components. Studies of radiation creep, of plastic instability in irradiated ductile materials, and of radiation driven changes in microstructure are also important. The resistance of metals under stress to crack growth is strongly affected by the presence of hydrogen or helium at the crack tip. The mobilities of these gases and their influence on cohesive energies need investigation. The enhanced atomic mobility under irradiation requires that post-irradiation testing be supplemented by a strong program of tests during irradiation.

Of nearly equal importance is the need to understand the effects of stress, radiation, and corrosive environments on fuel cladding materials. The cladding is the primary containment for fission products; breaches in its integrity impact directly upon the public safety, the operating economics of the facility, and the waste management problem. The zirconium-based alloys which are used as cladding materials because of their very low thermal-neutron capture cross sections resist corrosion in water and steam but are embrittled by hydrogen picked up during formation of the protective oxide. The influence of stress on the formation and disposition of embrittling hydrides needs study. A unifying theory of corrosion is needed to describe synergistic effects such as attack by solutes (e.g., oxygen) in the cooling water or by fission products (e.g., iodine) in the fuel during neutron irradiation. Temporary loss of cooling accidents lead to rapid temperature excursions with large internal pressures on the cladding. Study of oxygen diffusion and corrosion under these conditions is needed to predict the effects of such excursions on the material.

Void formation with concomittant macroscopic swelling is of major concern in the development of fast breeder reactors and merits continuing research. Currently the packing density of fuel elements must be reduced to accommodate swelling; this results in a severely reduced breeding ratio. Despite this heavy economic impact void research should be given lower priority than the topics listed above due to the uncertain prospects for breeder reactors. To provide a basis for the development of alloys which are more resistant to swelling, research leading toward a basic understanding of void nucleation, of defect absorption processes at sinks, and of radiation driven impurity segregation is particularly needed.

Tests in which large numbers of displaced atoms must be produced, as are needed for studies of swelling, require long irradiation times at neutron facilities. The effects of long neutron irradiations are most often simulated by charged-particle irradiations at orders of magnitude greater displacement rates. Much additional research is necessary to properly correlate charged-particle with neutron irradiations. In particular, better models are needed for electronic losses by energetic charged particles, for defect recombinations in cascades, and for surface effects which are important in charged-particle, but not neutron irradiations. A detailed knowledge of the temperature dependence of defect interaction parameters is also required because of the necessarily higher charged-particle irradiation temperatures for equivalent void growth conditions. Account must be taken of the different ratios of displacements to injections of hydrogen, helium, and metallic substitutional products in the two types of irradiations.

Additional materials research should be directed to understanding long-term aging and fatigue mechanisms of materials under stress and corrosive conditions. The combined effect of radiation and a corrosive environment should be investigated since the synergistic effects are often greater than would be predicted from the degradation rate due to either individual component. This effect arises in part from radiation driven diffusional changes in the composition of surfaces, from injection of contaminants by irradiation, and from selective hydriding of substitutional alloys.

With an increasing emphasis being placed on stretching uranium resources through increased fuel burn up, greater attention must be given to how changes in the chemical state of the fuel with burn up and build up of fission products and actinides limit the life of a fuel pin. Research is specifically needed in the areas of urania-fission product oxidation potentials, elemental diffusion in thermal gradients, measurement of reaction products and cladding-fuel-fission product reaction kinetics and equilibrium studies. Research is also needed in which investigations of atomic and ionic interactions and the energies associated with valence states and lattice defects are coordinated with measurements of thermodynamic and transport properties, so that equations of state and transport can be derived.

Future development of fast breeder reactors will require additional research and development of fuel and cladding materials that can perform reliably at the high fast-neutron fluxes and high burn-ups required. Significant efforts have already been expended on development of oxide fuels for breeders, but a better fundamental understanding is still required of their thermal, mechanical and chemical performance. Because the low thermal conductivity and low density of oxide fuels are drawbacks for breeder deployment, research on alternative fuels such as metals and carbides should receive increased emphasis, particularly from the standpoint of safety. Utilization of these higher density alternative fuels would provide higher breeding ratios and lower doubling times. Also, their higher thermal conductivities would permit more compact core arrangements, with resultant economic benefits. Additional research is needed on the mechanical and physical properties of and the effects of irradiation on these fuels before analytic predictions of their performance can be made.

E. Nucleonics

The present data base of nucleonics information (neutron cross sections, half lives, decay schemes) is generally adequate for the purposes of design work and comparative evaluations of alternative reactor concepts (when used in conjunction with semi-empirical corrections derived from test assemblies).

However, data inadequacies still exist and data of higher accuracy are needed to optimize selected fuel cycle strategies. In particular, more accurate fast-neutron capture cross sections of major structural materials and inelastic scattering cross sections for ^{238}U are needed. Better values of resonance cross sections are needed for understanding reactor dynamics. Capture and, in some cases, fission cross sections are inadequately known for ^{234}U , ^{236}U and transplutonium isotopes which are important at higher burnup or for assessing the feasibility of actinide element recycling. Direct decay heat measurements and additional nuclear data (fission yields, decay schemes, etc.) are needed to calculate decay heats for fast-neutron fission of the major fissile nuclides ^{233}U , ^{235}U , ^{239}Pu , and ^{241}Pu and the fertile nuclides ^{232}Th and ^{238}U more accurately. Fission-neutron yields and energy spectra are needed for all major isotopes as a function of incident neutron energy. Furthermore, there is a need for a more comprehensive, unified understanding of a broad range of nuclear phenomena such as nuclear level densities, distribution of nuclear charge, mass, and excitation energy between the fission fragments in thermal and fast neutron fission, and details of pre-scission neutron production.

F. Critically Evaluated Data Files

In addition to having the results of basic research available in the open literature, reactor design and operations personnel have a strong need for evaluated data files. In general, they do not have sufficient resources and time to conduct extensive literature searches and critical evaluations of data. The availability of critically evaluated nucleonics data files (neutron cross sections, decay schemes, half-lives, etc.) such as the ENDF evaluations (through the National Nuclear Data Center), the Nuclear Data Tables, the Table of Isotopes, IAEA evaluations, etc. has been important to the success of our nuclear energy programs and similar programs should be maintained and expanded to non-nucleonics areas, e.g., thermodynamic and transient properties of coolants and their reaction products, thermodynamic properties of fuels and fuel-cladding-fission products, etc.

G. Reactor Safety and Operations

In order to understand and cope with potential reactor malfunctions, research is needed in instrumentation, data management, mathematics and computer sciences, seismology, chemistry, materials, and nucleonics. Some research recommendations related to reactor operations and safety have already been given in other sections. For example, research has been discussed under "Reactor Materials Research" which is directed to understanding and developing materials that will function reliably for long periods of time in adverse reactor environments and

are less likely to fail under transient stress. Although many objectives are of an applied nature, the following statements and recommendations highlight the range of underlying basic research that can contribute to improved reactor safety and operations. The statements are deliberately broad in scope in order to avoid the risk of omitting useful alternatives.

Basic research should be directed to developing new more sensitive instrumental methods to reliably monitor the performance and status of reactors under normal operating conditions and during extreme transients of temperature, pressure, and shock. A better understanding of the propagation, attenuation and scattering of sonic energy in structural materials at elevated temperatures is needed to improve the efficiency and reliability of remote volumetric inspection of pressure vessels and containment boundaries. More sensitive methods for detecting and locating water/steam leaks into sodium in an LMFBR steam generator are badly needed. It would be desirable to explore the potentiality of using laser systems to measure trace amounts of fission product elements (or preferably isotopes) in gas or solution streams. Very high detection sensitivity would lead to earlier diagnosis of malfunctions and increase the usefulness of tagging techniques to locate malfunctions. A better understanding of the release mechanism of delayed-neutron precursors from fuels could possibly lead to development of new methods to monitor fuel conditions and performance. Non-destructive diagnostic techniques need to be developed for better evaluation and quality control of structural materials and diagnostic examination of physical states of reactor system, i.e., reactor vessel water level and density; pipe flow velocity and density; fuel and clad integrity.

Improved instrumentation is only one contribution that may be made to reactor operation. Operators are faced with massive amounts of data that could be difficult to interpret under abnormal or ambiguous circumstances. *A better understanding of the management of data derived from reactor instrumentation would greatly facilitate the correct choice of actions under abnormal reactor operating conditions.* The large amounts of data produced from existing and future sensors, the potential for ambiguous and erroneous responses, the short time scale for information assimilation--all militate in favor of computer-directed data management, display, and operator guidance. Much of this type of research is of a fundamental nature and common to many applications. Multidisciplinary studies could develop new approaches to this problem, leading possibly to real-time systems that analyze the instrument data, describe to the operators the probable cause of problem situations, and predict the effect of proposed actions.

Mathematical models and computer simulation have long been used to study the behavior of reactors. However, some areas

have been neglected; for example, the recent accident at Three-Mile Island illustrates the prudence of providing a strong secondary containment. Since this represents the last barrier preventing a major release, this accident clearly demonstrates the need for development of modeling techniques to evaluate containment responses to not only seismic and other natural events, but events brought about by human error such as airplane crashes or internal explosions. Containment analysis and evaluation should be equal in sophistication and level of confidence to the evaluation models for the primary system.

The applicability, effectiveness and credibility of modeling and simulation can be improved by additional research in mathematics and computer science. *Needed are new models and strategies that can be applied to analysis of extremely complex phenomena such as (1) the response of a reactor and its associated equipment to seismic disturbances, explosions and subsystem failures; (2) transient multiphase flow of material in complex and simple geometries; (3) risk assessments which take into account all components (including operators) of a reactor plant, their failure rates, and the stochastic nature of failure incidence.* Among the new features of these models would be a larger number of dimensions, use of "best estimates" instead of "most conservative" assumptions, and consideration of non-equilibrium processes. Even for existing models, the codes used for design and safety modeling are large, complex, and often exceed the capacity of existing computers. Computer science research has the potential of (1) developing better techniques for designing, developing, and validating these codes and (2) devising new algorithms, especially for vector and array computer architectures, which will reduce the magnitude of the computations.

Basic advances in the field of seismology are needed to reduce unnecessary conservatism in site selection criteria for fission power plants and in the design of buildings, fuel assemblies, major components, and structural supports to withstand earthquakes. In addition, progress is needed in techniques and instrumentation to anticipate earthquakes. Ongoing earthquake monitoring and prediction is generally directed towards the fairly ambitious goals of providing sufficient time (hours or days) to evacuate cities; however, reactors would benefit from minutes or even seconds of warning for shutdown and cooling.

Aqueous and molten sodium coolant chemistry research identifying and characterizing the behavior of impurity species from cladding, structural materials or cover gas is sorely needed. Furthermore, solution behavior of selected volatile fission products is needed to provide a data base for evaluation of reactor operation with breached pins. Basic research is needed to understand the physical and chemical phenomena

associated with corrosion processes and plating of radioactive materials on primary reactor surfaces. Such a basic understanding of solute-surface interactions could possibly lead to better choices of construction materials or operational procedures to minimize these deleterious effects. Furthermore, in order to decontaminate or decommission reactors and reprocessing and fabrication facilities more effectively, there is a need to develop new generic classes of chemical agents and techniques. Research should be directed to solution of the problems of cracking of stainless steel piping in BWR's, the denting behavior of PWR steam generators and the control of water coolant chemistry in all types of water moderated reactors.

H. Fuel Reprocessing

The recovery of fissile and fertile materials from spent nuclear fuel elements through chemical reprocessing is the most effective means of nuclear fuel utilization, particularly when employed in conjunction with breeder reactors. Use of such a strategy would substantially reduce our need for acquiring new sources of mined fuels and isotopic enrichment, if the problems surrounding the disposal of nuclear wastes and safeguarding of fissile materials can be overcome. During the past several decades, fundamental reprocessing chemistry studies and development of reprocessing facilities have focussed primarily on the PUREX process. Continued research is needed to solve short-term problems with PUREX and to determine its long-term suitability for use in a mature nuclear industry.

Short-term research to improve upon the PUREX process should be directed to development of a better extractant than tri-butyl phosphate (TBP) that would be more stable to radiation, have better solubility characteristics and lower water retention. TBP suffers from relatively high water retention and formation of a second solvent phase at high plutonium concentrations. Basic studies are also needed to develop electrochemical techniques in reprocessing. Oxidation/reduction cycles for actinides can be carried out electrochemically rather than by use of conventional oxidants and reductants and, thereby contribute to a reduction of wastes and solvent clean-up procedures. Research dealing with insoluble and colloidal compounds formed during fuel dissolution and reprocessing is needed. Additional information is required on rate and equilibrium constants for formation of actinide and fission product complexes, including hydrolysis constants.

The PUREX reprocessing strategy is based upon the isolation of uranium and plutonium and treats all of the other components as a single high-level waste fraction. Furthermore, PUREX was not developed as a low proliferation risk technology nor has it been optimized in terms of nuclear waste management. Basic research should now be strengthened to lay the groundwork for

development of the next generation reprocessing technology, optimized for disposal of nuclear wastes and, if possible, proliferation resistance. There are several advantages to be gained by development of a reprocessing scheme in which a number of elemental separations are performed on the high-level waste fraction. Partitioning the actinides and selectively removing the major short-term heat sources (e.g., cesium and strontium) will simplify waste management considerations. Because the transplutonium elements contribute appreciably to the long-term waste hazards, they could conceivably be recycled in reactors as added fuel value. Alternatively, removing the shorter-lived fission product heat producers from the wastes would greatly simplify the problems associated with incorporating these long-lived hazards in matrices for deep geological disposal. The shorter lived fission products could then be stored in near surface retrieval sites while they decay or are used for their low-grade heat value. Furthermore, sizable quantities of commercially important elements, e.g., stable palladium, could be removed from the process stream if a more detailed processing scheme is developed. In order to develop an optimum reprocessing technology, a better understanding of the aqueous chemistry of actinides and fission products will be needed. We must build-up our experimental and theoretical capability to design molecular extraction systems with more selective elemental complexing properties. Efforts should also be directed to exploiting relative chemical reaction kinetics as an additional variable in separations technology. In addition to developing new chemical systems, efforts should be directed to developing new separations and hardware methods such as high-speed contactors (to achieve greater efficiencies in separation and reduction in phase contact times thereby minimizing radiation damage effects to the organic solvent), gradient elution continuous chromatographs, and membrane techniques.

Some research effort should also be maintained on non-aqueous reprocessing (e.g., pyrometallurgical or volatility methods) with the goal of identifying next generation processes which would be more cost effective than PUREX, generate smaller waste volumes, and yield products more ideally matched to waste management strategies.

I. Nuclear Waste Management

The development of a technology to ensure safe disposal of radioactive wastes for tens or hundreds of thousands of years is one of the major barriers to the development of nuclear energy. The most promising method currently being investigated is emplacement of the radioactive wastes in deep geological repositories. Much of the scientific information and methods required to evaluate the geology and hydrology of a potential repository is already known and many of the scientific techniques required to gain additional specific data have already been or can with

confidence be developed. Comprehensive information exists on the properties of rocks, seismic activity of crustal bodies, ages of rocks, and genesis of rock formations. Scientific and engineering fields are established for studying rock mechanics, hydrologic properties, seismic simulation, age dating and petrology. However, in order to fully develop and attain confidence in the deep geological disposal concept, high priority should be given to fundamental research directed to developing stable waste-form materials to contain the radioactive wastes and to developing an accurate model of the transport of nuclear waste elements by water through geological strata. With a comprehensive understanding of waste-element transport, disposal sites can be selected with confidence which minimize the possibility of transport of the radioactive nuclides to the biosphere in the event of a catastrophic breach of the repository.

Incorporation of radioactive wastes into glass matrices is currently being actively pursued. However, many glasses have serious disadvantages such as devitrification at elevated temperatures and significant leaching and chemical attack in brine solutions at elevated temperatures and pressures. In addition to continuing research on glasses, other potential waste-form matrices should be investigated such as new high-silica glass forms, ceramics, synthetic rock preparations, and metal encapsulation of glasses or ceramics. Each of these candidate matrices should be extensively studied for its physical and chemical stability. Basic knowledge of bonding of fission products and actinides in candidate matrices, diffusion mechanisms, mechanism of cation partitioning in devitrified glasses, mechanisms of waste form dissolution in liquid media and the effects of intense radiation on all the above mechanisms are required for scientific and technical development of the optimum waste form. The effects of helium produced in alpha decay on the stability of the waste form needs to be understood as a function of time and temperature and related to diffusivity, bubble formation and induced strain. Transmutation effects and the effects of changes in chemical species, charge and ionic radii on crystal stability needs to be understood. More stable waste forms than those presently being considered may be identified by studying the structures of naturally occurring minerals that contain uranium or thorium and have been stable for hundreds of thousands of years.

Present empirical laboratory studies provide qualitative information on the rates of radionuclide transport by water through various geological materials. However, a detailed understanding of the fundamental reaction mechanisms involved is needed before quantitative assessments can be made as to the fate of nuclear wastes in actual geological media. Of importance, the chemical forms of the actinide and fission product elements leached from the waste forms and their thermodynamic stabilities in the geological environment near the repository

must be known. The rates of elemental migration depend strongly on the oxidation states of the actinides or fission products and on whether the elements exist as ionic or hydrolyzed species, colloids, silicate species or precipitates. The interaction mechanisms of these species in solution with geological materials must also be studied. In particular, it is important to know what specific sites in geological materials bind actinide and fission product elements, e.g., specific mineral constituents, grain boundary interfaces, secondary mineralization or deposition sites.

It is imperative that well defined field experiments be conducted as early as possible in conjunction with laboratory studies to establish confidence in extrapolations from laboratory to actual repository conditions. For example, in the area of radionuclide transport it is very important to conduct well defined field tests to determine if laboratory studies are being made under conditions appropriate to natural systems and if models of nuclide transport derived from laboratory experiments correctly predict nuclide transport by water under in situ conditions.

New experimental methods must be developed in order to study the chemistry of actinide and fission product species existing in waste-form matrices and in extremely dilute and complex ground water solutions. Several methods which may have important applications, if successfully developed, are fluorescent laser spectroscopy, laser thermal lensing, field flow fractionation, EXAFS, emission Mossbauer spectroscopy and charged-particle depth profiling.

IV. CONCLUSIONS

Recommendations for needed basic research covering the entire spectrum of activities in the nuclear fuel cycle have been given in this assessment. Because of the present lack of a National commitment to a specific nuclear energy development strategy, the research needed at this time to effectively pursue the numerous nuclear options available is extensive. During this period of uncertainty, it is important to maintain as strong a basic research component as possible to develop the scientific foundation needed to make future crucial decisions on nuclear options with confidence.

The two general areas identified in this assessment as meriting the highest priorities for basic research are:

- 1. Research in support of nuclear waste management and, in particular, the deep geological nuclear waste isolation concept.*

2. *Research directed to the development of materials with superior high-temperature, corrosion and radiation resistance for use in the reactor environments.*

Basic research in these two areas is of the utmost importance to most nuclear power options and is directed to the solution of a number of the major issues currently confronting the development of nuclear energy, e.g., the safe long-term disposal of nuclear wastes, reactor safety, more effective fission fuel utilization, and reactor economics.

During the course of this assessment, it was obvious that a number of specific fundamental research program areas presently being conducted by Basic Energy Sciences can have a broad and important impact upon the future development of a number of different components of fission-energy technology. For example: (1) Materials problems are the most commonly encountered barriers to the further development of a number of technologies. A continuing strong BES Materials Sciences Program will be very important to the development of the new materials which are needed. New materials are needed with superior high-temperature, corrosion, and radiation resistant properties for use in reactor environments. New materials, chemically inert to conditions prevailing in deep geological media and resistant to radiation effects, are needed for safe long-term encapsulation of nuclear wastes. (2) Strong continuing programs in actinide element research (currently funded through the Chemical Sciences, Nuclear Sciences and Materials Sciences Divisions) are needed to provide the data base for future developments in exploration, milling, isotopic enrichment, fuel element chemistry, reactor design and operation, reprocessing and nuclear waste isolation. (3) Continuing fundamental Separations Chemistry Research in the Division of Chemical Sciences is needed for future advances in leaching of ores in situ, milling, isotopic enrichment, reactor operations, and reprocessing technologies. Research in support of nuclear waste management is identified as one of the highest priority needs for development of fission-energy technology. Therefore, components in all BES Divisions that can contribute to nuclear waste management technology development should receive strong emphasis.

At this point we must also stress the obvious. Research and technological developments alone can no longer establish nuclear energy as a future major energy resource in this country without re-establishing public confidence in nuclear energy. This will be a long-term task involving not only a clear resolution of scientific and technical issues but also a considerable public educational effort on radiation hazards and the relative risk assessments of alternative energy technologies. The nuclear reactor industry must continually demonstrate safe, reliable performance. Furthermore, successful pilot development

of nuclear waste isolation repositories and successful operation of a major fuel reprocessing plant will contribute greatly toward establishing confidence in these technologies. In order to accomplish these tasks, a broad-based fundamental research program is required to provide the needed innovation and scientific foundation and continually point out the best path to follow.

APPENDIX

In preparing an assessment as broad in scope as this, the ANL Working Group felt that it was essential to seek recommendations from as broad a spectrum of experts as possible. The Working Group contacted a large number of experts in basic and applied research and development at industries, National Laboratories and universities by letter, telephone and personal visits seeking recommendations. The large number of recommendations received were then collated and critically reviewed by the Working Group and specific consultants. Because of the need to provide a short, concise critically edited document, many recommendations could not be included in this draft and other important recommendations had to be severely edited down to a few sentences in length. Because of the severity of this review and editing process, the contributors listed below should not be viewed as responsible for any shortcomings in this document or viewed as endorsing the recommendations made. We list the contributors here as an expression of our appreciation for their efforts in providing recommendations. A number of the contributors listed below have provided collective recommendations from the staff at their institutions.

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ASSESSMENT OF
BASIC RESEARCH NEEDS
AND PRIORITIES
IN SUPPORT OF
FOSSIL ENERGY

October 1, 1979

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INTRODUCTION

This document attempts a comprehensive delineation (for the DOE Basic Energy Sciences Office) of the areas in which basic research might make major contributions to the program of Fossil Energy development. It describes problem areas in which we believe that research in the physical sciences is needed and indicates the relative priority that we would accord such areas. Solution of most, if not all, of the problems will require applied research and demonstration efforts on a sequentially increasing scale. But most of the listed problem areas embody elements that basic research could address with varying probabilities of success and with varying degrees of impact after various (though seldom short) times. The relative priority accorded each item reflects our opinion of the probable value of the basic research contribution; it is not necessarily our assessment of the priority that the overall problem area (including its applied components) should have. We have not attempted to assess in detail the extent to which the on-going basic researches are commensurate with the need. Our conclusion that particular researches are needed does not, therefore, necessarily mean that present researches need augmentation.

In preparation of this document we have drawn upon previous studies that have done portions of this exercise and have had suggestions from our colleagues at the Oak Ridge National Laboratory. Moreover, we requested and obtained helpful advice from many knowledgeable individuals and institutions. These contributors - who submitted suggestions and/or commented upon one or more previous drafts - are gratefully acknowledged in Appendix A.

We have chosen to organize our discussion of the problem areas generally by fossil fuel source and subsequently by technology. To minimize repetition, however, we have found it convenient to first present a minimal list of (generic) researches that apply to several source materials and finally to list research needs for several technologies (i.e., Indirect Liquefaction) that apply to several or all of the source materials.

We are aware that the organizational format tends to emphasize the needs of present or presently conceived technologies. This tendency, if recognized, is not entirely bad. Technology frequently leads science. Pilot - or even larger scale - plants occasionally make breakthroughs that can lead to productive basic researches. At the same time, emphasis upon present needs tends to discourage funding of the truly speculative and innovative researches that we, along with many others, believe to be an urgent need.

Though virtually all of the research needs described below have applied components, we do not imply that BES should be made responsible for applied research even where such is clearly valuable or urgently needed. Nor do we imply that BES should be responsible for all of the truly basic research in DOE. Each applied mission of DOE needs to maintain the basic researches that are vital to that mission. The overall basic research program must adequately support the technologies and must also bear a major responsibility for ensuring the training of successive generations of needed scientists. That program must, accordingly, be of scope sufficient to assure the well-being of the scientific disciplines required. For this mission, it seems certain that increased funding for

basic researches in Fossil Energy is needed. It is certain that stability of that funding is absolutely essential.

The following sections list and very briefly describe problem areas in which research (including a complement of basic research) is clearly needed. The basic research component of each item - excepting brief expository statements - is assigned a relative priority rank ranging from modest (*) to very high (****).

RESEARCHES COMMON TO SEVERAL SOURCE MATERIALS

All of the broad domains (i.e., surface science) and most of the more specific areas (i.e., mechanisms of catalysis) of basic physical science can assist with problems in development of each of the fossil sources. In that sense, and at that level of categorization, there are very many researches that are common to several source materials. But most of the specific needs - and the thrusts of the needed studies - differ substantially among the several fossil sources and seem more appropriately described for the individual source or for a particular technology. However, a few basic research areas seem clearly to be common to most of the source materials. These are briefly described below and are not repeated elsewhere, though subsequent sections note associated researches peculiar to the individual source or technology.

ORGANIC CHEMICAL COMPOSITION AND STRUCTURE^a

In a chemical sense and with some oversimplification, the fossil source materials constitute a continuum ranging (in order of generally decreasing complexity) from coals through oil shale kerogens, tar sand bitumens, and heavy petroleums to "normal" petroleums with natural gas a much simpler special case. Problems in composition and structure are trivial for natural gas and are, probably, adequately solved for "normal" petroleums. But there are serious deficiencies in our knowledge of the structure - and even some facets of the composition - of the organic portion of other source materials. If we knew enough about the basic building blocks of these sources to understand how they respond to chemical and thermal forces, we could almost certainly improve presently envisioned processes for preparation, conversion, and upgrading of these materials. Moreover, such knowledge might reasonably be expected to lead (especially with kerogens and coals) to markedly different processes that would afford more useful products through gentler treatments and milder conditions.

Some of this understanding of detailed chemical structure can be gained by application of recently developed instrumental methods directly to the source materials. But some must be inferred from study of separated fractions after (for coals, kerogens and bitumens) depo-

^aThe organic materials in coals, oil shales, and tar sands are intimately admixed with inorganic materials. The mineral matter also deserves basic study as discussed under the individual source materials.

lymerization (liquefaction) through breakage of the more susceptible bonds along with more or less additional structural alteration.^a

Our knowledge of the nature and, in some cases, the quantity of elements other than carbon and hydrogen in the organic materials is insufficient to guide exploration of processes for removal of these elements during conversion or product upgrading. Improved rapid and direct methods for determination of oxygen and sulfur are needed.*** Methods are needed to determine occurrence of oxygen, sulfur, and nitrogen in substituent functional groups, in heterocycles and as ether or thioether linkages;**** nuclear magnetic resonance techniques applied to natural ¹⁵N, ¹⁷O, and ³³S may prove valuable.*** Identity and quantity of metallic species (generally present in trace quantities) in the organic matrix can be reasonably well determined by available methods, but methods for obtaining information about the nature of the metal-organic bonding are needed.***

The structure of the carbon skeleton with its functional groups and cross-linkages becomes much more complex as the sequence is ascended from petroleum to coals. Recent breakthroughs in instrumental methods - some applicable to solids as well as to liquids - should permit marked improvement in our understanding of structures of bitumens, kerogens, and coals. It is apparent, however, that complete understanding of organic structures, if realizable at all for the more complex materials, will require studies of many kinds over a long time span. Fortunately, it appears that understanding of certain key features of the structure may offer great assistance to technology development.

Definitive information about relative amounts of aromatic and aliphatic carbon and hydrogen is needed;** special nuclear magnetic resonance techniques can yield at least a part of this information.

For the more complex source materials much of the needed structural information must be obtained after depolymerization reactions that, by breaking the more susceptible chemical linkages (scissile bonds), produce smaller and more manageable entities. We need to know the number and nature of the bonds that are broken as well as the structures of compounds within the product materials.

The bonds broken in depolymerization reactions probably include some cross-linkages between macromolecular chains as well as reactive bonds within the chains. The frequency and the nature of network cross-linkages in coals and kerogens are poorly known and need to be determined.*** Identification of scissile bonds within the chains would be assisted dramatically by development of a suite of mild and selective

^aHere, as in many other places, problems arise as to what is "basic" research. As an example, a large fraction of a coal is solubilized by short-term heating with a hydrogen donor-solvent. Study of this liquid can be deemed "applied" since such study could reasonably be expected to lead to improvement of the donor-solvent process. But the liquid must contain many of the original coal building blocks, and careful study of its fractions can help to elucidate the structure of coal. We would consider its study for that purpose to be "basic."

reagents;** search for such should be encouraged though success can hardly be considered likely. Systematic study, as by use of labeled model compounds, of attack by available degradation reagents on bridging structures and substituent groups is still needed.***

Study of the degradation products would be markedly assisted by development of methods for more effective fractionation of the products both by molecular weight range and by nature of functional groups.*** Progress has been made in instrumental methods (such as nuclear magnetic resonance and photoelectron spectroscopy) in determination of functional groups in such fractions, but opportunities for improvement still exist and innovative ideas should be pursued.*** A better knowledge of molecular weights of separated fractions is needed. Number average molecular weights can be obtained by "osmotic" techniques, though difficulties persist in high-molecular-weight ranges; some improvement in such methods could probably be obtained.* But a small proportion of low-molecular-weight material in a fraction produces a large effect on such number average weights. Sound methods for determination of weight average molecular weights (perhaps by light-scattering, ultra-centrifugation, or by special source mass spectrometry) are badly needed.****

REACTION MECHANISMS AND KINETICS

A great many reactions could be considered as common to several of the fossil fuel sources. Reactions with hydrogen, for example, are clearly envisioned for use with coals, may be of value for oil shales, and may very well be used in product upgrading of materials from many fossil sources. We have chosen, however, to discuss hydrogenations under specific source and technology headings (see pages 17, 22, and 36). The reactions that seem clearly suitable for inclusion here are those involved in pyrolysis, in oxidation, and upon gasification of the source materials with steam at elevated temperatures.

Pyrolytic Reactions

Heating of the complex source materials to progressively higher temperatures in substantially oxygen-free atmospheres yields gases, complex liquids, and solid (and generally porous) carbonaceous residues. Composition and properties of the products of such pyrolysis vary with the character of the material used and with heating rate and ultimate temperature. Pyrolysis is a widely practiced technology by which gases, liquids, and cokes are produced from coals, petroleum bottoms, and tar sand bitumens (pages 14 and 23) and by which oils are liberated from oil shale kerogens (page 20). It is, moreover, a precursor in combustion processes and in many liquefaction and gasification operations in which solid or heavy liquid materials are heated with other reagents.

The reaction sequences in pyrolysis are obviously complex. Thermal cleavage of scissile bonds (with progressively stronger bonds cleaved at higher temperatures) generates free radicals. The radicals may abstract labile hydrogen to form relatively small molecules or may combine with each other or with the macromolecular matrix material. By continuation of such sequences at successively higher temperatures most of the hydrogen appears in volatile gases and liquids - whose escape is hindered by the viscous liquid or semi-solid reaction medium - and a fraction of the

carbon remains as coke or char. An important long-term research goal is a much improved understanding of the sequences, mechanisms, and rates of these important reactions.*** Recent studies with model compounds (such as 1,2-diphenylethane or ethylbenzene in benzene solution) at high temperatures have shown that electron spin resonance techniques can detect, identify, and quantify the free radicals involved. Cracking of such compounds, and of even more simple ones, are important reactions in pyrolysis; mechanisms and rates of such decomposition seem amenable to direct study. Extension and elaboration of such techniques should permit study of more complex compounds (though only the total number of radicals could be determined in pyrolysis of a complex material such as coal) and would offer a powerful tool for study of pyrolytic and related reactions.****

Oxidation Reactions

Oxidation reactions are clearly of great importance since, in addition to many practical problems caused by ambient-temperature oxidation, it is the fate of a very large portion of the fossil materials, generally after some upgrading, to be burned as fuel in some type of combustion system.

Ambient attack by air results in deterioration of some coals (and probably other freshly mined or exposed sources) and, in some cases, to fires during transportation and storage. Mild oxidation is used to destroy unwanted caking propensities of coals. Studies of reaction rates and mechanisms are needed for oxidation of pertinent source materials under ambient conditions and on mild heating.**

Basic studies of oxidation reactions needed in support of combustion systems are complex in character and several in number. An improved understanding of the mechanisms and kinetics of the elementary reactions under realistic combustion conditions is needed in many areas.*** Mechanisms and rates should be determined for high-temperature oxidation of hydrocarbons and pertinent oxygenated species under a range of oxygen-fuel stoichiometrics.*** Such studies should depend upon several modern diagnostic techniques such as variants of laser spectroscopy and (where pertinent) on the tools of surface physics to elucidate the nature of surface oxides on intermediate chars. Studies are required on nucleation and condensation mechanisms that control formation of soot and smoke particles** (see also page 16). Mechanisms and rates of reactions responsible for pollutants (i.e., NO_x and carcinogens)*** and for control of NO_x (in particular) by staged combustion*** need study. Mechanisms by which NO_x results from combined nitrogen in coal- or oil shale-derived fuels need to be known.** Fundamental studies on the synthesis of chemical and complex fluid flow phenomena are needed to allow identification of dominant or rate determining processes in applied combustion science.****

Reactions with Steam

A complex suite of chemical reactions occurs when source materials (usually coals or heavy petroleum ends) or the cokes and chars derived from them are treated with steam at elevated temperatures. The raw source materials react by complicated and poorly understood pathways that probably differ with different gas atmospheres to yield methane and

heavier hydrocarbons plus residual char. Important reactions of the char are:

In addition, the gaseous species further react by:

The water-gas and Boudouard reactions are highly endothermic; the methanation reactions are highly exothermic, and the shift reaction is mildly so. For reaction at high temperature, where reactions are rapid and equilibria favor CO and H₂ with little methanation, the required heat is supplied by oxidation of part of the feed. If the source materials, rather than chars, are used, pyrolytic reactions precede or accompany the reactions above. This important suite of reactions is used in gasification (see page 15) of fossil fuels to provide - after purification of the product gases - a spectrum of gaseous fuels (page 15), SYNGAS mixtures for methanation (page 16) or indirect liquefaction (page 34), and H₂ for hydroliquefaction (pages 17 and 21), product upgrading (page 36), or other purposes.

Temperature and pressure dependence of the several equilibria is adequately known. However, the simple stoichiometries indicated above give no indication of the reaction complexity. Detailed mechanisms for all these reactions are needed;*** such studies, which should be done under realistic conditions with the several reactions preceding simultaneously, will need to use techniques suggested above for "Oxidation Reactions". Kinetics of the several reactions under realistic conditions are also needed;*** it is probably important to note that kinetics of char reactions need to be done with "nascent" carbon prepared in various gas atmospheres as well as with carbons that have been "aged" in various atmospheres for varying periods.

MATERIALS OF CONSTRUCTION

Most of the technologies associated with the fossil sources could benefit from, and some can hardly be developed without, improved materials of construction. Screening of commercially available materials has produced, in many cases, adequate solutions to specific problems of the several technologies. Such screening (accompanied by studies that establish causes and mechanisms of deterioration) is often essential in providing the data base for appropriate materials development programs. Several such studies (for coal gasification systems, for example) are in progress. For many areas, however, little fundamental understanding of the problems has been developed. Some particular problem areas - requiring applied as well as basic research - are noted under the specific technologies. These problem areas are quite diverse, but many of them have elements in common.

Improved alloys, ceramics, and a variety of composite materials will certainly be needed along with effective means of fabricating, joining, and bonding of these materials. Limitations on service life will derive, in a generic sense, from erosion and wear, from corrosion (often assisted by erosion), and from possible mechanical failure due to multicomponent and cyclic stresses assisted by aging as well as by corrosion and erosion.

Metals and Alloys

The obvious goal of this research is to provide the basis for development of an optimum alloy for each application. In addition, the studies should facilitate development of useful alloys that are less expensive or less dependent upon critical or imported metals; specifically, steels in which Ni and Cr are replaced by more available elements need to be developed.*** To meet these needs, the thermomechanical treatment and the composition of the alloy must be balanced to meet requirements imposed by temperature, state of stress, and multicomponent chemical environments. Fundamental research of high priority should be directed to understanding of the mechanisms of phenomena that limit service life and the dependence of these mechanisms on material composition and properties. Understanding of the behavior of classes of alloys must be the goal since the number of potentially useful complex alloys is so large as to preclude study of all combinations. Development of theory and correlations that can lead to prediction of structure and properties of complex alloys should be encouraged.***

Erosion and Wear

These degradative processes limit service lifetimes in a spectrum of applications from use of mining, drilling, and grinding equipment to operation of turbine blades exposed to very hot gases containing particulates. The importance of the problems (in fossil energy and in many other industries) has prompted much applied research and led to many improved materials, but only a meager fundamental data base exists to guide the development effort. The basic mechanisms of material wastage - though they may differ substantially over the range of service conditions - need first to be defined and understood.** As these are developed, both theoretical and practical understanding can be invoked to provide alloys with the desired structural and other parameters desired.** The properties required for abrasion- and wear-resistant surfaces will seldom be desirable for the bulk metal; accordingly, composite materials (see subsequent discussion) will often be required.

Corrosion

Many of the process environments expose the alloy to several corrosive agents (including sulfur compounds) at low oxygen partial pressures or even strongly reducing atmospheres; in some systems, solid or liquid deposits are likely and synergisms with erosive processes compound the problem. The active species in the corrosive fluids seem to be identified in most - but probably not all - cases. A markedly improved understanding of the mechanisms by which alloys corrode in realistic complex environments is needed.*** This simple statement of a host of complex problems represents an immense undertaking in which carefully designed applied research must play a large part. Basic thermodynamic

data (such as stability of simple and complex sulfides and activity of species in stable and metastable alloy phases) is needed in many cases.*** These data, along with diffusion coefficients of the rate-controlling species in the bulk alloy and in films and coatings,*** will often be necessary before corrosion mechanisms can be verified or, in some cases, developed. Establishment of the dependence of the mechanisms on material and process parameters should permit selection or development of improved alloys. The required studies will include both laboratory experiments upon the isolated processes and studies in realistic systems to include the possible synergisms.

Mechanical Failure

Mechanical failures pose problems in fossil energy development (as in all industries), and the needs for basic research go far beyond testing under uniaxial stress. Research is needed on mechanisms that lead to failure at high temperatures through multicomponent and cyclic stresses in the presence of aggressive environments.**** The role of grain-boundary-active species (such as sulfur) needs attention.*** Lower-temperature processes in need of study include mechanisms of hydrogen embrittlement and stress corrosion phenomena.***

Materials Engineering

Fabrication and welding are often considered too complex for basic research, but many components of the problems should be amenable to productive study. Innovative fabrication techniques have had major impacts on other industries (eg., single-crystal jet engine turbine blades; laser-processed electronic components); fossil energy development, with its wide variety of problem areas, should profit from far-ranging fabrication research.

A particular need is for research in joining dissimilar materials.*** Mechanisms (and their prevention) of cracking in welds between austenitic and ferritic steels and effective transitions between metals and ceramic components are obvious examples.

Failure of alloys (and particularly of weld-affected zones) due to precipitation (aging) in long-term service at elevated temperatures is a related phenomenon that needs basic study.*** Recent techniques from evaluation of radiation damage may be used to accelerate such aging so that multi-year processes can be studied on a time scale commensurate with materials development.**

Ceramics

Chemical stability and high-temperature capability make ceramics attractive materials for combustion chambers, process vessel linings, heat exchangers, and turbine blades. Ceramics are generally more inert, less ductile, and less well understood than metals, and their use presents problems largely different from those with alloys.

Research is needed to develop an understanding of deformation processes,** of thermal shock resistance,*** and of grain boundaries and grain boundary phases*** that determine high-temperature properties. Castable ceramics with improved creep strength are needed as liners in process vessels.** Improved basic understanding of corrosion and erosion behavior of ceramic materials in appropriate environments is

needed.*** Fundamental study of fabrication techniques and of ceramic-ceramic and ceramic-metal joining is necessary.*** Applied research - which basic study can assist - is needed to devise methods for design of components using these brittle materials.

Composites

Some service requirements cannot be met by monolithic metals or ceramics, and for others only very expensive materials will suffice. For such cases, two or more materials can frequently be combined in a composite that will fill the need. Several general classes of such composites are used. Those based essentially upon metals and alloys include claddings and overlays - where protective but expensive layers coat cheaper substrates, hard-faced materials - where brittle wear-resistant surfaces are produced on a tough metal core, and surface-modified materials - where surface composition is altered to achieve specific properties. Composites of metals and ceramics include refractory linings - used for chemical protection or thermal insulation, and surface coatings - as of polymers, oxides, or other materials. More recent innovations include fiber-reinforced composites, which may be of ceramic-metal or ceramic-ceramic composition.

These materials offer a vast opportunity for innovative research into more effective, more efficient, or more economical ways of achieving the required property combinations. Research areas that seem ripe for attack include the bonding interface between dissimilar materials,*** the development of multilayer gradations between external layers with desired properties,** the development of in-situ application of coatings (as is the case of oxidized surfaces),** and the "invention" of protective layers that will be self-repairing in the service environment.*** Ion implantation, used in the UK to markedly improve lifetime of nozzles in oil-fired power stations, may find expanded application to these needs.

Nondestructive Examination

Nondestructive examination, also needed in many other industries, attempts to assure the initial integrity of components and to detect incipient failures in time for repair. Techniques, especially for initial examination, are available and in common use, but precision of defect location and description is lower than desirable. Research to provide a better quantitative model for defect-signal coupling is needed.** Better techniques for the continuous, or at least periodic, inspection of operating equipment (without shutdown) are also needed.*** This requires development of probes capable of operation in chemically and thermally hostile environments.*** Inspection techniques for composite materials are needed** - for example, for the in-situ measurement of the integrity of coatings and surface-modified layers.

MISCELLANEOUS

Many of the conversion and upgrading technologies require hydrogen in large quantities, and some require separated oxygen. Both of these requirements add significantly to the process cost, and more economical production methods are highly desirable. It seems likely that a portion of the fossil fuel must be used to provide the hydrogen via gasification

with steam followed by shifting and purification; basic studies listed for this technology (page 15) should assist with the economics of H₂ production. Recent studies in which slurries of coals or cokes serve as the anode in electrolysis of water may provide a lead to new approaches to H₂ generation; mechanisms seem not to be understood and might well be the subject of basic study.** Separation of oxygen from air is a mature technology whose economics will probably prove hard to improve. It is easy to say that innovative ideas should be pursued, but it is difficult to suggest specific basic research areas. Recently reported development of coordination complexes of manganous salts with tertiary phosphines that reversibly sorb and release oxygen at ambient temperature simply as a function of O₂ partial pressure may offer a lead worth basic study.**

There seems to be a need for an accessible bank of organic materials (particularly liquids) derived from fossil fuels for use by researchers so that results from a variety of techniques can be compared among the various laboratories.*** Provision of such a bank is hardly basic research, but it would fill a need that basic researchers share.

ABOVE-GROUND PROCESSING OF COALS, OIL SHALES, AND TAR SANDS

The research needs associated with source materials and with the several technologies that are, or may be, employed for their above-ground conversion into usable or upgradable products are described under this heading. In-situ conversions may be used to convert these materials, as well as heavy oils or otherwise irrecoverable petroleums, to gaseous or, in some cases, to liquid products. Such in-situ conversions of the several source materials seem to contain enough research needs in common to justify their description under a single heading in a later section of this document. Moreover, the additional topics of research needs in Indirect Liquefaction (synthesis from SYNGAS), Product Upgrading and Combustion of Refined Products all seem sufficiently source independent to justify their inclusion as separate items in the final section.

COAL^a

Our fundamental understanding of coals at present is generally perceived to be inadequate. Coals, excepting those of the highest rank, are remarkably reactive materials, but the basic factors responsible for this reactivity are poorly understood. Some researches are common to several technologies presently envisioned for effective use of coal or seem to be necessary if superior technologies are to be discovered; our listing of these is presented under "Generic Research Needs" below. Other areas are of primary interest to a single coal technology; these are presented under that technology, though knowledge so gained may well be of value elsewhere. Many of the listed needs contain needs for in-

^aAs used here, "coal" includes all of the diverse materials, ranging from lignites through anthracites, that constitute the coalification series. In addition, it should be realized that peats, though not generally considered to be coals, share many of the listed research needs.

vention or development of accurate and automatable analytical and physical measurement techniques.

Generic Research Needs

Coals share all of the research needs listed (pages 2-9) as common to several fossil sources. Additional needs of value to several coal technologies are described in the following.

Chemical Composition and Structure (see also pages 2, 3)

Coals offer complexities that are not shared by the other fossil sources. Chemical composition and behavior vary markedly with maturity (rank) in the progression from peats through lignites and bituminous coals to anthracites. Moreover, the organic portion is a mixture of petrographically distinguishable ultimate constituents (macerals) that differ in appearance, optical properties, chemical composition, and reactivity.

Consequently, ancillary needs in the study of coal composition and structure are for new or improved methods for separation of coal macerals (especially those other than vitrinite)*** and for innovative approaches to study such macerals as individual grains without separation.** The systematic changes in chemical structure of the macerals from coals selected to represent a range of ranks, geological antecedents, and petrographic compositions need to be determined.**

Coals appear to contain a small quantity of relatively simple organic compounds trapped within the porous structure or very loosely bonded to the structure; the identity and abundance of these trapped organics need further study.** Vacuum evaporation at relatively low temperatures can provide useful information. Extraction with supercritical fluids appears to remove these materials (along with various depolymerization products). Basic study of such super-critical extraction is needed;** study should include characterization of the physical and chemical structure of the residues.

Depolymerization sequences (with solvents and mild reagents, see page 3) are particularly important in study of chemical structure of coals. Many treatments have been used, but much work remains to establish, by a variety of studies that include ^{14}C -labeled model compounds, the reactions and reaction sequences that occur.**** In general, reagents capable of rapid depolymerization at low temperature should be preferred with emphasis upon the structure of the asphaltol fractions.

Coals also contain mineral matter as discrete - and, in principle, removable - bands and as particulate matter intimately admixed with the macerals. Further knowledge of the identity and quantity of inorganic species, identity of the specific minerals (along with their particle size range and degree of interaction with the macerals) is needed.*** The goals here should include understanding (via systematic geochemical study) of why a coal contains its particular suite of minerals.*** In addition, we need to identify the chemical reactions of the minerals upon heating (and with added inorganic species where pertinent) and the phase behavior of the resultant products*** as a basis for understanding ash, slag, and clinker formation. [Coals also contain small quantities of metallic species organically bonded in the structure; studies directed to these were discussed previously (page 3).]

An ultimate and very long-range goal is an understanding of the structural and other factors that are responsible for reactivity of coal with at least a few pertinent reagents. To that end, measurements of relative reactivity (versus rank and composition) are needed for reagents such as H_2O and H_2 .***

The program implied above will, at best, require a large and long-term effort. Some of the desired information will require study of coals of several ranks. It is essential, however, to limit the detailed studies to a relatively small number of carefully chosen coals.

Physical Structure and Properties

The internal surface area and the pore size distribution of coals change systematically and markedly with rank. These features of coals and of the cokes and chars produced by pyrolysis (see pages 4 and 14) control reagent access and product egress during conversion and combustion. Systematic comparative information (as by sorption-desorption equilibria with a variety of gases and vapors and by small angle x-ray scattering) is required on the surface area of a variety of selected and carefully pretreated coals and on the changes in these areas upon treatment with heat and with reagents.*** Determination of absolute surface areas is desirable but less essential.* Systematic understanding of pore structure and pore size distribution (by modern transmission electron microscopy, modified small-angle x-ray scattering, sorption equilibria and kinetics and rates of diffusion of gaseous species) of coals, chars, and other solid reaction products as functions of pretreatment or processing conditions is necessary.**** The overall goals include fundamental understanding of the nature and number of active sites in the coals and chars, of their interaction with chemical species, of the effects of reagent and product diffusivity on reactivity, and of mechanisms for modification of pore structure for improved reagent accessibility.

Physical properties of coals are important for many technological applications, but needs for systematic basic researches appear to be relatively few. A systematic investigation of electrical conductivity and dielectric constant as functions of electric field polarization and direction of travel would be valuable (especially if correlated with other coal properties) in design of remote electromagnetic instrumentation for monitoring within a coal medium.***

Some coal technologies desire fine particles, but others find coal fines unusable. Study to establish the relationship among physical and mechanical properties of coals and rates of application of compressive energy to particle size distribution of the comminuted product would be valuable.**

Engineering Research

Effective scale-up of conversion and combustion systems and systematic development of more efficient systems require an improved understanding of the complex interactions in reactive gas-solid (i.e., fluidized beds) and gas-liquid-solid (i.e., slurry contactor) systems. We need a markedly improved synthesis of the complex chemical, heat transfer, and solid-fluid flow phenomena in such reactor systems (including wall effects and surface effects) to permit identification of

the dominant processes and realistic modeling of the systems.**** Such researches will require experimentation in engineering equipment (of small to moderate scale) dedicated to obtaining basic data rather than process improvements. Diagnostic instrumentation capable of defining the reaction zones, sensing key chemical reactions, and determining rates of movement of solids and fluids in reactors and in associated conduits is needed.*** Development of sound and sufficiently detailed models of the process and iterative testing of the models are required.*** Such experimentation and theoretical modeling will require a variety of scientific disciplines in an integrated effort and will be expensive even on equipment of moderate scale. But the basic understanding is urgently needed, and the cost of a demonstration plant failure for lack of such data is very high.

Coal technologies must all be expected to produce gaseous and liquid effluents that must be released to the environment and to yield solid wastes that must be controlled. Information concerning identities and concentrations of noxious species in specific process wastes would properly be the subject of applied research. However, much basic knowledge (such as phase behavior, partition coefficients, etc.) is needed if optimal engineering (including bioengineering) processes are to be developed for removal of noxious materials from effluents, if processes for leaching and dispersal of noxious materials from storage piles and disposal sites are to be understood and controlled, and if processes for recovery of values from residues, ashes, and slags are to be developed.** Specific, though by no means exhaustive, examples are given under individual technologies below.

Materials of Construction

All researches described previously (page 6) apply particularly to materials of construction for the coal technologies, which expose the structural metals to environments with a wide range of redox potentials, a multiplicity of corrosive agents, and additional complications from abrasive materials and formation and deposition of condensates, ashes, and slags. Specific materials research needs are described under the separate technologies below.

Needs in Mining, Beneficiation, and Transportation

It seems certain that future thrusts in underground mining of coal will be directed to improved mine safety, improved recovery of coal from the mine, and to the ability to mine deeper seams. Improved basic understanding of rock mechanics, of the mechanical properties of coal, and of factors influencing support strength of pillars can assist with these goals.** Development of automatic or remote controlled mining systems is an important applied effort that may well have a major economic impact. Basic understanding of coal and rock cutting (in combination with water jets or sonic intensifiers) can probably assist such development;* basic studies of physical properties (see page 12) might offer assistance with guidance systems for such machines.**

Future thrusts for surface mining seem certain to be reduction of environmental impact without undue economic penalties. Digital terrain modeling appears useful in such planning, but additional basic study is

needed to improve ability to model hydrological and air movement phenomena.**

Fundamental relationships among characteristics of minerals (particularly sulfur-bearing minerals), physical properties of coals and optimal grinding regimes are needed to assist in optimization of physical, gravity, magnetic, and surfactant separations of minerals from coals.** Basic understanding of surface and interfacial properties would assist surfactant separations, froth recovery of coal fines, and purification of pipeline transport water.**

Some coals show a pronounced and rapid degradation in heating value (and in other properties) after removal from the seam, and coals (especially those of lower rank) sometimes burn spontaneously during transportation or storage. The changes in physical structure upon drying, need systematic study,*** as do the mechanisms by which ambient-temperature oxidation (possibly assisted by other phenomena) leads to spontaneous combustion.** Mechanisms for reaction of coal slurries with pipeline transport water need to be established.* Basic studies of contaminants in water after prolonged exposure to slurried coals can probably assist with effective cleanup of such water before discharge.*

Environmental contamination by sulfur-bearing species from mines and storage piles could probably be reduced by improved knowledge of mechanisms for oxidation (including bio-oxidation) and leaching of sulfurous compounds.**

Fundamental relationships among alloy composition and microstructure and abrasive wear need to be developed so that wear-resistant alloys can be optimized for handling of coal-mineral systems.** The goal is development of abrasion-resistant alloys that offer better performance or alloys with minimal concentration of strategic constituents for use in mining, grinding, beneficiation, and transportation equipment. We need, in addition, to understand performance of polymers and films to assess possibilities of these relatively inexpensive materials for use in slurry pipelines.**

Needs in Production of Gas, Tar, and Coke by Pyrolysis (see also page 4)

Pyrolysis is used to convert coals (and heavy petroleums) to hydrogen-rich gases and upgradable liquid products and hydrogen-poor cokes, carbons, or chars. Though coal gas and coal tar were once valuable fuels and chemical intermediates, metallurgical cokes (from coals) or petroleum cokes have, in more recent years, been the primary product. Needs to establish the complex chemical sequences involved were previously described (page 4); these are rendered more complex in the case of coals by the porous nature of the material (the product egress problem) and of its semi-solid and solid products (see page 12).

Standard tests - largely empirical - to determine the ability of coals to form sound cokes have long been available, and existing rules for mixing coals for satisfactory coking appear entirely adequate. Coke manufacture is a mature art, but little is known in detail about the behavior of coals in the plastic state, where volatiles are evolved and cracked, the coal behaves as a liquid, liquid crystals are observed, and the porosity seems still to exist. We need to understand the chemical processes, the physical properties, and the surface physics and chemistry as coking coals are heated through the plastic range.***

Needs in Combustion and Gasification

Though the desired end-products are different, these technologies have many features in common. Both include pyrolysis and devolatilization of the coals, both attempt complete reaction of the carboniferous matter, both, in large part, rely on gas-solid reactions at high temperatures to produce gaseous products, and both must deal with coal minerals and ash.

Improved understanding of the detailed mechanisms and kinetics of the pertinent elementary reactions under realistic conditions (as described generically on pages 4-6) are needed for both technologies.***

Several gasification processes and some combustion systems cannot use caking coals. Mild oxidation is frequently used to destroy agglomerating propensities of coal. Study of mechanisms of such destruction might lead to more effective methods with even smaller losses in energy content of the coal (see also page 4).*

High-temperature behavior of the mineral matter in coals is important to both technologies. Understanding of the phase behavior of coal minerals and their reaction products and of fluid properties of slags are needed to assist in design of gasifiers and combustion equipment.** The inorganic materials that volatilize from ash and slag need to be identified, and the mechanisms of nucleation, condensation kinetics, and the chemical and surface processes that lead to formation and deposition of fly ash and soot need to be understood.*** The catalytic activity of coal minerals and their reaction products and the mechanisms of such activity need to be established both for combustion and gasification reactions.**

Other basic studies of catalysis and of catalyst deactivation are of especial interest to these technologies. Study (page 5) of mechanisms of oxidation might suggest interesting possibilities for catalyzed combustion or of CO (producer gas) generation that could be examined.** Understanding of mechanisms of catalysis of the shift reaction and of deactivation of such catalysts might lead to improved catalysts or to extended catalyst life.** If CO and H₂ (as for shifting to SYNGAS mixtures) are the desired products, steam gasification must be accomplished at relatively high temperatures where the water-gas reaction is at a favorable equilibrium; these reaction rates are rapid, and catalysis will offer only moderate advantages. Such SYNGAS can, of course, be used (after purification) for methane production at relatively low temperatures; mechanisms of CO-H₂ methanation seem relatively well understood. A valuable applied study, which basic studies could assist, is development of more rugged and sulfur-resistant catalysts and catalysts for methanation at higher temperatures (as to produce superheated steam).***

Methanation reactions (page 5) are strongly exothermic, while the water-gas reaction is strongly endothermic. If the suite of reactions could be catalyzed to yield useful reaction rates at temperatures of 400-600°C, nearly adiabatic methanation of coal carbons could be attained in a single stage. Alkali-metal compounds at relatively high concentration appear capable of such catalysis at temperatures as low as 700°C. Identification of mechanisms of such catalysis is needed to assist the search for more effective catalysts at even lower temperatures.****

Gasification of coal at 700° to 1000°C by short-time treatment (less than 10 seconds and with shorter times at the higher temperatures) with hydrogen at pressures generally above 50 atmospheres is a promising possibility. Basic study of mechanisms and kinetics of such short-residence-time hydrogasification is needed.*** For such studies improved instrumentation for measurement of gas temperature and composition will be valuable.*** Variants of this process (using shorter times or lower temperatures - see page 17) can also produce liquid products. Whatever the desired product, presently available data are insufficient to permit an engineering balance of carbon conversion and quantity and quality of product against the obvious difficulty of providing sufficient heat to the small reaction zone required for short residence times. Production of acetylene and olefins is possible by very high-temperature (as by plasma or laser heating) treatment of coals or carbons with hydrogen followed by very rapid quenching of the products. Mechanisms and kinetics of formation (and retention) of these products need to be identified.*

We need (see also page 12) to synthesize the complex chemical, heat transfer, and flow phenomena (as in fluidized beds or entrained flow systems) into realistic and testable models of combustion and gasification systems.*****

Combustion systems and gasification plants present particularly harsh environments for structural materials, and most studies previously described (page 6) are pertinent. Systematic testing of commercial and developmental alloys and ceramics in realistic environments (with emphasis upon the causes and the mechanisms for deterioration and failure) is necessary both to provide a sound basis for near-term choice of useful materials and to provide the data base upon which to establish an appropriate materials development program.*** A fundamental understanding is needed of mechanisms of corrosion/erosion of metals and ceramics by the hot gases plus inorganic condensates, soots, ashes, and slags.*** Many more specialized problems could be mentioned.

Removal of SO_x from combustion gases and separation and purification of coal gasification products are successfully accomplished at present, but better and more economical methods - particularly for application at elevated temperatures and, in some cases, pressures - are needed. Basic study, both of chemical mechanisms and kinetics and of engineering principles, can almost certainly benefit stack gas scrubbing of SO_x and conventional and relatively low-temperature purification of product gases.* Studies on promising candidates for regenerable high-temperature SO_x sorbers would be more valuable.*** Improved understanding of gas-solid reactions, interactions of gases with high-temperature liquids, selectively permeable membranes, etc., might lead to separation and purification of gasification products at high temperatures and pressures.*** Success here would lead to economies through minimized need for compressors, expanders, heat exchangers, etc., in conventional gasification plants and may prove necessary if gasifier-gas turbine systems are to be possible or gasifier-shift-methanation sequences are to be genuinely economic.

The general problems associated with environmental contamination (page 12) are shared by coal combustion and gasification. Coal combustion emits particulate smokes and fly ash in stack gas; degradation of

these materials in the environment and their effects on ecological systems are subjects needing basic study in physical and biological sciences.** Some gasifications yield tars, and all produce H_2S and NH_3 ; these are recovered, but such recovery produces water that must be purified before discharge. Both technologies produce solid residues containing noxious chemicals. Basic study of mechanisms and rates of leaching from such solids and of dispersal of the dissolved materials is needed to establish what disposal measures are required.** Some of the ashes and slags may yield valuable by-products (uranium from some lignites and alumina from some coal ash, for example), but such possible recovery is likely to be process-specific and would generally be classified as applied research.

Gasification of lignites and coals by biological processes does not appear to be a viable option. However, biological conversion of peat should be studied as an alternative route to production of medium- or high-Btu gas.**

Needs in Direct Liquefaction

Coals can be converted to upgradable liquid products by (1) removal of carbon by pyrolysis (pages 4 and 14) or (2) by addition of hydrogen through treatment with H_2 under pressure. Most processes for such hydrogen addition (Direct Liquefaction) slurry the coal in a process-derived pasting oil; they may or may not use an added catalyst (either in a fixed bed or "once through") and may or may not catalytically hydrogenate the pasting oil in a separate (fixed-bed) operation. Process conditions vary but generally use H_2 pressures of a few thousand psi and temperatures near $450^\circ C$. However, direct liquefaction can also be done by flash hydropyrolysis in which finely divided coal particles are heated with H_2 (typically at 1000 psi) and are quenched after residence times of less than a second at temperatures generally below $1000^\circ C$ (see also page 16).

Direct liquefaction by any of these variants obviously involves radicals produced by thermal and other modes of bond cleavage (see pages 4 and 14), along with capping of the radicals by hydrogen and by carbon monoxide (via formate ion) to diminish their recombination to form large entities. We need to understand the chemical reaction paths (including the nature, concentration, and fate of the free radicals) and to establish the relative roles of CO and of hydrogen from molecular H_2 , from the solvent, and from hydrogen-rich moieties in the coal.**** We need to understand the extent to which the pasting oil (called a donor solvent if separately hydrogenated) is incorporated into soluble chemical structures and is decomposed into gaseous and char products.*** Studies with ^{14}C -labeled model compounds incorporated in the solvent can help with these problems. The fate of heteroatoms in hydroliquefaction with and without donor solvents needs to be established.*** Extent of organically-bound metals in hydroliquefaction products must be determined.*** Many of the studies will require separations, identifications, and molecular weight determinations previously described.

Several types of catalysts and several operating modes have been proposed for coal slurry hydroliquefaction. Solid materials in granular or pelletized form may be used as essentially fixed beds in the main

coal slurry stream or in a side stream for hydrogenation of the (donor solvent) pasting oil. Molten salts may be used, as essentially fixed beds in the main stream, as hydrogenation and hydrocracking catalysts to produce a reasonably large yield of relatively light hydrocarbons in a single step. Mechanisms by which such catalysts assist in hydrogen transfer (and otherwise) need to be identified to assist development of improved catalytic materials.**

In general, the coal hydroliquefaction environment is a harsh one for catalysts. Initial catalyst activity rapidly diminishes to a more or less steady value and then more slowly diminishes to an uneconomical level. Mechanisms of such deactivation and failure need to be better defined to aid in development of more rugged catalysts, to assist with catalyst regeneration and (for molten salts) recovery, and to understand the differences in poisoning capacity of various coals and coal liquids.***

This inevitable harshness of the liquefaction environment and the relatively high cost of these fixed-bed catalysts tend to encourage use of quite inexpensive catalytic materials in a once-through disposable mode. For this, the minerals present in coal (or their reaction products), some of which seem to be active, represent the ideal. The catalytic effect of specific coal minerals and of cheap possible additives and the mechanisms for their catalysis need to be defined.** In addition, study of the modes of action and means of recovery of once-through catalysts such as Sn and Mo with added acid that are (though expensive) highly effective at low concentration is still needed.**

The variables that control behavior in three-phase liquefaction contactors (see also page 12) must be understood to permit realistic modeling of chemical, heat transfer, and fluid flow behavior for effective testing and scale-up of systems.*** Development of such models, which should hopefully contain specific properties (i.e., aromaticity, functional group distribution, etc.) of coals as parameters, will require advances in diagnostic instrumentation to define changes in chemistry, viscosity, and flow behavior within the subsystems (i.e., the pre-heater).***

The basic data to describe the physical properties of the complex coal liquids are poorly known. Elementary properties (such as vapor pressures, heat capacities, viscosities, and densities) are unknown at high temperatures even for pure heavy aromatic compounds and their derivatives. We know relatively little about complex mixtures - and especially about mixtures with functional and polyfunctional groups. Moreover, the semi-theoretical correlations long available for distillability of petroleum liquids apply very poorly if at all. We need to know the solubility and the rates of diffusion and migration of H_2 , CO, and other small molecules in coal liquids under realistic conditions.** Physical property measurements and thermodynamic data, especially for mixtures containing heavy components, are badly needed, as are semi-theoretical correlations necessary for sound engineering design.**** Such information, which would be considered applied research if done for a particular coal liquid, is necessary if costly "overkill" conservative designs or potential design failures are to be avoided.

In common with many other fossil fuel technologies, direct liquefaction exposes its structural materials (largely metals) to quite hostile environments. The basic studies suggested previously (page 5) are all applicable. Special features of direct liquefaction are the presence of high pressures (1000 psi and above) of H_2 at moderate to very high temperatures with reducing fluids containing abrasive solids. Mechanisms of corrosive attack and material failure need to be understood; these will include embrittlement by hydrogen and stress corrosion phenomena (lower-temperature processes) and the effect of creep-fatigue interactions during cyclic loading in hostile environments at higher temperatures.*** It should be noted, however, that (erosion problems excepted) petroleum hydroprocessing has faced these same problems with general success; this oil industry know-how should be drawn on wherever possible. Hydrogen and impurities that segregate to grain boundaries have complex interactions that are poorly known and worthy of separate study.*** Fundamental study of corrosion of metals by molten salt catalysts plus process conditions needs to be continued to offer possibility of use of more economical alloys in such processes.** This overall effort will, of necessity, include studies of engineering materials in service and of model systems that will lead to fundamental understanding, with the synthesis of these efforts leading to materials less restrictive to the system operation.

Separation of solids from coal liquids is difficult. We need to know the composition, the mineral species, the size range, shape, density, and the surface physics and chemistry (especially the electrokinetic properties) of the solids present in the coal liquids to assist in electric field coagulation, electrophoretically-assisted filtration, magnetic separation, and, especially, in solvent or anti-solvent deashing.** The mechanisms (both those affecting the liquid and the particle surface) of solvent and of anti-solvent deashing need to be determined.*** Phase relationships are needed for light hydrocarbons (C_5-C_8) and heavy hydrocarbons ($>C_{14}$) at conditions near critical values for the light fraction.** Solids removal by thermal diffusion and after coagulation by sonic forces may be worthy of study.** Sedimentation and filtration theory need to be extended to regimes with viscous fluids, hindered settling, and a wide range of particle shapes and sizes.** Moreover, the fundamentals of particle behavior need to be known as solids concentration increases and liquid properties change during distillation or flash evaporation.**

Most direct liquefaction technologies propose to furnish the hydrogen by use of the water-gas shift reaction sequence on the less volatile liquid fractions and unreacted carbonaceous residues produced in liquefaction. Research needs for this are essentially those described previously (page 15) under Gasification (but see also pages 4 and 5).

Coal liquefaction plants will produce aqueous streams from which inorganic as well as organic materials must be removed before the water can be discharged. Different processes and different feeds will produce different specific problems that will call for applied researches. But there are several contamination problems (i.e., phenols, sulfides, ammonia) that could justify basic studies in both bioscience and physical science.** We need better understanding of biological effects of a

variety of organic materials to define reasonable releases.** Basic studies of biological processes for removal of traces of noxious materials from effluents are required.**

Most coal-derived liquids will require upgrading before ultimate separation into final products for use as fuels or special fuel materials. The research needs of such upgrading are described as part of the final section of this document. It is worthy of note here, however, that many of the coal-derived liquids are relatively unstable; the reactive species responsible for this instability need to be identified to aid in development of methods for stabilization of these liquids so they can be satisfactorily stored and transported.**

OIL SHALE KEROGENS

Domestic oil shales constitute an energy source of great potential value both because very large quantities are available and because the organic matter has several favorable characteristics. Oil shale kerogens, particularly those in the western shales, are markedly less aromatic, contain less organically combined sulfur, have a less complex chemical structure, and have higher hydrogen-to-carbon ratios than do coals. Devonian oil shales, found in vast quantities in many eastern states, are of a somewhat different character. When subjected to standard assays, the eastern shales generally yield considerably less oil than do the western shales though their organic carbon content is not markedly inferior. The eastern shales have received less attention, and their development into useful fuel sources seems likely to lag behind exploitation of the western shales. The numerous research needs discussed below apply to both classes of shales.

Generic Research Needs

Oil shale kerogens, like coals, share essentially all the research needs listed (pages 2-5) as common to several fossil fuel sources. Additional researches of value to several possible routes to recovery of shale oils are described in the following.

Chemical Composition and Structure

Our knowledge of the composition and structure of the organic kerogens and of the oils derived from them is far from complete. As a consequence, many of the basic structural researches previously described (pages 2 and 3) are needed to guide development of more effective and more economic processing for these materials.

Oil shale kerogens lack some of the complexities (i.e., the presence of maceral types) of coals, and their structures appear to be somewhat simpler than those of coals. Particular needs are for the quantity and functionality of heteroatoms (especially N and S),**** structure of the carbon skeleton,** and number and nature of the cross-linkages** in kerogens and, especially, in the derived oils. As for coals, the overall goal is an understanding of the scissile bonds and of the reactive configurations within the molecules. The nature and extent of organically-bound metals (arsenic appears to be a frequent trace component) in the kerogens and oils need determination.* Though kerogens apparently lack distinctions corresponding to rank in coals, differences in structure as functions of geologic province, formation age, etc., would be of interest.**

These studies will require mild depolymerization reactions using solvents, reagents, and heat and effective separation, molecular weight determination, and compound identification techniques previously described (pages 2, 3, and 11). It seems certain that study of carefully selected model compounds will prove useful.

"Ash" content of the oil shales is very high. More complete definition of the inorganic components and of the specific minerals, especially carbonate minerals, is needed*** along with correlations of those with geologic history of the materials.**

Pyrolytic Reactions

It seems likely that recovery from oil shales will be accomplished by thermal treatment although (page 22) additional reagents may be used. Whether such treatment is accomplished above-ground (page 22) or in-situ (page 33), the basic mechanisms of kerogen pyrolysis need to be understood. These are probably generally similar to those previously discussed (pages 4 and 14). However, the paths, mechanisms, and energetics of dominant reactions that produce volatile products and chars need to be known as shales are pyrolyzed under essentially inert atmospheres,** and in low oxygen partial pressures plus CO and steam as when heat is supplied by combustion of char and a part of the kerogen.*** Pyrolysis of oil shales under hydrogen has apparently received little study; such study as has been done suggests that such treatment may be valuable. Basic studies of pyrolysis of kerogens (including those from Devonian shales) under hydrogen atmospheres, with emphasis upon differences in dominant reaction modes and upon product liquid composition, heteroatom functionality, and oil and char properties are still needed.*** The goal in all of this is an understanding of the marked effect of retorting conditions upon composition of the liquid products.

Reactions of the large inorganic fraction of the oil shale upon pyrolysis (or hydropyrolysis) and interactions with the reacting organics need to be understood. Chemical and mineralogical reactions as the shales are heated need to be determined.*** Changes in porosity and interconnecting pore structure of the complex inorganic matrix with extent of pyrolysis need to be determined and understood,* as do heat transfer and mechanical properties of the matrix as reactions progress.** Mechanisms (if any) by which the minerals or their reaction products catalyze pyrolysis, gasification, or combustion of the organic materials need to be determined.** The identity and quantity of inorganic species in (and especially organically combined in) the liquid shale oil must be determined.** The factors that influence adsorption of the pyrolytic products by the inorganic mass plus char need to be known.**

Combinations of pyrolysis with solvent action have apparently received much less attention for oil shales than for coals. Recovery of liquid solvents from the large inorganic mass is likely to be difficult. A basic study of super-critical fluids as solvents might lead to valuable insights as well as possible processing methods;** super-critical fluids that have good hydrogen donor capabilities would be an interesting possibility.**

It is obvious that the behavior of heteroatoms (particularly N) in all these reaction sequences needs to be determined.*** The specific

functionalities occurring in the liquid products are needed to guide possible methods for product upgrading*** (page 36). Specific functionalities responsible for instability of the thermally produced oils need to be known.*** Rheology of oils and possible gel formation are especially important.***

The extent of char formation is almost certainly a function of process type and conditions. Factors that influence quantity of char and char reactivity need to be understood.**

Needs for Shale Processing

Shale oil can be recovered by retorting (pyrolysis) and, perhaps, by hydropyrolysis or other techniques. Alternatively, the kerogens could be gasified by use of steam with heat supplied by partial oxidation or even (though less likely) by partial oxidation alone. Most of these operations could be performed above-ground or in-situ (page 24).

Above-ground operations will require mining of the shale and its comminution to fragments of suitable size. Mining of oil shale will benefit from basic study (as indicated for coal) of physical and mechanical properties and fracture mechanics of the shales, and geophysics and rock mechanics of the adjacent strata.** Mining, short-haul transport, and crushing operations will be assisted by fundamental study of abrasion- and wear-resistant alloy compositions.**

Effects of controllable variables (rubble size, pressure, heating rate, etc.) upon product yield and quality must be systematically established.*** Kinetics of oil-droplet coalescence, appearance of oil mists, and collection on surfaces as function of gas flow, size, and geometry of passages, etc., need to be known.** Study (see also above) of changes in frictional properties, porosity, and pore distribution, etc., of the rubble particles will be needed as functions of temperature and state of decomposition.** As for coals, improved diagnostic instrumentation to evaluate chemical and physical property changes in the system is needed.** The overall goal of these studies - in combination with others (pages 4 and 12) - is the development of realistic and testable models that can guide scaleup and improved design of the process.**** Such development will require both experimental study and closely coordinated physical and theoretical modeling.

Distillative separation of retorted shale oil may be practiced, though this may be postponed until after product upgrading (page 36). Though shale oils are more petroleum-like than are coal liquids, physical property and thermodynamic data and semi-theoretical correlations are needed to guide sound designs of separative processes.***

Basic researches on mineral separations processes might lead to recovery of important mineral constituents (nahcolite and dawsonite, for example) from the shale.** Some oil shales in the Eastern United States contain appreciable concentrations of uranium; better understanding of its occurrence, its mineralogy, and its reactions upon retorting, etc., will assist in its possible recovery along with the oil values.**

Materials problems in shale retorting seem somewhat less severe than for coal liquefaction. Improved materials for large retorts will require basic studies of degradation mechanisms (see pages 6 and 18).* Gasification processes would need materials studies generally similar to those indicated for coal (page 16).

It is likely that a major problem with above-ground recovery of shale oil will be possible environmental effects. Process water will be contaminated with organic materials as well as inorganic species, and studies (similar to those described for coal liquefaction, page 12) will be required to assess the contamination, its environmental consequences, and its removal to tolerable levels.** The shale residue must be dumped - or otherwise disposed of - so that it does not adversely interact with the environment. Basic investigations concerning possible airborne pollutants** and contamination of surface aquifers by species leached from the spent shales will be needed.** Many benefits may accrue from returning the spent shale to the mine and to spent in-situ retorts. Such operations will require study (much of which is applied research) of the flow properties of spent shale slurries and of mechanisms and rates of their re-solidification and cementation.**

TAR SAND BITUMENS

The tar sand bitumens of the conterminous United States have received rather less attention than most of the other fossil sources primarily because they were, until relatively recently, believed to constitute a very small resource. Their study has received some increased emphasis in recent years since (though still the smallest of the fossil sources considered here and far smaller than the Canadian sources whose commercial exploitation now appears to be economic) they are now estimated at about 30 billion barrels. Usable, though perhaps not optimal, methods are available for conversion of the recovered bitumen to petroleum-like liquids and for upgrading of these materials to refinery feedstock. It is fair to say, however, that our understanding of the domestic tar sand bitumens is inadequate and that basic researches (several of which are in progress) might be very productive.

Generic Research Needs

Studies that deserve, and are receiving, highest priority at present are those associated with detailed definition of the resource in selected major tar sand deposits. Such studies would obviously be assisted by improved, better controlled, and more economic drilling methods** and by improved techniques for obtaining and preserving of cores under realistic in-situ conditions.** These needs, which are also important for other operations (in-situ conversions, natural gas explorations, oil recovery, etc.) to be described subsequently, are noted here and elsewhere (see pages 26, 30, and 33) because of their importance though it is not obvious how basic research leads to their satisfaction.

Some fraction (which is not certainly known but which may be near 20%) of the domestic tar sands lie near the surface and are amenable to mining and above-ground recovery of the bitumen for conversion and upgrading. The deeply buried materials must, presumably, be recovered by pumping from the reservoir after their viscosity has been reduced by heating (via steam addition or partial in-situ combustion) or, possibly, by addition of solvents or chemicals. In either case, a better understanding of the interactions among bitumen, water, and the formation minerals is needed. The Athabasca (Canadian) tar sands are complex materials consisting of fine-grained (99.9% <1000 μ m) quartz

admixed with clay minerals in which each sand grain is enveloped by a film of water that is surrounded by a layer of bitumen (comprising 1 to 18% and averaging 12% by weight) and with connate water filling most of the balance of the void volume. At least some of the domestic tar sands lack the intermediate water layer, and the sand may, accordingly, be more difficult to free from the bitumen. On the other hand, some of the domestic sands contain considerably less clay than do the Canadian ones; water recovery and recycle may be appreciably simpler. More complete definitions of the mineral species, their particle size range, and the degree of hydration, along with their variation among deposits, are needed.** Details of the surface forces among the bitumens, the water, the colloidal clays, and sands need to be determined and understood.*** Such understanding will probably require study of the response to combinations of mild thermal treatments with aqueous surfactants or solvents.

Recovery of the deeply buried bitumens will require techniques essentially identical to those of thermally assisted enhanced oil recovery. Consequently, such researches (pages 25, 28) are generally applicable. In addition, basic understanding of the physical properties (particularly density, viscosity, and surface and interfacial tension) is needed as functions of temperature and bitumen quality.***

Once the bitumen is above-ground and essentially freed from minerals, a variety of processes appear to be possible. In general, these materials can be effectively cracked (by thermal treatment with or without added hydrogen at under 500°C) to distillable liquid products, gases, and relatively small quantities of coke. To guide development of optimum primary processing, we need a better understanding of the composition, and the variability in that composition, of the bitumens in domestic tar sands;** relationship of these to location and geologic history of the formation is needed.** As for most of the fossil organic geodeposits (see page 2), we need to know the heteroatom content and the functionalities of the heteroatoms.*** In addition, we need to understand the factors responsible for the high viscosity and adherent nature of the bitumens.** These organic structural problems will require some of the depolymerization researches, and the separation, identification, and molecular weight determination techniques previously indicated (pages 3 and 11). We need, in addition, to understand mechanisms and rates of dominant pyrolytic and hydropyrolytic reactions of these complex materials.***

The liquid materials obtained by pyrolysis (or hydropyrolysis) of the bitumens seem to be relatively normal petroleums with moderately high sulfur content. Basic studies of their physical and thermodynamic properties seem to have only a modest priority.* It seems likely that they would be upgraded (see page 36) at the production site, but some short-term storage would be necessary even so. Basic studies may be able to assist if storage instabilities (gum or sludge formation) are problems.**

Needs for Recovery and Conversion

It seems likely that some of the domestic sands will be mined for bitumen recovery above-ground. Such mining poses materials problems primarily because of the abrasive nature of the materials. Commercial

operations with the Canadian deposits appear to have developed adequate solutions to the materials problems, but longer-lived abrasion-resistant materials for use in the mining and conveying operations are still needed (see page 13).

Conversion of the bitumen to distillable products (plus some gases and coke) is apparently possible without separation of the mineral matter. It seems more likely, however, that separation (by frothing after treatment with steam and hot alkaline water) of the bitumen will be used. Basic research needs for above-ground separation of bitumens from sand and clay minerals seem to lie primarily in surface physics and chemistry. If clean separations are to be made in the complex bitumen-water-clay-sand system, fundamental understanding is needed of the processes by which mild heating plus surfactants free the bitumen.** In the Canadian operations, settling of the colloidal clay minerals (contaminated with some bitumen) for recycle of the water is exceedingly slow and difficult in spite of considerable study; the large settling basins required may be the source of the worst environmental concerns about above-ground processing of Athabasca sands. Innovative basic researches in these surface chemistry areas are a real need at least for those domestic deposits that contain appreciable quantities of clay.**

Intensive study (both in the U.S. and in Canada) has shown encouraging (~50%) recovery of the bitumen after steam injection or fire-flooding techniques. Such recovery operations will be aided by basic studies very similar to those described (page 28) for thermally assisted enhanced oil recovery. In addition, it may be necessary to enhance permeability of the formation (perhaps by hydraulic or explosive fracturing) as indicated (pages 30 and 33) for unconventional gas recovery or in-situ conversions.

Additional study (generally applied research assisted by the generic studies noted above and on pages 3 and 5) will be needed to optimize pyrolytic or hydrocracking processes for primary conversion to liquid and gaseous products along with coke. And finally, the high-sulfur primary liquids obtained must be upgraded (present methods use hydrogenation) before they can be used as feed to conventional petroleum refineries (see page 36).

UNDERGROUND OPERATIONS

Under this general heading are included the basic (plus much applied) research needed in Enhanced Oil Recovery, in obtaining Natural Gas from Unconventional Sources, and in In-situ Conversion as it may be practiced with several fossil source materials.

ENHANCED OIL RECOVERY

For more than two generations the sophisticated research arm of a powerful industry has focused upon production of petroleum. Rewarding areas for basic research certainly remain in study of methods for enhanced recovery - that is, for recovery beyond that available by flooding with water alone. But selection of these areas needs more than usual care to avoid duplication and to complement existing knowledge.

Development of economical methods for enhanced recovery is difficult because of the extreme complexity of the system. Crude oils are

complex chemical mixtures; reservoir rocks are mixtures of many mineral forms and, in addition, they can vary considerably in porosity and permeability both areally and vertically; connate waters are generally complex brines. Moreover, the oil-rock-brine system, which matured through millions of years, has generally been perturbed by years of waterflood recovery operations. As a consequence, our understanding of the rock-oil-brine system is, at best, incomplete.

Methods for enhanced recovery must disengage the oil from pores of the formation and cause it to flow through the inhomogeneous formation to recovery wells. Several options exist, in principle, to accomplish this. Thermal methods, using steam or the products of partial in-situ combustion, can be applied. Massive injections of gases (particularly CO_2 and, possibly, $\text{CO}_2\text{-SO}_2$ mixtures) at high pressures can be used. Both of these methods may use surfactants or other chemical additives. In addition, many variants of water flooding - with combinations of added organic solvents, chemicals, surfactants, foaming agents, and polymers - are under study. Major research needs involve a combination of sensitive surface physics and chemistry of multicomponent systems and complex flow behavior with the complexities introduced by inhomogeneities (both in chemistry and in permeability) of the reservoir.

Generic Research Needs

Methods for determination of quantity and distribution of oil remaining in a reservoir frequently disagree. Improved methods that can sample a large volume of the formation are clearly needed.***

It is obvious that one needs reliable estimates of the potential for recovery from each stratum of the formation. For this one needs the best possible three-dimensional description of the reservoir in terms of mineral types and location, oil saturation as a function of permeability, variation in areal and vertical porosity, and permeability of the formation, and composition of the connate brines. Such a description would be markedly assisted by improved techniques for obtaining and interpreting data from down-hole instrumentation. Such data are obtained from measurements of many types including sonic, electrical, radioactive, magnetic, gravimetric, microwave, and seismic. Exploration of basic physical concepts that could lead to more detailed information about reservoir properties by these and any other available techniques is a major need.*** Improved methods for synthesis of this data into a suitable model of the reservoir are also needed.** Though the difficulties are large, it is probably true that economical methods for obtaining accurate reservoir descriptions (including inhomogeneities) are the major need in enhanced oil recovery.

All enhanced recovery techniques require effective flow through generally inhomogeneous porous media, inevitably with gradients of density and viscosity, and usually with liquid-liquid, gas-liquid, or even with gas and two liquid phases. One needs to know the flow patterns fluids can take, the relationships of these patterns to parameters usually measured, and the fraction of the oil that can "see" an injected displacing agent. Better understanding of the porous media, the properties of the fluid phases, and their interactions is critical to success of the processes. More complete definition of pore-size distribution, pore shape and void fraction, as well as inaccessible pore volume typi-

cal of reservoir rocks is needed.** Changes in mineral composition and texture need to be correlated with pore characteristics and with reservoir inhomogeneity.** Existing information on dispersion in flow under the influence of favorable and unfavorable density and viscosity gradients in specific media should be expanded and general principles established; extension to multiphase flow is required.*** The coalescence and breakup of oil droplets in aqueous-oil liquid phases and their movement through constrictions in pores as functions of interfacial tension, interfacial viscosity, brine viscosity, and wettability of pore surfaces are necessary in understanding the mechanisms of mobilization of oil banks, in untangling the relative importance of interfacial tension, interfacial viscosity, and other factors, and in interpreting the movement of various components in core-flood experiments.*** The goals of such studies are better modeling of floods and better control of sweep, fingering, and oil-bank mobility in floods.

Adsorption on surfaces is an important additional interaction, particularly for chemical and chemically assisted flooding. Adsorption causes loss of oil-recovery chemicals - surfactants, polymers, etc. - and may change the composition of injected slugs in disadvantageous directions. Research elucidating the adsorption of organic compounds, substituted with various hydrophilic groups, on hydrophilic and oleophilic solids typical of formation constituents, is needed, both for prediction of difficulties and for identification of remedies such as competitive adsorbates.*** Properties of many surfactants and polymers are strongly affected by presence of multivalent ions of opposite charge. Distribution of common inorganic ions between minerals and aqueous solutions is needed to define the level of hardness that chemical systems must tolerate and to assess suitability of candidate ions as tracers for water flow.**** In this connection, basic studies of complexing of ions by organic ligands would aid development of sequestering agents for hardness control.*

Wettability is another important fluid-solid chemical interaction. For assessment of optimal recovery approaches the factors [perhaps including nature of the minerals, the residual oil composition and properties, the brine composition (particularly pH in alkaline floods), and electrokinetic effects] that control whether the surfaces are water- or oil-wet need to be understood.*** With oil-wet formations, the three-phase contact angle between water, oil, and the reservoir matrix may be of critical importance, even if the customary emphasis on interfacial tension reduction is adequate for water-wet solids.**

Understanding of interfacial behavior of the oil-water system is important not only during the mobilization operation but in the necessary emulsion-breaking step after the oil is recovered.** Removal of particulate solids from some recovered oils is also required.*

Some basic efforts may be needed for characterization of the heavy crude oils recovered to decide upon optimum uses or alteration of processing or refining techniques.*

It should be noted that materials problems persist even in this "mature" technology. Deterioration of well casings in "sour" gas and oil wells is rapid; the severity of the problem is such that quite expensive alloys are undergoing test. Here it is clear that better and less expensive alloys need to be developed.***

Needs in Thermal Recovery

Thermal methods, mostly by injection of steam from the surface and limited to suitable reservoirs at less than 3000 ft depth, are currently the only commercially successful tertiary recovery processes. Fire-flooding (partial combustion) and combination steam- and fire-flooding seem likely to be used for recovery of tar sand bitumens and other viscous petroleums. It appears that improved techniques for monitoring advancing steam-oil fronts would be beneficial.* Injection of steam (plus CO_2 and N_2) by burning of fuels at the formation level can minimize heat losses, deliver higher-quality steam to needed areas and can probably make treatment of deeper reservoirs profitable. Basic studies of the effects of elevated temperature plus massive CO_2 injections on mobilization of the oil and upon the chemistry and surface chemistry of the formation can probably be valuable.** Both thermal and miscible gas (see following topic) recovery methods need improved methods for control of fluid movement (mobility control) in highly non-uniform media. Foams have been used with some success, but mechanisms by which they act are poorly understood and need study.*** Soluble polymers that are useful for mobility control at elevated temperatures are needed.*** Combinations of added surfactants, etc., perhaps as preconditioners of the reservoir or added after the steam may prove valuable. Fundamental studies of combustion in porous media are pertinent.** Several applied researches can be suggested, but except for the Generic Studies described above, few other basic studies seem called for.

Needs in Gas Flooding

Since the value of natural gas is now such as to virtually preclude its use, gas flooding seems likely to be limited to use of CO_2 (with CO_2 - SO_2 mixtures as possible alternatives) at pressures near or above the critical value.

Basic study of phase behavior of the gas-hydrocarbon and gas-hydrocarbon-brine systems is still needed,** as is knowledge of the physical properties of the fluids under reservoir conditions.** Mechanisms of oil displacement by gas interactions are poorly understood and need basic study.*** As for thermal flooding, mobility control (as by foams or by some novel method) seems likely to be needed.** The mechanisms and rates of reaction of CO_2 with reservoir formations need attention; carbonate etching and reprecipitation occur over considerable flooding periods and cause permeability and well-bore blockage problems.*

Use of CO_2 flooding will require large quantities of gas that will not be cheap and may, in any case, not be readily available. Basic studies (as on page 16) may suggest more economical means for CO_2 (and SO_2) recovery. However, recovery and reuse of the injected gas will clearly be required. Study of such recovery must be considered applied research, but it is an area to which basic study of gas separation and recovery could contribute.*

Needs in Chemical Flooding

We include under chemical flooding use of surfactants or alkali, and of mobility-control polymers with or without surface-active agents, along with cosurfactants, biocides, hardness-control agents, competitive adsorbates, or other additives.

A broad and complex series of problems is posed by the fact that interfacial tensions, which have been empirically related to phase behavior in micellar systems, must lie in the millidyne/cm range; for a given surfactant such values occur over narrow ranges of salinity, temperature, surfactant and cosurfactant concentrations, and hydrocarbon composition, and are strongly affected by presence of other ions in formation brines and minerals. Information on all these, including effects of concentration changes by adsorption, is necessary input in mathematical modeling of floods.

Study is needed of the effects of variation in monomer structure (particularly that near the hydrophilic group), salt composition and concentration, surfactant concentration, and temperature upon the size and structure of micellar and microemulsion aggregates.*** Traditional methods such as ultra-centrifugation and light scattering can help, and recent refinements of neutron and x-ray scattering, NMR, ESR, and Raman spectroscopy may be useful. Newer techniques such as quasi-elastic light scattering should be evaluated.**

Considerable basic information exists on thermodynamics and phase behavior of well-defined aqueous-hydrocarbon-surfactant-alcohol systems, and there are extensive parallel data concerning systems with petroleum and practical oil-recovery surfactants. There appear to be qualitative differences between these classes - liquid crystal regions versus microemulsion phases, etc. Bridging the gap between these studies of systems containing mixtures of known compositions of surfactants and hydrocarbons would increase the value of the literature to applications. Study should not be limited to petroleum sulfonates, synthetic sulfonates, and non-ionic surfactants now projected for use, but should include carboxylates and phenolates, because of their pertinence to alkaline floods and their potential as an alternative source of surfactants.**** There is much interest in surfactants that have mixed and anionic/non-ionic character. The mechanisms of caustic recovery, including in-situ soap formation and emulsification, need specific attention. Relationships of critical micelle concentrations of mixed surfactants to those of pure surfactants should be established, because of possible importance in surfactant adsorption.* Studies should extend to chemically similar systems in which micelles are not formed; free energy and enthalpy measurements on one-phase systems would be helpful.** Kinetics of formation and reversion of liquid-crystal phases need study.** These phase equilibrium studies should include attention to effects of various (particularly multivalent) ions and to distribution of components between phases.*** Excess concentrations of surfactant in interfaces would be interesting if methods for their determination could be developed.* Understanding and predictability of water-salt-surfactant-hydrocarbon phase behavior have importance beyond establishment of mutual solubilization of oil and water since clarification and understanding of the relationships between interfacial tension and phase behavior (at present controversial) are worthwhile goals.

Addition of polymers for mobility control can improve water floods as well as surfactant floods and may be helpful in miscible-gas and thermal processes. Traditional basic research in polymers - such as relationship of structure, shape, and size to solution viscosity and to shear degradability - should be strengthened.** We need to know how to

tailor soluble polymers as viscosity builders, especially in the deeper reservoirs where concentrated brines and 200°F temperatures exist.** Polymer solutions tend to be non-Newtonian, so shear-thinning and (more controversial) shear-thickening behavior is important.** Factors affecting compatibility of surfactants with polymers need investigation.** The possibilities of alternative mobility control techniques, for example by gradations of surfactant slugs, emulsions, or foams, can be explored by investigations of viscosity properties of these systems.**

Fundamental study of mixing and solubilization of polymer flood additives may be necessary to minimize or prevent polymer gel formation in the solutions.* Such gels must be removed before injection to minimize plugging of the reservoir; alternatives to DE filtration for this operation are badly needed.** In general, water treatment requirements must be expected to become more demanding as tertiary treatments become more severe and environmental pressures on sludge disposal increase. Basic research that could lead to treatment alternatives are needed.*

Chemical costs are a major factor in micellar flooding. Cheaper materials or ways to use less material are needed. Studies outlined above to delineate mechanisms and needs of the process should help. Basic study of synthesis of the organic materials should also help.* Biopolymers produced by microorganisms are among the candidates for use in mobility control; a broad basic investigation of gumforming organisms might lead to improved and cheaper products.** Preliminary indications that surfactants can be produced microbiologically should be followed up.** It is likely that useful cosurfactants and sequestering agents can be so produced.*

Better analytical techniques, particularly for surfactants and polymers in presence of oil, would substantially accelerate progress.**** More convenient and reproducible techniques for measurement of interfacial tension and of interfacial viscosity are desirable.**

Aqueous-oil systems can be made miscible by addition of alcohols and/or low-alkyl-substituted organic electrolytes, though not at levels that appear economic. Systematic investigation of the effect of various classes of components might lead to a feasible non-micellar displacement system.*

It is certain that not all reservoirs will prove amenable to enhanced recovery methods. Useful energy might be extracted from such deposits by in-situ gasification or partial combustion (page 33), or perhaps by in-situ conversion by microorganisms. For the latter, most emphasis seems to have been placed on aerobic processes. Evaluation of anaerobic species for such purpose would appear worthwhile.**

NATURAL GAS FROM UNCONVENTIONAL SOURCES

Among the possible unconventional sources, the most promising are generally considered to be the low-permeability or "tight" sands, shales, carbonates, etc. Additional possible sources include very deep reservoirs, salt-water aquifers containing natural gas, methane-bearing coal deposits, and deposits of hydrocarbon hydrates. Applied research needs in support of eventual recovery from such sources occur in many areas. Basic research needs appear to be substantially fewer though still numerous.

Recovery of natural gas shares with other technologies, notably In-situ Conversions (page 33), a real need for improved drilling methods and, especially, for improved capability for precise directional (including essentially horizontal) drilling. Improved drill-bit materials and improved (i.e., jet-assisted) drilling techniques are areas in which basic studies should be able to contribute.* Precise non-vertical drilling techniques will be needed to intersect natural and artificially produced fracture systems in tight formations and for recovery of natural gas from coal seams. Development of improved guidance systems and sensing devices can almost certainly be assisted by basic studies.*

Natural gas is not uniformly distributed in the tight formations. A most important practical problem, accordingly, is recognition of high yield areas. Geochemical and biostratigraphical study of these formations is needed to define basinal trends in the key parameters (organic carbon content, thermal maturity, etc.) so that areas of high potential can be located.*** This can, given time and money, be provided by analysis of recovered cores, and many such analyses must be done; techniques for recovery of cores (applied research) under in-situ conditions would be valuable.** However, a most important need is for down-hole sensing and logging techniques for direct examination of the key parameters such as porosity, permeability, and water saturation; basic researches that can assist with this problem area should be encouraged.***

A better understanding of permeability of fine-grained rocks (including cap rocks) and of fluid flow (water, brines, and pertinent hydrocarbons and associated gases) within the reservoir is needed under in-situ conditions.*** Greatly improved understanding of the methane entrainment mechanisms (adsorption, trapping in molecular-sized pores, and content of larger pores) plus related methane release and transport mechanisms is essential to definition of the resource base and the producible fraction for shales, clays, and very fine-grained sandstones.*** Research to define the mechanisms controlling low-pressure gas accumulations in tight sandstone synclines and the minimum gas-filled porosity required for transport is critically important.**** The pore structure, the nature of the wetted surface, and electrochemical effects on flow are required.** Definition of temperatures and pressures at which various rock types can be expected to have negligible permeability might set limits to depths at which gas could be expected.* Solute composition of water needs to be determined and related to pressure (and pressure changes), temperature, and mineral constituents.** Instruments capable of down-hole logging of porosity, permeability and fluid saturations in tight formations would be valuable, and basic researches that could lead to such tools are needed (see also page 26).***

Physical properties (particularly viscosity), phase equilibrium correlations, and thermodynamic data are needed for low molecular weight hydrocarbon mixtures with high concentrations of CO₂, N₂, H₂S, etc., at temperatures and pressures approaching the critical state.*** The goals here include understanding of sulfur precipitation and assistance with mechanisms for corrosion of materials.

Economical recovery of gas from tight reservoirs will require some method for enhancement of the formation permeability. Hydraulic or che-

mical explosive fracturing seem most likely to be used though some benefits may be possible by use of acid or chemical treatments or by heat. Optimum use of fracturing techniques requires basic data on the mechanical properties and fracture mechanics of the gas-bearing formation and the sealant rocks,** as well as careful attention (though not basic research) to economics of recovery versus cost of chemical explosives. Improved means are needed to monitor fracture propagation and to define fracture geometry**; the mechanisms of fracture propagation and of fracture healing in a number of rock media need to be understood.*** For some exotic fracturing fluids (such as liquified petroleum gas-polymer gels), basic PVT data and rheological data are needed along with data on the miscibility of the fluids with water and hydrocarbons.** Mechanisms by which fracture fluids affect gas flows through interaction with the reservoir rock and with the brines in the formation need to be understood.* Mathematical models of the fracturing process are needed for correlation with field tests to define pressures and pressurization rates for optimal production of the fracture system.*** Models of sophistication sufficient to predict distribution of solid proppant materials in the fractures are desirable.** Mechanisms by which in-situ combustion of a portion of the resource improves bed permeability should be determined.* Treatment of clayey sandstones with HCl-HF solutions often yield gelatinous suspensions that block flows; mechanisms for such blockage and for its elimination (as by use of ethylene glycol derivatives) need study.* Better acid treatment methods for carbonate rocks are desirable.*

Many subsurface brines, particularly along the United States gulf coast, contain substantial quantities of dissolved methane and other hydrocarbons. Studies of such occurrence as functions of salinity, depth, temperature, and pressure are desirable along with means for hydrocarbon migration in such aquifers.** Laboratory determination of pore volume compressibility, relative permeability to gas for fractional water saturation in excess of 90%, brine compressibility, and the effect of gas in solution upon the compressibility and viscosity of brines is needed for pressures in the range of 6000-20,000 psi at the reservoir temperatures associated with these high reservoir pressures.**** We need to know whether such sources are of possible economic value, whether they contain other resources (Br_2 or I_2 , for example), and if they point to the existence of more conventional resources.

A better understanding of sorption-desorption equilibria of methane and other gases with coals and two-phase (water and gas) flows through seams is needed for possible recovery of natural gas from Western deposits.** In many Eastern coals permeability seems largely associated with fractures. A much improved understanding of permeability of the natural fracture systems in coals and in the changes as stresses are relieved is needed.*** Improved understanding of fracture mechanics of coals is needed so that systematic and useful fracture systems can be obtained.*** As in other reservoirs, detailed and testable models of gas and water flows and their interactions are necessary.**

A basic study of physical properties (thermal conductivity, heat capacity, electrical resistivity, and sonic velocity), multi-phase fluid transport properties, and thermodynamic properties of reservoir rock

containing hydrocarbon hydrates is needed to assess producibility of methane from hydrates underlying permafrost and the deep ocean floor.**

Many of the operations suggested above have severe materials problems. Corrosion is commonly severe in the wells producing H₂S-contaminated gases, especially from deep high-temperature formations. Mechanisms of deterioration and of cracking of pipes are needed to direct developments of improved alloys.*** Mechanisms of inhibition, and improved inhibitors, especially in high-temperature and highly saline environments, is a particularly important area.***

IN-SITU CONVERSIONS

In-situ gasification with steam with heat for the process derived by partial combustion of the material can, in principle, be applied to any of the fossil sources. In-situ liquefaction (by pyrolysis) seems likely to be used for recovery of oils from shales and may possibly be used to produce liquids from coal. Such in-situ pyrolysis, gasification, and combustion processes share most of the generic needs described in pages 2-5 and under the individual sources, above. But many problems - some of which have basic research components - are added or intensified by underground operation of the processes. Underground reaction chambers must be created by drilling process wells and linking them together (as for coal seams) or by generating beds of rubble in underground caverns between process wells (as for oil shales). Ingress of extraneous water must be avoided, and escape of products through defects in the formation must be minimized. Remote control of the process must be accomplished in spite of inevitable lack of uniformity in fluid flow patterns, heat transfer rates, and reaction rates both in space and time.

Basic understanding of mechanical properties, fracture mechanics, permeability, etc., and the changes in these with thermal treatment is needed for the formations that bound the source material.*** Location of natural fractures, the presence and size of aquifers, and location of particularly permeable areas all need to be known.*** Many geometric and geomechanical details are needed for the source material; nature and location of fractures and joint systems are important as are porosity and permeability of the formation and the non-uniformity of such properties.** Many of the implied researches are obviously applied. They would obviously be assisted by markedly improved and better diagnostic instrumentation for down-hole logging (see pages 26 and 30); basic researches that can assist this should be encouraged.*** Basic studies of rock mechanical properties of the source materials and their change with thermal treatment are needed.***

Practical problems exist in linking of process wells in coal seams. Horizontal drilling, which may be used, can benefit from researches previously suggested (page 34).** Creation of more or less uniform beds of rubble for shale processing would be assisted by basic studies of rock fragmentation by explosives;*** such studies should include shale of various grades, should be done with a free surface and should attempt to define the size distributions of fragments and voids. Flow distributions (perhaps by gas-tracer dispersion studies) through such rubblized beds are needed as are testable mathematical models for such flow.***

Process operation must obviously be remotely controlled. Remote detection of the burn front, of subsurface ground motion and pressure,

and flow and composition of the products are needed.***

Markedly improved and testable models for in-situ processes are needed.**** The ultimate goals are models that directly incorporate water influx, product losses, solids motion and include a complete linking of chemistry and source recovery. A stable and long-term program - carefully coordinated with basic chemical and other studies - of iterative modeling and field testing would seem to be required.

In-situ conversions will obviously require materials (as for casings and down-hole equipment) capable of service at high temperatures in hostile environments; basic researches (of the type described on pages 6 and 16) can assist with these problems.**

Consequent environmental concerns may pose difficult problems for all in-situ conversion processes. Careful studies of rock mechanics (as noted above), including the effects of heat and of volume change in the source materials, will be needed for prediction and modeling of land subsidence and possible alteration of hydrological flow regimes.**** Basic studies of leachability, mobility, and removal of both organic and inorganic species are needed to predict and control contamination of usable aquifers during, and especially after, in-situ conversion operations.****

"SOURCE-INDEPENDENT" TECHNOLOGIES

Several of the technologies described previously can be applied - with some modification - to more than one of the fossil source materials. However, only Indirect Liquefaction (catalytic conversion of $\text{CO} + \text{H}_2$ or $\text{CO} + \text{H}_2\text{O}$ mixtures that can obviously be obtained from any source), Product Upgrading, and Final Product Combustion, both of which will differ in some degree from source to source, are included in this Section.

NEEDS IN INDIRECT LIQUEFACTION

Catalytic conversion of reactive gases to fuels, chemicals, or chemical intermediates is here referred to as Indirect Liquefaction, even though some of the chemical intermediates so produced may be gaseous. Gases fed to the converters are usually relatively pure CO-H_2 (SYNGAS) mixtures though $\text{CO-H}_2\text{O}$ mixtures can be used for some syntheses. Any of the fossil source materials could be gasified (above-ground or, perhaps, in-situ) with steam to impure CO-H_2 mixtures or by partial combustion to impure CO . The CO-H_2 mixtures would require shifting to provide proper SYNGAS stoichiometry. Both the SYNGAS and the CO would require purification - especially for removal of sulfur compounds - before conversion (see pages 5 and 15 for discussion of Gasification).

The ultimate goal of both basic and applied researches in support of this technology is demonstration of new or much improved processes for SYNGAS conversion. A wide variety of applied researches (many of which are undoubtedly under way) could be suggested. Fundamental researches should clearly focus on identification of mechanisms of catalysis and of catalyst deactivation and poisoning. To that end, both sophisticated experimentation and theoretical study will be needed.

Experimental study, using several of the modern tools of surface science, of pertinent reactions occurring on well characterized catalyst surfaces is needed.*** Nature and concentrations of adsorbed species

and reactive intermediates on catalyst surfaces need to be known under realistic reaction conditions;*** infrared spectroscopy and solid state NMR presently appear best suited for study of adsorbed species under such conditions, but higher sensitivity needs to be obtained for ^1H and ^{13}C NMR. Other techniques need to be developed to provide improved physical and chemical probes of catalytic intermediates.*** Electron energy loss spectroscopy can detect C_2 and CH structures on surfaces; studies leading to improved resolution by this technique are needed.** Particular needs are for mechanisms of carbon chain growth and for formation of oxygenated species; use of ^{14}C - and ^{13}C -labeled reagents can markedly assist such studies. Three-dimensional aspects of the mechanisms (which metal orbitals participate in adsorbate bonding and the spatial relationships of the reacting species) need especial study.*** Theory of surface electronic structure, surface geometry, and energetics and dynamics of formation and breaking of adsorbent-surface bonds is required.*** Such studies of catalytic mechanisms should include homogeneous catalysts and the interface (microcrystals, cluster ions and compounds, and organometallic compounds) between heterogeneous and homogeneous catalysts.*** Interactions of catalysts (especially in small particle sizes) with catalyst support materials need study.**

Few catalysts operate at their intrinsic activity level in practical systems; they are usually poisoned to a lower activity level. It is especially important to understand the mechanisms of such poisoning to guide development of less sensitive catalysts or effective means of catalyst regeneration.***

Examples (but not an exhaustive list) of catalytic systems that presently seem to deserve such fundamental studies are the following: The reaction paths and the mechanisms by which shape-selective zeolite catalysts produce a narrow range of hydrocarbon products from methanol need to be understood.*** Such study might well lead to other shape-selective catalysts for specific reactions. Synthesis of zeolites is still largely an art; fundamental study of synthesis of zeolites with desired pore sizes could be valuable.** Shape-selective catalysts with transition metals in their surface structure or with metallic particles or cluster compounds on internal surfaces should be of interest.**

A very important long-term goal is the development of catalysts with good efficiency and high selectivity for synthesis of (1) gasoline and diesel fuel hydrocarbons, (2) oxygenated chemical intermediates, and (3) olefinic intermediates by Fisher-Tropsch ($\text{CO} + \text{H}_2$) or Kolbel-Englehardt ($\text{CO} + \text{H}_2\text{O}$) processes. Edisonian approaches must be used, and they may solve the problem, but better information about mechanisms of C-C bond formation and processes for chain-growth termination would certainly help and may be necessary;*** here it is especially apparent that ^{14}C - and ^{13}C -labeled compounds can be of great assistance. A specific goal here is understanding that can lead to catalysts whose mechanisms are not limited by the Anderson (Schulz-Flory) product distribution.

Improved catalysts for synthesis of methanol, dimethyl ether, and higher alcohols (under lower temperatures and pressures) are desirable,** as are SYNGAS catalysts with higher tolerance for sulfur compounds.**

In general, processing conditions (though at elevated temperatures and pressures) in indirect liquefaction plants are relatively simple and benign. Basic studies (see pages 6 and 16) leading to improved materials of construction could be of modest benefit as could basic engineering studies that could lead to improved plant design and, in some cases, improved product separation.* But indirect liquefaction is, given the purified SYNGAS, a relatively inexpensive operation; cost of producing the SYNGAS from coal or other fossil fuel is a very large fraction of the product cost, and it is there (see page 15) that the major gains from engineering and materials researches can be made. Indirect liquefaction plants (but not their SYNGAS suppliers) seem also to have only relatively minor problems in control of environmental contamination.*

NEEDS IN PRODUCT UPGRADING

Most, though not all, of the products derived from fossil fuel sources will require special upgrading before use. The clean and (relatively speaking) simple liquids produced by indirect liquefaction processes require (for methanol) only simple distillative separation or (for the Fischer-Tropsch products) catalytic reforming by more or less conventional petroleum technology. Much of the petroleum procured by enhanced oil recovery techniques and some of the heavy petroleums can presumably be subjected to "standard" refinery practices. Neither of these upgradings is considered further in this discussion. Some of the liquids produced by direct liquefaction of coal, oil shale retorting, or tar sand treatment may be used as utility boiler fuel; it is possible that the fraction so used would not require extensive upgrading procedures, though some stabilization treatments to permit effective storage and transport may well be required. However, a large fraction of these complex and relatively dirty liquids must be extensively upgraded before component fractions can be used as chemical feedstocks, transportation fuels and, perhaps, even boiler fuels. Some, and perhaps most, of such upgrading will be done at the site of primary liquid production (as is now done - by hydrogenation - for liquids from tar sand bitumens).

For service as transportation fuels, these liquids, and particularly those from direct coal liquefaction, must be enriched in hydrogen. Organic sulfur and nitrogen concentrations must be markedly reduced, as must the concentrations of metallic constituents. As a consequence, most upgrading processes under study at present involve catalytic hydrogenation of the liquids. The hydrogen, presumably, would be provided by gasification of still-bottoms remaining after product recovery or, lacking these, from the source material at a less advanced processing stage. Since hydrogen is an expensive material, there are strong incentives to discover and develop alternative processes and to develop processes and process conditions that use hydrogen more effectively.

Key problems, which are the subject of much applied research, are the effective and selective removal of organic nitrogen compounds from shale oil, and of organic sulfur plus nitrogen from bitumens and, particularly, from coal liquids, accompanied by reduction of average molecular weight of the organic materials. Basic researches can assist in several ways, most of which have been emphasized in preceding sections.

A sound knowledge of the heteroatom bonding and functionality (repeatedly emphasized in the document) will be most valuable in guiding development of hydrogenation and alternative removal processes;**** an easy removal of nitrogen from shale oil, as an obvious example, might well be possible. Metallic contaminants often appear to present problems in product upgrading. Nickel and vanadium are present in liquids from bitumens, arsenic is generally present in shale oils, and coal liquids frequently contain titanium. Improved knowledge of the physical and thermodynamic properties of complex liquids and structures of important compounds (also emphasized elsewhere) could certainly assist such development.***

If hydrogenation is to serve as the processing method, a key issue for basic research will be study of mechanisms of catalyzed hydrogenation and especially of mechanisms by which the catalysts are poisoned (see page 35) in these inherently dirty systems.*** The following problems may be cited as specific, but far from exhaustive, examples of practical areas needing sophisticated basic study. Metals (such as vanadium or nickel) in heavy oils irreversibly poison hydrodesulfurization catalysts; this poisoning is assumed to be due to plugging of the catalyst pores, but the mechanism is not known. It has recently been shown that prior extraction of phenols from coal liquids permits hydrogenation (including denitrification) of the remaining liquid with much smaller hydrogen consumption and at considerably milder conditions. Knowledge of the mechanisms involved might well lead to improved catalysts or regeneration procedures.

Materials problems, engineering problems and environmental concerns of the upgrading plants will be generally similar to, but less formidable than, those for direct coal liquefaction (page 17). Basic studies suggested there should (except for concerns about solid residues) be applicable.

NEEDS IN FINAL PRODUCT COMBUSTION

Some of the mined coal will be burned, generally after beneficiation, in large devices to provide electric power or heat for industrial operations. Basic research needs for such combustion have been noted previously (see pages 5 and 15). A very large fraction of the gaseous and liquid products derived from the several fossil sources will also be burned as fuels; a wide range of devices (utility boiler systems, gas turbines, domestic stoves and furnaces, internal combustion engines, as well as fuel cells and MHD systems - neither of which is included in this study) will be used. Basic researches in mechanisms and rates of pyrolysis and combustion reactions pertinent to all these systems have been noted (see page 4) and in materials of construction for such devices (see page 6).

It is clear that optimal combustion of a variety of liquid products in a wide range of special devices will require solution of many specific problems. Most of these problems will require what would properly be called applied research, and no attempt is made here to enumerate them. Some especial areas in combustion of relatively clean liquid fuels that require basic researches other than those previously emphasized are noted in the following.

Mechanisms and kinetics (see also page 5) of combustion of hydrocarbon fuels need study near the lean-limit (as in stratified-charge engines) and near the rich-limit (as in staged combustion devices).** Basic studies of soot formation as influenced by trace elements in the fuel and by cooled walls of the combustion devices would be helpful.** Improved diagnostic tools for chemical species, temperatures, velocity components, etc., in combustion devices are needed.*** Burning of liquid sprays under both laminar and turbulent flow conditions needs both experimental and theoretical study.** Modeling techniques and specific models that use the available and expanding data base and that can be tested and refined as experimental information becomes available are needed for many systems.***

Basic studies of structural materials (described on pages 6 and 16) are needed to assist in development of improved ceramics and alloys for many high-temperature combustion applications. Particular attention should be paid to mechanisms of corrosion-erosion behavior in the presence of trace elements and abrasive particulates.** Use of coal-derived liquids (or even gases) as gas turbine fuels may subject the equipment to traces of alkali metal compounds and require understanding and control of corrosion by these materials.** Such basic (as well as many applied) studies will assist in decisions as to the extent of purification and upgrading of the fuels that is necessary.

Basic study, both in biological and physical sciences, is required to determine permissible emission limits for SO_x , NO_x , particulate soots, ashes, etc., and selected organic materials.*** Basic studies, to which geosciences can contribute in a major way, are needed to assess the important problem of the global effect of massive additions of CO_2 .*** Such studies are clearly important, but their details are properly the subject of a companion assessment.

APPENDIX A

The preceding document (dated 1 October, 1979) represents the third version of this assessment. Before preparation of the first version (12 April, 1979 PRELIMINARY DRAFT), we solicited personal opinions as to major research needs from nearly 150 individuals in Universities, Energy Technology Centers, Research Institutes, National Laboratories, and Industry. Many scientists gave us helpful advice in the very short time available. We sent that PRELIMINARY DRAFT to essentially the same large list of individuals with a request for their suggestions, criticisms, and comments. Again, many individuals responded with material that was helpful in preparation of the second version (1 August, 1979 REVISED DRAFT). In turn, we sent that version to a slightly smaller number of scientists, including some who had not seen the previous version. Again we had helpful and constructive criticism and advice from many scientists. It is a very great pleasure to acknowledge our gratitude to those listed below who sent us suggestions and/or comments upon one or more of the DRAFT versions.

We need to note here that as of 10 October, 1979, none of the individuals listed below have seen the present version of the assessment. They are, accordingly, not responsible for whatever may be the shortcomings of the document, and inclusion of their names in our grateful acknowledgement does not necessarily indicate their endorsement of its conclusions.

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BASIC RESEARCH NEEDED FOR THE DEVELOPMENT OF GEOTHERMAL ENERGY

by

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September 25, 1979

INTRODUCTION

This report was prepared as part of the "Technical Crosscut" program of the Office of Basic Energy Sciences of the U. S. Department of Energy. The purpose of the report is to identify the basic research needed to facilitate the development of geothermal energy.

An attempt has been made to make the report representative of the ideas of productive workers in the field, and it is hoped that busy BES research administrators, as well as geoscience researchers, will find it useful.

The plan of the report is to discuss the present state of knowledge of geothermal energy, and then to list specific recommendations for further research, with priorities. The discussion is limited to a small number of very widely applicable concepts, namely:

- 1) The origin of geothermal flux.
- 2) Transport of geothermal energy.
- 3) Geothermal reservoirs.
- 4) Rock-water interactions.
- 5) Geophysical exploration.

The origin of geothermal flux.

Oceanic Crust: The flux of heat from the oceanic crust was thought for many years to arise from the mantle by conduction. The theory of plate tectonics, according to which new oceanic crust spreads out from oceanic ridges for thousands of kilometers at the rate of a few centimeters per year, and finally descends in subduction zones, has given a new picture of oceanic heat flow: For about 120,000,000 years, the heat flow from the ocean bottom arises from cooling of the crust.¹⁻² After this time some conduction through the crust from the mantle is needed to sustain the flux.

There are indications of extensive hydrothermal activity near the ocean ridges, where this crustal heat first arises. It may be expected that studies of these regions will yield important information for possible advanced geothermal energy systems.

Subduction Zones: Most of the heat flux through the ocean floor was carried into the crust by convection at the oceanic ridge; the downward sinking crust at a subduction zone gives rise to another region of increased heat flow, and such regions, near the boundary of continents and island arcs, are the location of most of the world's geothermal energy systems. A major cause of this volcanic activity over subduction zones may be the hydrated (and consequently lower melting point) sediments which cover the descending plate.³

Continental Heat Flow: The anomalous heat flows described above are restricted to regions near subduction zones. An interesting question for geothermal research is whether or not ancient subduction zones exist in the continental interior. If so, they may be potential geothermal resources.³

The radioactivity originally present throughout the earth appears now to be preferentially concentrated in the continental crust. The radioactivity generates heat, and the heat flow through the continental crust can be separated into two parts, a flux from the mantle and a flux generated by radioactivity in the crust. Birch et al, Roy et al, and Lachenbruch⁴⁻⁷ made the remarkable discovery that over wide regions ("heat flow provinces"), a plot of heat flow vs heat production in surface rocks is linear, with a finite value of heat flow at zero heat production, as in Fig. 1, which is taken from Lachenbruch.⁶ As Lachenbruch showed, if different amounts of rock have been removed by erosion at the various locations where measurements were made, and the relation has remained true during all this time, then the radioactivity must be distributed exponentially in the rock, decreasing with depth into the granite. Such a distribution has the property that if the rock is sufficiently thick the integral of all the heat generated below a depth, z , where the local heat generation is $A(z)$, is equal to $DA(z)$, where D is the vertical distance in which the heat generation falls by a factor of e . From the data of Fig. 1 it can be shown that $D = 10$ km in the central Sierra Nevada region where the data were taken. The left hand intercept of the curve is taken to be the contribution from the mantle, about 17 mW/m^2 in this region.

Fig. 1. Radiogenic Heat Production vs Heat Flow in Sierra Nevada.

This study of the heat flux from within the earth is a good example of the kind of basic research which has important consequences in geothermal energy extraction. It also shows that the question, "What basic research is needed to facilitate the extraction of geothermal energy?" involves a contradiction because of which it cannot be answered precisely, i.e., if the research is truly basic, the results of the research will be unexpected. Conversely, if the research results can be predicted, then very little new (or basic) information can be expected from the research.

The distribution of radioactivity in rock is of special interest to the geothermal energy program because of the possibility of finding reservoirs in the Atlantic Coastal Plain which derive their heat from buried granitic plutons, or of artificially creating reservoirs in granitic ranges such as the White Mountains of New Hampshire. Many questions remain as to the general applicability of this exponential distribution in rocks of various kinds with various emplacement histories; some regions where the heat flow is not linear with surface radioactivity have been found.⁷

Transport of Geothermal Energy

Volcanos provide impressive evidence that the earth's internal heat may sometimes be delivered to the surface at a very high rate. Large hydrothermal areas with surface manifestations of steam and hot water also require heat fluxes much greater than normal to support them. These two phenomena typify the two main aspects of a natural hydrothermal system, firstly, transfer of heat from the mantle into the upper part of the crust and secondly, transport of heat within this upper region. Sensible heat may be transferred by conduction or by convection of water or molten rock, so it is of interest to examine these processes separately, and relate them to various geothermal energy systems.

Conductive transport: Rocks are good thermal insulators with high heat capacity, so it is not surprising that it is difficult to extract the heat from a large body of rock. The thermal conductivity, k , of a typical crystalline rock is 3 w/(mK). The thermal diffusivity, η is $k/(\rho c)$, where ρ is the density and c the specific heat per unit mass. Typical values

of ρ and c for crystalline rock might be 2700 kg/m^3 and $1000 \text{ joule/(kg K)}$ making $\eta \approx 1.1 \times 10^{-6} \text{ m}^2/\text{s}$. The distance, L , from which heat can be extracted by conduction in time τ is $L \approx \sqrt{\eta \tau}$. Values of L for $\tau = 1$ year, 100 years, 10^4 years and 10^6 years are 6 m, 60 m, 600 m and 6 km, respectively.

The mean geothermal flux over the whole earth is $\sim 0.06 \text{ W/m}^2$. The temperature gradient corresponding to the flux is $\sim 20 \text{ K/km}$ in crystalline rock. A heat flux much greater than the mean, if sustained by conduction alone, requires correspondingly higher temperature gradients, with very high temperatures at the base of the crust. Mechanisms other than simple conduction appear to operate in regions of abnormal heat flow.⁸

Convective transport. The depth to which water might penetrate the crust is uncertain. In tectonically active regions water-filled cracks may extend to 10 km or so.⁹ Although fractures probably seal rapidly from mineral transport and deposition at water temperatures above 300°C ,¹⁰ new fractures are formed by the tectonic activity to maintain access to the heating zones and to provide permeable reservoirs for storage of hot fluid.¹¹

The lithosphere is a poorly defined region above the partial melt zone, in which the mantle and crust behave as a solid. Its thickness is 150-200 km under the continents, and non-radiogenic heat must penetrate this region to supply a hydrothermal field. If conduction and water convection are limited to a few kilometers, some other mechanism must be invoked. The association of known hydrothermal fields with volcanism suggests that the mechanism is "penetrative convection" of magma,¹² in which a bubble (perhaps many kilometers wide) of magma rises from a region of the mantle in which the temperature has been temporarily raised by some undefined process (e.g., subductive friction). After some millions of years, during which complicated processes such as crustal melting, stoping, and recrystallization at the base of the bubble occur, the bubble rises high enough to begin to supply heat to a hydrothermal system above it, perhaps with an intervening region of conductive transport. This process may not be necessary to the formation of warm water reservoirs with little surface manifestation, but must apply to large hydrothermal reservoirs like the Taupo district of New Zealand, which is described below.

Geothermal Reservoirs

Hydrothermal systems. The term "geothermal energy" at present is almost synonymous with hydrothermal energy--other types of reservoirs are under development, but are unproven. In the U.S., geothermal energy produces about one one-thousandth of the total electric power production. A recent estimate of the energy which might be recoverable from known and undiscovered hydrothermal reservoirs at temperatures above 90°C and depths above 3 km is 2400×10^{18} J, which could contribute 100-150,000 MW of electricity for 30 years, together with $230-350 \times 10^{10}$ J of beneficial heat.¹³ If this estimate is compared with present U.S. electric power consumption of 250,000 MW and total yearly energy use of 80×10^{18} J,¹⁴ it is seen that hydrothermal systems may provide a useful supplement to U.S. energy needs, but are not a long-term answer.

Some hydrothermal systems have been extensively studied. A good example is the Taupo geothermal district in New Zealand. This region, in an area of 2500 km², contains two major hydrothermal areas, Waiotapu and Wairaki, plus a number of small ones, and has an average heat flow about 35 times the world average.¹⁵ There is geological evidence that this activity has persisted for more than one million years. It is concluded that this reservoir is driven by a magmatic intrusion which lies within a few kilometers of the surface.

Geopressured systems. These systems are differentiated from hydrothermal systems in that no natural fluid convection system exists. However, sufficient fluid may be present in the rock, and the rock permeability may be high enough, so that heat may be extracted from the rock for extended periods simply by drilling into the reservoir. By definition, a geopressured rock contains fluid at pressure greater than would exist at the same depth in a column of water extending to the surface, i.e., hydrostatic pressure.

The geopressured reservoirs of interest for geothermal energy are located near the gulf coast in Texas and Louisiana. The reservoir rocks were deposited as sediments in river-bed, delta and marine environments, resulting in intermixtures of sandstone and shale rocks. When expulsion of pore fluids from the sandstones is restricted (the shales are almost impermeable), fluid pressures above hydrostatic arise from compaction

and from alteration of the shale by heat and pressure. The water temperature may be in the range 100-200°C depending on location and depth. The water is assumed to be saturated with methane, so three kinds of energy are theoretically available from a well--kinetic, thermal and chemical. Since there is essentially no convective heat loss from a geopressured reservoir, and the reservoirs are overlain by sediments of low conductivity, it is not necessary to postulate intrusive volcanic rocks as heat sources for the geopressured reservoir--the heat may have been deposited by normal heat flow over tens of millions of years. However, the depth to a given isotherm varies by a factor of two over the geopressured region¹⁶ and study of the origin of the heat may be fruitful.

Estimates of the recoverable geothermal and methane energy range from $270 \times 10^{18} \text{J}$ to 2800×10^{14} and $158 \times 10^{18} \text{J}$ to $1640 \times 10^{18} \text{J}$, respectively.¹⁶ These estimates are uncertain because of lack of production experience in geopressured wells, and lack of knowledge of the in situ permeabilities of undercompacted sandstone and shale, especially as fluid pressure drops during production.

Conductive Systems. Hydrothermal convective systems, discovered and undiscovered, are estimated to contain only one percent of the 10^{24}J of igneous-related geothermal energy present to a depth of 10 km¹⁷, much of the remainder must be locked up in relatively dry rock. About $3 \times 10^{25} \text{J}$ is estimated to reside in rock showing no recent igneous activity, at depths above 10 km.¹⁷ A hot dry rock experiment has been carried out in which approximately 5 MWT was extracted for 75 days, with negligible water losses, from impermeable crystalline rock at the Fenton Hill site near Los Alamos, New Mexico.¹⁸ The prospect for several times this much power for 20 years or more from a single pair of wells is promising and is being actively investigated. Artificial geothermal systems will be of many kinds, depending on the permeability of the rock and the fluid pressure in its pores. These reservoirs will range from high-pressure circulation systems in very impermeable rock to hot water convective systems with reinjection of all the extracted fluid, which may equally well be called stimulated hydrothermal systems. Since these reservoirs will be constructed (and, ideally, engineered), new methods of

securing information about the reservoir rock and the growth of the reservoir are needed. Knowledge of the directions and magnitudes of the principal earth stresses, joint patterns, pore fluid pressure, rock permeability and temperature gradient would be useful in the initial design of an artificial reservoir, and knowledge of fracture shape and the fluid flow paths is needed during operation.

When rock is cooled it undergoes thermal stress cracking, which may enlarge artificial reservoirs and extend their life almost indefinitely. Study of this process where it occurs in nature, i.e., in "lava lakes" near active volcanoes, in near-surface intrusions and at oceanic ridges may be valuable in designing artificial geothermal reservoirs.

Rock-Water Interactions

Basic research into the chemical interactions between hot water and rock has provided valuable tools for understanding natural hydrothermal systems. Several geothermometers have been developed.¹⁹⁻²⁰ These are based on measurement of the concentration of various common rock elements in the water from hot springs and the assumption that these concentrations arise from solution equilibrium between the water and rock at the reservoir temperature, and are unchanged as the water rises to the surface. In many cases it is even possible to correct for the effects of mixing of surface waters with reservoir water.

Geochemical analysis of this kind has been successfully used to locate fourteen producing geothermal wells in the Central Phillipines.²¹

Scaling and corrosion have been the principal obstacles to the development of liquid-dominated geothermal reservoirs. Scale is principally composed of silica, carbonates, metal sulfides or sulfates or mixtures of these. It is usually formed by loss of CO_2 (which changes the pH), concentration of dissolved materials by flashing or by changes in temperature of the fluid. Methods of scale control such as injection of acids or organic scale inhibitors, use of binary cycles to prevent flashing, and development of fluidized bed heat exchangers²² are currently under study. Corrosion is due to high temperature fluids with high chloride or hydrogen sulfide content combined with low pH and high oxidation potential. Methods for the control of corrosion in geothermal

systems have been developed,²³⁻²⁴ but much work remains to be done in order to achieve more understanding of corrosion mechanisms.

Geophysical and Geochemical Exploration

Various geophysical measurements have been successfully applied in exploration for hydrothermal systems. New Italian geothermal fields at Cesano, Torre Alfina, Bagnore, Piancastagnio and Poggio Nibbio, all without surface manifestations, were discovered by exploration techniques including reflection seismic surveys, gravity contouring, resistivity surveys, and measurement of geothermal gradient in shallow boreholes. Wells were successfully drilled in the region of highest heat flow.²⁵ In Leyte, in the Phillipine Islands, geochemical thermometric measurements in hot springs have indicated where the highest grade geothermal energy resource was located.²¹

Geophysical exploration techniques were originally developed for petroleum and mining exploration and well logging. In geothermal exploration some of the anomalies of interest, such as low resistivity at depth, may or may not arise from hot water or brines. Some such ambiguity cannot be avoided, but it is likely that new geophysical tools can be developed specifically for geothermal energy exploration. Examples of unique phenomena applicable to geothermal energy systems are the presence or movement of magma within a few kilometers of the surface, weak seismic signals from thermal-stress cracking, thinning of the crust in regions of extension, and temperatures above the Curie point at shallow depths. Geophysical effects from all these phenomena have been detected, but have not yet been widely employed for geothermal exploration. Corresponding geochemical phenomena are isotope ratios in rocks and water as well as new information which may be deduced from the concentrations of chemical species. Recent developments in both geophysics and geochemistry are given by White and Guffanti.²⁶

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Research Recommendations

All of these recommendations belong in the Engineering, Mathematical and Geosciences program of the Office of Basic Energy Science, Department of Energy. Relative importance has been indicated by asterisks, one asterisk corresponding to the least importance or urgency.

Fundamental geological studies on the cause and distribution of elevated isotherms within the North American Plate.

- ***(a) Regional Curie isotherm analysis of available aeromagnetic and magneto-telluric data.
- *(b) Conduct deep crustal seismic reflection surveys using shear wave or combined compressional and shear wave vibrators.
- ***(c) Using distant and regional earthquakes, map seismic velocity and attenuation variations, with special attention to depth to the Moho.
- ***(d) Study of relationship between gravity surveys and regions of anomalous heat flow.
- * (e) Map contours of saturation temperature using geochemical thermometric data from hot springs.
- * (f) Age-date youthful volcanic events.
- * (g) Study distribution of radioactivity in plutons.
- ***(h) Emplacement mechanisms of igneous intrusions.

Physical Properties and Behavior of Rock-Fluid Samples at Elevated Temperatures and Pressures.

- *** (a) Metamorphism--dissolution, recrystallization, diffusion.
- ** (b) Sealing of cracks--necessary conditions, mechanisms, time scale.
- * (c) Study of magma-water system--vapor pressure, diffusion rates, phase changes vs water content, pressure and temperature.
- * (d) Mechanisms involved in cooling of magmatic intrusions--study of phenomena in lava lakes.
- ** (e) Geochemical thermometers--factors affecting accurate interpretation such as the approach to low-temperature equilibrium; use of new chemical species and/or isotopes.
- * (f) Physical and chemical interactions of gases in hydrothermal systems.
- ** (g) Phenomenology and kinetics of the precipitation of calcium carbonate and silica from geothermal brines.

Hydrothermal Evolution of Geothermal Systems

- * (a) Depth of circulation of water in hydrothermal systems.
- * (b) Formation of geopressurized reservoirs.
- * (c) Effect of tectonic stresses and activity on permeability.
- ** (d) Convection and recharge in geothermal reservoirs--favorable sites for reinjection of cooled geothermal fluids.

Development of New and Improved Geophysical Probes

- ** (a) Deep seismic soundings--continuation of succesful attempts to improve resolution at great depths.
- ** (b) Deep magnetic, electric and electromagnetic soundings--relation of earth stress to asymmetries in resistivity at depth.
- ** (c) Study of short and long period variations in altitude of continental surface--new satellite techniques for measuring earth swelling and subsidence may reveal deep processes.
- * (d) Study of short and long period variations in horizontal position or differential position (earth strain) of continental surface--earth-tide strains may reveal deep inhomogeneities.
- ** (e) Development of three dimensional algorithms for interpretation of seismic data.

SERI/TR-351-358

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BASIC RESEARCH NEEDS AND
PRIORITIES IN SOLAR ENERGY
VOLUME I
EXECUTIVE SUMMARY

TECHNOLOGY CROSSCUTS FOR DOE

T. S. JAYADEV
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FOREWORD

This executive summary condenses the findings of a SERI technical report which identifies basic research needs that are important to the development of solar energy. The report was prepared in response to a request from the Associate Director for Basic Energy Sciences, Office of Energy Research, U.S. Department of Energy. The full technical report is Volume II of SERI/TR-351-358.

The project was led by T. S. Jayadev of the Research Division and David Roessner of the Analysis Division. Michael Genest, a summer intern from the University of California, Berkeley, served as Research Associate on the project and made a major contribution to this report. Members of the SERI task force assembled to carry out the project were:

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PREFACE

OVERVIEW OF SOLAR ENERGY TECHNOLOGY

By: J. Charles Grosskreutz

Solar energy conversion can be categorized by the processes of the physical interaction of solar radiation with matter (SERI 1979, MR-12-207). Figure P-1 is a schematic representation of the two major absorption processes: the production of heat and quantum interactions. Both processes, by means of suitable conversion mechanisms, can lead to useful energy products. These two general conversion processes or paths are referred to as Thermoconversion and Photoconversion. Given today's knowledge, they are the only two paths currently available. The most common conversion technologies that use the two primary interactions are flat-plate collectors which convert the heat produced by thermoconversion to hot water or air, and photovoltaic cells which convert the electron-hole pairs created in semiconductors by photoconversion to an electric current.

A more detailed view of the multiple conversion pathway with thermoconversion and photoconversion is shown in Figs. P-2 and P-3. These figures are arranged so that from bottom to top one moves from already or nearly commercialized technologies to those which are not yet out of the basic research stage. Similarly, the photoconversion paths may be placed above the thermoconversion paths so that the same vertical axis takes one from relatively simple mechanical and structural systems in thermoconversion to highly sophisticated, solid state biological and chemical systems in photoconversion.

Another way of viewing the phenomenological framework shown in Figs. P-2 and P-3 is to use the horizontal axis to designate how far a particular conversion mechanism has progressed along the RD&D sequence. The wavy shaded line denotes that (fuzzy) boundary between what is already known, understood, or developed (the area to the left); and the region where research is still required to advance the technology (the area to the right). Clearly, lowhead hydro and wind turbine technology are in various stages of engineering development, while photobiological and photochemical conversion still require research in the mechanisms of primary product formation. Photovoltaic research is now concentrating on conversion mechanisms and device technology, with single-crystal silicon much further advanced than other materials such as gallium arsenide or amorphous silicon.

Any new conversion technology must fit into this overall scheme, either deriving from primary quantum processes or from the heat produced in some absorber. Note, too, that storage of the energy produced along any of these paths can occur at any point along the horizontal axis; e.g., storage of the final electricity product in batteries, or of the primary excited photochemical states in a suitably stable chemical compound.

Furthermore, the horizontal axis is a continuum in mission-oriented research. Domains of fundamental research occur near the left side. These evolve into mission-oriented research as one proceeds to the right and begins engineering research and development, market and policy analysis, and the commercialization activities required for the marketplace to accept the technology. The position of the wavy shaded line expresses qualitatively the kind of research still required and distinguishes the near-term technologies from those far removed from application.

Figure P-1. Solar Radiation Processes and Conversion Paths

Figure P-2. Detailed Framework for Solar Thermoconversion Paths

Figure P-3. Detailed Framework for Solar Photoconversion Paths

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SECTION 1.0

INTRODUCTION

1.1 BACKGROUND

Energy supply and use issues are likely to command the attention of government policy makers from now until well into the next century. Tax revenues will continue to be spent to influence consumer energy choices and to develop and accelerate the commercialization of new energy technologies. Tax revenues will also continue to support the fundamental research needed to ensure a broad range of future energy options. How these research monies should be allocated among the myriad promising avenues is a continuing concern of energy policy makers. This report seeks to address that concern by providing the U. S. Department of Energy (DOE) with the results of an effort to identify the basic research needs and priorities in solar energy.

Research in solar energy must develop knowledge about how both the physical and social systems function. Achieving the nation's current solar energy goal, to produce 20% of the total energy consumed in the year 2000 through solar energy conversion, will be a challenge for both physical and social scientists engaged in solar energy research.

Current solar energy conversion technologies are probably not adequate to achieve the 20% goal. The solar energy conversion systems of the twenty-first century will be very different from today's systems. In this report we have tried to identify areas of research that will lead to new concepts for the year 2000 and beyond, in addition to those areas of research which must be pursued to develop nearer-term technologies. The products of solar energy are heat, electricity, chemicals, and fuels. Various physical phenomena can be exploited in order to convert solar radiation to each of these end products.* Conversion to heat is relatively straightforward and current programs, especially those conducted by DOE's Office of Energy Technology (ET), cover this area. But in the areas of conversion to the other end products, research is generally in the embryonic stage. Conversion of solar energy to electricity—either directly or via thermal processes—is still an emerging field where new concepts based on physical processes in solids, liquids, and gases seem certain to emerge in the near future. Research needs in these areas are described in the sections on Materials Sciences, Engineering, and Advanced Energy Research Projects. Conversion of solar radiation to fuels and chemicals, and to electricity via chemical and biological processes, is also a very promising and exciting area of research. Research needs in these areas are described in the sections on Chemical and Biological Sciences.

With the exception of conversion of solar energy to heat and biomass conversion, solar technologies will not mature for ten to twenty years or more. To reach maturity, these technologies will require research support in basic and applied sciences. This support must come from programs that focus on the special needs of solar energy as well as from the current programs which are organized according to scientific disciplines.

Public action will be taken over the next several decades to increase the number of available solar energy supply and use options; improve the cost, performance, and reliability of developing solar technologies; provide incentives to increase the market for

*See the Preface to this report, "An Overview of Solar Energy," by J. C. Grosskreutz.

solar technologies; and remove institutional and legal barriers that inhibit solar energy applications. If these actions are to be effective while also minimizing economic, social, and environmental costs, better understanding is needed of how consumer and industrial markets for energy supply technologies operate, what consequences are likely to result from large-scale use of solar technologies, and how government policies affect energy choices and private investment in the development of new energy technology. Such understanding must come from research in the Behavioral and Social Sciences.

Our society is built on the belief that knowledge about ourselves, our social system, and our physical environment will help us solve the problems we face. Energy issues now seem almost intractable in their complexity and show little promise of becoming simpler as the years pass. Immediate and near-term solar energy policy decisions hopefully will be illuminated by current, state-of-the-art knowledge. If future decisions are to be still better informed, government must invest now in basic research that can bear fruit in usable knowledge and analytical tools ten, twenty, thirty, or more years hence. The Behavioral and Social Sciences section of this report suggests areas of basic inquiry that we believe have the greatest likelihood of contributing to the appropriate development of solar energy within that time frame.

This assessment of basic research needs in the field of solar energy was undertaken at the request of DOE's Office of Basic Energy Sciences (BES). Specifically, BES requested that SERI identify the "lines of research (that) should be covered," provide guidance in assessing the relative importance of those lines of research, identify research areas "deserving very special emphasis," and identify the "principal issues concerning basic research" related to solar energy. Choice of the methods to be used in preparing the assessment was left to SERI's discretion with the understanding that it should represent the views of the broad scientific community and should not be limited to the opinions of SERI scientists alone. BES was hopeful that the finished document would be useful in "comparing priorities across divisional lines within BES."

1.2 METHOD

A committee composed of ten SERI scientists representing the major scientific disciplines important to solar energy was formed following the BES request. The first decision the committee faced was how to develop a representative description of research needs in solar energy. Wallace S. Sayre notes that scientists traditionally have been represented by outspoken, self-appointed, individual spokespersons; by small elite groups, some self-nominated, some the designees of government officials; by various scientific associations with broad scientific constituencies; or by specialized associations of scientists (Gilpin and Wright 1964). Thus, there is no existing group that can claim to represent "scientific opinion," nor is there an established, clearly defined group of scientists engaged in solar energy research.

Various methods for sampling the opinions of working scientists were considered, but many were deemed impractical, inefficient, or beyond the resources available to SERI. The method finally adopted rested on the knowledge that SERI scientists were in excellent positions to know the scope of solar energy research and identify key researchers in their fields. Each scientist on the committee sought the opinions of leading scientists in his or her field engaged in or knowledgeable of solar-related research. Initially, more than 120 scientists were interviewed by telephone to obtain their views on needed research topics. From these interviews, a preliminary draft listing these research topics by discipline was prepared and mailed to most of the scientists interviewed. Each was

asked to review the draft and suggest changes in the list of research needs identified as well as to assign priorities within his or her field of expertise. This final version incorporates the responses to the first draft.

The committee scientists relied heavily on the opinions of scientists polled but occasionally deleted, augmented, or combined the specific recommendations of individuals polled in order to resolve contradictions and make comparisons more uniform. In addition, committee members weighted their own recommendations and opinions at least as heavily as those of the scientists they polled. The result is an amalgam of national scientific opinion representing the viewpoints of key researchers in relevant disciplines and of SERI research staff opinions.

The researchers queried are not fully representative of the full spectrum of solar energy scientists. Undoubtedly, many important and knowledgeable solar energy scientists were omitted. This was inevitable, given the time and resource constraints on the overall effort. Nevertheless, a broad range of scientists working at each major type of research institution contributed their opinions on research needs and priorities in solar energy. The report does not represent a national consensus or even a consensus among the groups surveyed, but we believe the result is a close approximation to "the scientific community's" views on research needs in solar energy.

1.3 THE PROBLEM OF SETTING PRIORITIES

Perhaps the most difficult and controversial aspect of this effort was the setting of priorities. While there is abundant literature on the question of policy choice in resource allocations to science, it generally approaches the question from a broad national perspective. For example, it addresses the problems of choice among broad areas of federally funded research such as medicine and space but seldom touches on the issues inherent in choices among narrow fields of research such as photochemistry and photobiology.

Alvin Weinberg provides some insight into this more specific type of scientific choice (Weinberg 1963, 1964). Weinberg proposes three sets of criteria for scientific choice—"scientific merit," "technological merit," and "social merit." "Social merit" is a broad concept having to do with considerations of national prestige, health, welfare, and military power. "Technological merit" refers to the balance between research costs and probable benefits attributable to a given line of research. ["Technological merit" is closely related to C. F. Carter's economic criterion (Carter 1963). Carter suggests that scientific effort be distributed in such a way as to maximize the flow of wealth to society.] "Scientific merit," the "internal criterion," depends upon the maturity of a field or technique for exploitation and the caliber of the practitioners who will be engaged in the research. While Weinberg did not propose these concepts as criteria for the more detailed level of scientific choice that this report addresses, "technological merit" and "scientific merit" are concepts that can be useful in assigning priorities to research topics within broad fields such as solar energy.

In applying the criterion of "technological merit" to specific research projects, four parameters must be estimated: the probability that a project will result in a viable new technology, the likely benefit to society attributable to that technology, the time required to complete the research, and the likely cost of the research. Clearly, these parameters are extremely difficult to estimate accurately. How many scientists would be willing to assign a precise probability to the chances for success of a specific project? In the likely event that different scientists assigned widely different probabilities

to the same project, who would choose the "correct" one? If estimates are pooled or averaged, would each be weighted equally or would some be given more credence than others? Efforts by committees of the National Academy of Sciences to apply this kind of thinking to setting research priorities in several fields of science have not been successful (Reagan 1969, pp. 270-302).

Nevertheless, consideration of these four parameters undoubtedly plays a part in scientific choice by public policy makers. No attempt was made, however, to formally incorporate a consideration of these parameters into the priority setting process in preparing this report. A methodology for doing so has not yet been developed.* It is likely, however, that many of the respondents considered such questions informally in making their recommendations.

Undoubtedly, the criterion of "scientific merit" was also considered by the respondents. Scientists are more aware than any other group of the readiness of a field for exploitation and of the caliber of practitioners available for doing the research. Again, no attempt was made to formally consider "scientific merit" in preparing this report for reasons similar to those just presented. Based on the priority rankings and substantive recommendations received from respondents, the committee scientists were asked to assign to each research topic one of three priorities. The levels of priority were defined as follows.

Crucial: work that is essential if progress is to be made in an important area of solar energy; without research on this topic we have little hope of further significant progress in the field.

Important: work that is likely to produce immediate payoffs either in improved technology or in scientific understanding of an important area of solar energy.

Needed: work that has a fair to good chance of helping to further the development of an important area of solar energy.

The committee chose these definitions over a simple "high," "medium," and "low" ranking system in an attempt to suggest the criteria of "technological merit" and "scientific merit." While these definitions partially capture the elements of these criteria, with the exceptions of research costs and caliber of practitioners available (estimates of these parameters were thought to be more appropriately left to BES decision makers and national laboratory administrators), they clearly are more suggestive than definitive. In practice, committee scientists found that the distinctions between the categories were blurred and, in assigning research topics to one or the other of these categories, they often relied heavily on personal judgments.

Since each committee scientist was responsible for a specific discipline, it is not possible to use the priorities as a basis for comparing research priorities across different disciplines. What is crucial to thermochemical conversion may be no more vital to the nation than what is important to photochemical conversion, or vice versa. BES clearly needs to make these kinds of comparisons, but this report cannot serve as the basis for doing so. Such comparisons are particularly difficult to make among fields in basic research. Federal agencies, of necessity, have been making such comparisons for many years. John G.

*Some interesting work along these lines has been done by S. James Press and Alvin J. Harman of Rand. See Press and Harman; Methodology for Subjective Assessment of Technological Advancement. Rand; Santa Monica, CA: April 1975; R-1375.

Wirt et al. have described the various techniques these agencies have used (Wirt et al. 1974). While they do not attempt to evaluate these techniques, their description may prove helpful to BES in its efforts to design a method for making these difficult comparisons.

1.4 THE FORMAT OF THE REPORT

Each major section covers one scientific field, corresponding to the organizational structure of BES. With the exception of the section on Behavioral and Social Sciences (which is arranged according to generic areas of research needs) the sections are composed of subsections, each of which covers one scientific discipline. Each subsection was written by a committee scientist specializing in the discipline discussed. At the end of each subsection, there is a table of research needs within that discipline, arranged by priority classification. Priorities, always underlined, also appear in the text.

This format was chosen to facilitate quick access to the relevant parts of the text for readers interested only in particular disciplines.

SECTION 2.0
CHEMICAL SCIENCES

2.1 THERMAL CONVERSION OF BIOMASS

The crucial needs in thermal conversion of biomass are (1) for improved mechanistic and kinetic characterization of pyrolysis, gasification, and liquefaction, including the effect of catalysts; and (2) for better chemical and physical characterization of biomass and for exploratory electrochemical research.

Table 2-1. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: THERMAL CONVERSION OF BIOMASS

Research	Priority
1. Fundamental studies of slow and fast pyrolysis.	<u>Crucial</u>
2. Thermodynamic, thermophysical, and optical property information of biomass and chars.	<u>Crucial</u>
3. Development of catalysts for gasification and liquefaction.	<u>Crucial</u>
4. Research on the fundamental reaction chemistry in liquefaction in aqueous and nonaqueous media.	<u>Crucial</u>
5. Research in the area of electrochemical processing of biomass.	<u>Crucial</u>
6. New formulations of organic reaction mechanisms under extreme thermal or photo fluxes.	<u>Important</u>
7. Novel methods of temperature and composition measurement in heterogeneous systems.	<u>Important</u>
8. Kinetic studies of secondary cracking of primary pyrolysis products.	<u>Important</u>
9. Basic engineering studies of prototype reactors.	<u>Important</u>
10. Demonstration of novel thermal processing methods (e.g., molten salts, microwave).	<u>Important</u>
11. Characterization of environmentally hazardous conversion by-products.	<u>Needed</u>

2.2 THERMOCHEMICAL AND THERMOELECTROCHEMICAL CONVERSION OF SOLAR ENERGY

The crucial research needs in both thermochemical and thermoelectrochemical conversion of solar energy relate to the laboratory demonstration of the feasibility of novel cycles to produce chemicals, fuels, or electricity.

A detailed discussion of electrochemical research areas is contained in a report prepared for NSF entitled "Energy Workshop on Electrochemistry. A Report on Discussion of Energy-Related Basic Research in Electrochemistry" (Osteryoung et al. 1974).

Each of the subject areas just discussed is included in a forthcoming NAS report to NSF entitled "High Temperature Science: Future Needs and Anticipated Developments," which should be completed in 1979. Another report, being prepared for DOE by the NAS Committee on Chemical Science, will address aspects of basic research in the chemical sciences, including specifically solar energy, biomass energy, electrochemistry, and high-temperature chemistry.

Table 2-2. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: THERMOCHEMICAL AND THERMOELECTROCHEMICAL CONVERSION OF SOLAR ENERGY

Research	Priority
1. Demonstration of the feasibility of cyclic, dissociative, or N-fixing schemes.	<u>Crucial</u>
2. Demonstration of thermally regenerable EMF cell cycles.	<u>Crucial</u>
3. Study of modified electrodes, electrocatalysis.	<u>Crucial</u>
4. Acquisition and critical evaluation of thermodynamic data.	<u>Important</u>
5. Basic studies in reversible chemical systems for heat transport and storage.	<u>Important</u>
6. Research to discover new solar-driven processes in metallurgy and biomass gasification.	<u>Important</u>
7. Search for new solid electrolyte anion, cation, and gas conductors.	<u>Important</u>
8. Microscopic description of ionic and electronic processes at solid/electrolyte interfaces.	<u>Important</u>
9. Studies of novel high-temperature dissociated gas separation techniques.	<u>Needed</u>
10. Studies of solar-assisted gasification of coal.	<u>Needed</u>
11. Research on the use of ZrO_2 in high-temperature electrolysis of steam, CO_2 .	<u>Needed</u>

2.3 PHOTOCHEMICAL CONVERSION AND STORAGE

Significant scientific advances in basic research are difficult, if not impossible, to predict. There is no way of deciding a priori when, or in what way, basic scientific exploration will "pay off." If such things could be forecast with any accuracy at all, there would be little point in doing the research (Thomas 1978). The specific opportunities listed in the table outline the kinds of research that are required in order for photochemical conversion to emerge as a self-sufficient technology. This research will provide a significant part of the knowledge required to develop new approaches to conversion and storage of solar energy.

Table 2-3. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: PHOTOCHEMICAL CONVERSION AND STORAGE

Research	Priority
1. Photosensitization:	
Define photophysical and photochemical parameters required for efficient capture and primary conversion of solar quanta.	<u>Crucial</u>
2. Redox Catalysis:	
Synthesis and characterization of molecules capable of serving as stable intermediates in sequential electron-transfer events.	<u>Crucial/Important</u>
3. Coupled Systems:	
Specific matching of spectroscopic, photophysical, electrochemical, structural, and catalytic properties of photosensitizers and redox catalysts in heterogeneous media to effect useful photochemical reactions such as water splitting and reduction of N_2 or CO_2 .	<u>Crucial</u>
4. Unimolecular Storage:	
Mechanisms of direct and sensitized photoisomerization reactions and development of specific catalysts for the reverse processes.	<u>Important</u>
5. Theoretical Studies:	
Accurate, quantitative predictions of molecule properties.	<u>Important</u>
6. Instrumentation:	
Application of new techniques and development of new instrumentation.	<u>Crucial/Important/Needed</u>

2.4 PHOTOELECTROCHEMICAL ENERGY CONVERSION

Photoelectrochemical energy conversion is based on photoactive semiconductor electrodes which absorb visible light, thereby creating electron-hole pairs which separate in the space charge layer produced at a semiconductor-liquid electrolyte interface. These separated electrons and holes are injected into the electrolyte to drive chemical reduction and oxidation reactions.

Photoelectrochemical cells can be configured to produce electricity (electrochemical photovoltaic cells) or to drive chemical reactions (photoelectrosynthetic cells). Chemical reactions driven uphill in energy (endoergic) produce fuels (for example, splitting of H_2O into H_2 and O_2); chemical reactions can also be driven downhill in energy (exoergic) to produce useful chemicals (for example, reduction of N_2 to NH_3). For the endoergic case, solar energy is converted into chemical energy, while for the exoergic case, solar energy provides the activation energy for chemical reactions.

Photoelectrochemical systems have a high theoretical conversion efficiency (25%); they can be operated with inexpensive polycrystalline and/or amorphous electrodes without drastic loss of efficiency; and simple inexpensive photochemical reactor systems based on photochemical diodes in a slurry- or colloidal-type system can be utilized. However, the major problem preventing the implementation of these advantages is the lack of sufficient photochemical stability in the semiconductor electrode materials that have band gaps in the optimum range (1.0 to 2.0 eV). For electrochemical photovoltaic cells, efficiencies of 12% have been achieved with GaAs electrodes. For photoelectrosynthetic cells, H_2O has been split with simulated sunlight at 1% of efficiency, and N_2 and CO_2 reduction has been demonstrated using visible light and p-GaP electrodes.

The research needs in electrochemical photovoltaic cells include work on (1) theory and models, (2) semiconductor materials with high efficiency and stability, (3) new electrolytes and compatible redox couples, (4) in situ energy storage, (5) toxicology of candidate semiconductor electrodes, and (6) establishment of the relationships between the behavior of single-crystal and polycrystalline electrodes. For photoelectrosynthetic cells, research needs include work on (1) theory and models, (2) catalytic effects and their relationship to electrode overvoltage, (3) new semiconductor electrodes and structures, (4) new and novel photoelectrochemical reactions (such as nitrogen fixation and carbon dioxide reduction), and (5) photochemical diodes (particulate systems) and photocatalytic systems.

Table 2-4. SUMMARY OF RESEARCH NEEDS AND PRIORITIES:
PHOTOELECTROCHEMICAL ENERGY CONVERSION

Research	Priority
<u>Electrochemical Photovoltaic Cells (ECPVC)</u>	
1. Development of models and theoretical understanding of ECPVC.	<u>Crucial</u>
2. Development of new electrolytes and compatible redox couples which promote the stability of potential, high-efficiency, semiconductor electrodes.	<u>Important</u>

**Table 2-4. SUMMARY OF RESEARCH NEEDS AND PRIORITIES:
PHOTOELECTROCHEMICAL ENERGY CONVERSION
(concluded)**

Research	Priority
3. Study of in situ storage in ECPVC.	<u>Important</u>
4. Toxicology—environmental effects of apparently hazardous and toxic materials.	<u>Important</u>
<u>Photoelectrosynthetic Cells (PESC)</u>	
1. Theory and models of PESC.	<u>Crucial</u>
2. Catalytic effects and their relationship to electrode overvoltage.	<u>Important</u>
3. New and novel photoelectrochemical reactions.	<u>Important</u>
4. Photochemical diodes.	<u>Important</u>

SECTION 3.0

BIOLOGICAL SCIENCES

3.1 BIOMASS

To develop a Biotechnology of Biomass Processing for producing fuels and chemicals, basic work is crucially needed in genetics, biochemistry/physiology, and biochemical engineering.

Biomass production could be advanced by adequate research support in plant physiology, agronomy, and tissue culture. It is important that such research be focused on a systems approach; that is, with conversion in view.

For improving the efficiency of conventional fermentation processes, microbiological and biochemical engineering work is crucial. The development of product- and temperature-tolerant strains is crucial. The present energy inefficiency of product recovery should be improved by basic chemical engineering research; optimal control of biological processing is important/crucial.

To bring the processing of lignocellulosic biomass to a commercial level, a long-term application of basic research is crucially required. The mechanism of action of hydrolyzing enzymes is not yet understood. Physiological and biochemical engineering features of mixed culture processing should be investigated. A basic understanding of the genetics of industrial microorganisms and of the possibilities for hybrid construction by gene transfer is lacking. The unconventional engineering features of bioreactors for processing solid biomass require investigation, and there is a lack of information on the fluid dynamic properties of slurries.

Extensive biochemical and genetic work is needed to advance the development of extraction processes for producing oily hydrocarbons and other chemicals from both lower and higher organisms.

Table 3-1. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: BIOMASS

Research	Priority
<u>Biomass Production</u>	
1. Tissue culture.	<u>Crucial</u>
2. Agronomic development (genetics).	<u>Crucial</u>
3. Plant physiology.	<u>Crucial</u>
4. Plant biochemistry and development.	<u>Important</u>
<u>Biomass Conversion</u>	
1. Biological pretreatment.	<u>Crucial</u>
2. Membrane biochemistry.	<u>Crucial</u>

Table 3-1. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: BIOMASS (concluded)

Research	Priority
3. Strain development (Genetic Engineering).	<u>Crucial</u>
4. Product recovery energy efficiency.	<u>Crucial</u>
5. Novel bioreactor engineering.	<u>Crucial</u>
6. Immobilized cell research.	<u>Crucial</u>
7. Biosynthetic pathway manipulation.	<u>Crucial</u>
8. Process control.	<u>Important/Crucial</u>
9. Mechanism of cellulose action.	<u>Important</u>
10. Hemicellulose conversion.	<u>Needed/Important</u>
11. Pentose metabolism.	<u>Needed/Important</u>
12. Lignin conversion.	<u>Needed</u>
13. Xylanase mechanism.	<u>Needed</u>
14. Slurry rheology.	<u>Needed</u>
<u>Biomass Extraction</u>	
1. Plant production of hydrocarbons.	<u>Important/Crucial</u>
2. Microbial production of chemicals.	<u>Important/Crucial</u>
3. Biochemistry and genetics of marine microorganisms.	<u>Needed</u>

3.2 PHOTOBIOLOGICAL CONVERSION

Although it is difficult to predict the relative importance of basic research in different areas, it is clear that studies which address metabolism or the relationship between structure and function in photobiological systems (especially the energy transfer processes in photosynthesis) are crucial. Work directed towards understanding the mechanisms and regulation of in vivo energy transducing systems is also crucial during the near term. Research on component stability and coupling mechanisms in in vitro systems is important to crucial over the long term.

**Table 3-2. SUMMARY OF RESEARCH NEEDS AND PRIORITIES:
PHOTOBIOLOGICAL CONVERSION**

Research	Priority
1. Primary processes and electron transport.	<u>Crucial</u>
2. Stability of biological systems.	<u>Important</u>
3. Metabolism of biological systems.	<u>Important</u>
Hydrogen production by photosynthetic bacteria	<u>Crucial</u>
4. In vitro systems.	
Short term	<u>Needed</u>
Long term	<u>Important to Crucial</u>

SECTION 4.0

MATERIALS SCIENCES

4.1 METALLURGY AND CERAMICS

The design and fabrication of metal and ceramic components for solar applications must meet critical and often contradictory demands for low cost, high reliability, and long life. Present understanding of fabrication processes and degradation mechanisms are inadequate to insure reproducible performance or to predict service lifetimes with confidence. These are pervasive problems which limit all technological applications of metals and ceramics as well as those in solar energy conversion. Research which is crucial to the improvement of this situation is listed in the table accompanying this section.

Table 4-1. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: METALLURGY AND CERAMICS

Research	Priority
1. Improve the understanding of the processes involved in the reproducible fabrication of metal and ceramic components. These processes include: <ul style="list-style-type: none"> A. kinetics of nucleation, phase transformations, and solidification; B. behavior of fine particles and how their shape and surface properties affect their rheology and subsequent ceramic or powder metallurgy fabrication. 	<u>Crucial</u>
2. Improve methods to detect flaws in fabricated metal and ceramic components and thereby improve their reliability: <ul style="list-style-type: none"> A. determine origins of flaws; B. develop physical techniques for the nondestructive detection and measurement of flaws. 	<u>Crucial</u>
3. Improve methods for predicting the degradation of metal and ceramic components in service: <ul style="list-style-type: none"> A. improve the understanding of atomistic mechanisms at the tip of a growing crack; B. model complicated chemical reaction processes in multiphase, multicomponent systems. 	<u>Crucial</u>
4. Improve the nonequilibrium, nonlinear thermodynamic theory required to describe the processes in A-C above.	<u>Important</u>

4.2 MATERIALS CHEMISTRY

Major research efforts should be carried out in materials chemistry to elucidate mechanisms of degradation in solar-stressed environments that reduce the solar system performance, in order to (1) guide modifications of materials to minimize the effect of the detrimental processes; (2) understand the influences of structure, bonding, and composition that provide stability; (3) devise materials preparation and fabrication processes that yield the desired chemical, electronic, physical, or mechanical properties; and (4) devise new experimental techniques to study and/or measure the important materials properties.

In summary, a number of studies are crucial, important, and needed for impacting solar energy conversion technologies. These are listed in the accompanying table. It is crucial that the studies be carried out on the most promising materials to elucidate the synergistic effects of solar stresses such as UV, temperature, atmospheric gases and pollutants, daily and annual thermal cycles, etc.

In addition to those people contacted, as given in Appendix B, the information in this section has been assembled using several reference documents (Call 1979; Somorjai et al. 1977; U.S. DOE 1979b; Solar Optical Materials Program Activity Committee 1979; Solar Glass Coordinating Committee 1979; Pohlman and Staehle 1979).

Table 4-2. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: MATERIALS CHEMISTRY

Research	Priority
1. Work on the most promising materials for potential application when exposed to solar-stressed environments.	<u>Crucial</u>
2. Study enhanced stability/reactivity resulting from interfacial contact between different materials.	<u>Crucial</u>
3. Elucidate mechanisms of degradation reactions at s/s, s/l, and s/g interfaces.	<u>Crucial</u>
4. Elucidate mechanisms of photoenhanced degradation of polymers and ion transport in transmitting materials.	<u>Crucial</u>
5. Study gas/solid reactions and co-chemisorption processes at atmospheric pressure.	<u>Crucial</u>
6. Study diffusion in coatings and thin films including atom transport and accumulation at grain boundaries.	<u>Crucial</u>
7. Understand bonding, compositional, and structural relationships in adhesion.	<u>Crucial</u>
8. Understand reactions at s/l interfaces.	<u>Crucial</u>
9. Work on the stability of polycrystalline materials.	<u>Important</u>

Table 4-2. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: MATERIALS CHEMISTRY (concluded)

Research	Priority
10. Understand diffusion and segregation at grain boundaries.	<u>Important</u>
11. Study nucleation and growth at interfaces.	<u>Important</u>
12. Determine interfacial effects on optical properties.	<u>Important</u>
13. Understand adhesion of s/s interfaces, including polymer/metal oxide(s).	<u>Important</u>
14. Study adhesion of dust onto transmitting materials.	<u>Important</u>
15. Conceive and test theoretical models of polycrystalline systems.	<u>Needed</u>
16. Conceive and test theoretical models of atomic forces in adhesion.	<u>Needed</u>
17. Study growth or modification processes to alter properties of films, coatings, glasses, and polycrystalline materials.	<u>Needed</u>
18. Develop advanced instrumentation for preparing new or modifying existing materials.	<u>Needed</u>
19. Characterize interfacial properties of polycrystalline materials.	<u>Needed</u>
20. Develop equipment to detect incipient stages of diffusion, segregation, chemisorption, etc.—processes that cause changes in properties.	<u>Needed</u>

4.3 SOLID STATE PHYSICS

Solid state physics plays a very important role in solar energy conversion. One of the solid state energy conversion techniques, photovoltaics, is currently being actively investigated by Energy Technology (ET). But there are other energy conversion technologies that need to be studied from both basic and applied points of view. It is crucial to develop a research program in solid state energy conversion technologies, as they will open alternate avenues for solar energy conversion. Further, some of them may be particularly suited for certain applications. For example, thermoelectrics may be more suitable than photovoltaics in solar total energy systems or as a topping cycle for a solar steam power plant. It is crucial to conduct a broad program of research in thermal and optical properties of materials in support of energy conversion technologies. It is crucial to conduct a comprehensive empirical and theoretical search to identify promising materials for solid state energy conversion. It is crucial to develop an experimental research program in new semiconductor materials such as amorphous semiconductors or organic semiconductors. This will open up interesting possibilities for thermoelectric and

other solid state energy conversion processes. In fact, it may be possible to take a fresh approach to photovoltaics. Some scientists believe that a radical reduction in cost of solar cells could be achieved by an imaginative research program to uncover a very cheap thin-film material that has optical and electrical properties suited for solar cells. In addition, there are several areas of basic and applied research which have to be pursued in support of ET activity. The crucial ones are studies of self-compensation, basic properties of reactive melts, and a diagnostic study of plasma used in formation of thin films. Chemical thermodynamics and kinetic studies of gas phase reactions, compound formation at interfaces, thin-film nucleation and electromigration, and thermodynamic studies of semiconductors are important for further solar cell improvements.

Table 4-3. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: SOLID STATE PHYSICS

Research	Priority
1. Solid state energy conversion processes; thermal and optical properties of semiconductors; thermodynamic studies of semiconductors.	<u>Crucial</u>
2. Theoretical approach to identify new materials for energy conversion.	<u>Crucial</u>
3. Experimental research on new semiconductor materials.	<u>Crucial</u>
4. Theory of hetero- and homojunctions.	<u>Important</u>

In support of ET program in PV

1. Self compensation studies; diagnostic study of plasma in formation of thin films; basic properties of high-temperature reactive melts.	<u>Crucial</u>
2. Chemical thermodynamics and kinetic studies of gas phase reactions; compound formation at interfaces; nucleation and growth of thin films; electromigration.	<u>Important</u>
3. Electron affinity measurements, doping, and solubility in III-V compounds.	<u>Needed</u>

In support of Photoelectrochemical Energy Conversion Research

1. Research involving electrochemical photovoltaic cells (ECPVC), including studies of:	
A. semiconductor materials, with high conversion efficiency and long-term stability;	<u>Crucial</u>

Table 4-3. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: SOLID STATE PHYSICS (concluded)

Research	Priority
B. polycrystalline/single-crystal electrodes.	<u>Crucial</u>
2. New semiconductor electrodes and structures for photo-electrosynthetic cells.	<u>Crucial</u>

SECTION 5.0

ENGINEERING AND MATHEMATICS

5.1 ENGINEERING

There is a vital need to conduct engineering research in support of DOE programs in solar energy. It is important to solve hydrodynamic problems related to salty solar ponds. Research in heat and fluid mechanics is important in order to support solar collector development. Several research problems are important to solar cooling, such as endothermic cooling methods and dessicant cooling. Despite common belief, several basic problems, such as multizone convection, need to be solved in support of passive solar technology.

Table 5-1. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: ENGINEERING

Research	Priority
1. Hydrodynamic problems in solar ponds.	<u>Important</u>
2. Heat transfer and fluid dynamics problems in collectors.	<u>Important</u>
3. Solar cooling—endothermic and desiccant cooling, chemical heat pumps.	<u>Important</u>
4. Multizone convection, soil heat conduction in support of passive solar technology.	<u>Needed</u>

5.2 MATHEMATICS

As the basic research needs of the solar community are better defined, it is expected that mathematical and numerical modeling will play an increasingly important role in accelerating the development of these technologies. Although the mathematical and computer science research communities are actively participating in the development of other energy technologies, they have not been made aware of the analytical and computational needs of the solar research community. For this reason, a DOE-sponsored workshop to better define the problem areas is considered important. It is also important to support additional research in the area of finite difference and finite element techniques for partial differential equations and other closely related areas, such as the numerical solution of large systems of linear and nonlinear equations. Additional research is needed in the areas of numerical solution of ordinary differential equations and integral equations, stability analysis, asymptotic analysis and perturbation methods for partial differential equations, nonlinear and stochastic optimization techniques, optimal control techniques, statistical and time series descriptions of solar insolation data, and the development of efficient simulation methods.

Table 5-2. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: MATHEMATICS

Research	Priority
1. Workshop on mathematical and computational needs.	<u>Important</u>
2. Numerical solution of partial differential equations and related areas.	<u>Important</u>
3. Numerical solution of ordinary differential equations and integral equations.	<u>Needed</u>
4. General applied mathematical techniques such as stability analysis, asymptotic analysis, and perturbation methods.	<u>Needed</u>
5. Nonlinear and stochastic optimization techniques, optimal control problems.	<u>Needed</u>
6. Statistical and time series descriptions of solar insolation and wind data.	<u>Needed</u>
7. Efficient simulation methods.	<u>Needed</u>

SECTION 6.0

ADVANCED ENERGY RESEARCH PROJECTS

AERP is currently supporting high-risk innovative concepts and is playing a very important role in the DOE program. However, the magnitude of effort is much too small to meet the needs of solar energy, which is in dire need of new concepts. It is therefore crucial to enlarge the activity of supporting innovative research in solar energy. Presently, there is a gap between basic energy research as supported by BES and technological development as supported by ET. It is crucial that the area of applied science, particularly applied physics, be covered by AERP. There also is a gap in energy conversion processes, because there is no branch in ER which provides the opportunity for sustained development of new concepts in these areas. Examples are thermoelectrics, ferroelectrics, thermionics, etc. It is crucial to develop the area of energy conversion sciences, particularly the ones dealing with high temperatures, as they may hold the key for making solar technology viable by the turn of the century. It is suggested that activity in these two areas—applied science and energy conversion—be brought into focus, perhaps by creating branches for each within the AERP division.

Table 6-1. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: ADVANCED ENERGY RESEARCH PROJECTS

Research	Priority
1. Support of high-risk research as in the past, but on a larger scale to meet solar needs.	<u>Crucial</u>
2. Support of applied science research, perhaps as a branch (particularly applied physics).	<u>Crucial</u>
3. Support of energy conversion research, perhaps as a branch.	<u>Crucial</u>

Figure 6-1. Peak Cycle Temperature Achievable by Concentrating Solar Flux

Figure 6-2. Maximum Theoretical Conversion Efficiency as a Function of Achievable Collector Temperatures

SECTION 7.0

BEHAVIORAL AND SOCIAL SCIENCES

7.1 INTRODUCTION

An office of Science and Technology Policy working group recently concluded that "A notable weakness (in DOE research) is the tendency to view obstacles to adoption of new energy systems as purely technological. Important obstacles to the adoption of new energy systems or expansion of existing ones will increasingly be recognized to be to some degree political, sociological, economic, institutional, and environmental in character. Research which could assist in addressing these issues is virtually nonexistent within the DOE" (U.S. Executive Office of the President 1978, p. 9).

This finding sets the stage for the following description of generic areas of need for basic and applied Behavioral and Social Science research that would support solar energy development. These needs can be addressed through research undertaken in the traditional disciplines of the Behavioral and Social Sciences: sociology, political science, economics, and psychology; and in newer, applied, and multidisciplinary fields such as environmental studies and policy sciences.*

We have organized research needs by broad area of research rather than by discipline, because in most cases several disciplines have made efforts to address the same issue and because many social problems cannot be addressed through the perspective of a single discipline. For example, even in the case of "basic" research on consumer decision making, psychologists, sociologists, and economists have attempted to develop explanatory and predictive theory. We have not distinguished between basic and applied social science research because precise distinctions are both difficult to make and likely to be irrelevant for present purposes. Research needs are divided into six subject areas: Behavior of Individuals; Behavior of Organizations and Communities; Political, Social, and Economic Processes; Social and Economic Impacts; Policy Analysis; and Research Methods and Conceptual Bases for Research.

7.2 BEHAVIOR OF INDIVIDUALS

By the year 2000, a substantial portion—perhaps 25%—of solar energy will be generated by technologies purchased by individual consumers. If public agencies desire to accelerate the acceptance of these technologies, they need to understand what influences individual energy choices. In particular, it is crucial that analyses of the consumer decision process be conducted, including the effect of external factors on consumer decisions, product attributes, risk and uncertainty, and value and use of information. Research is needed that focuses on the effect of individual lifestyle or changing lifestyle on individual energy choice.

*Definitions of the social sciences can be found in Appendix A.

Table 7-2.^a SUMMARY OF RESEARCH NEEDS AND PRIORITIES: BEHAVIOR OF INDIVIDUALS

Research	Priority
1. Analysis of the consumer decision process, including the effect of external factors, on consumer decisions, product attributes, risk and uncertainty, and value and use of information.	<u>Crucial</u>
2. The effect of individual lifestyle or changing lifestyle on individual energy choice.	<u>Needed</u>

^aThere is no Table 7-1. The tables were numbered so that they would coincide with section numbers.

7.3 BEHAVIOR OF ORGANIZATIONS AND COMMUNITIES

The bulk of energy technology purchases are made by organizations: government units, industrial and commercial firms, utilities, etc. Despite their importance in determining the extent of solar energy use over the next decades, little is known about how and why organizations decide to adopt or reject new technological products, particularly new energy supply technologies. It is crucial that research be supported that analyzes the significance that external factors and organizational strategies and objectives have on energy supply choices. It is important to expand and improve economic decision models, particularly through continued development of generic models of utility company behavior, and to identify the influence that risk and uncertainty have on industry and utility decisions. Finally, research is needed that would analyze the impact of bureaucratic incentives, organizational structure, and objectives on decisions to adopt and use new energy technology. In addition, research is needed on the value and use of information in community and organizational decision making.

Table 7-3. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: BEHAVIOR OF ORGANIZATIONS AND COMMUNITIES

Research	Priority
1. Assessment of the significance of external factors on organizational and community energy supply decisions.	<u>Crucial</u>
2. Analysis of the influence that organizational strategies and objectives have on energy supply choices.	<u>Crucial</u>
3. Improvement and expansion of economic decision models, particularly through continued development of generic models of utility company behavior.	<u>Important</u>
4. Identification of the influence of risk and uncertainty on industry and utility decisions.	<u>Important</u>

Table 7-3. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: BEHAVIOR OF ORGANIZATIONS AND COMMUNITIES (concluded)

Research	Priority
5. Analysis of the impact of bureaucratic incentives, organizational structure, and objectives on decisions to adopt new energy technology.	<u>Needed</u>
6. The value and use of information in community and organizational decision making.	<u>Needed</u>

7.4 POLITICAL, SOCIAL, AND ECONOMIC PROCESSES

This category of research focuses on a very broad range of socioeconomic and political processes such as the diffusion of new technologies, shifts from centralized to decentralized energy economies, and energy supply economics. It is crucial that better understanding of the factors that influence the rate and pattern of diffusion of new technologies (market penetration) be achieved, that the implications of a major shift toward a decentralized energy economy for the social system and for social values be identified, and that the impact of introducing renewable energy technologies on conventional supply economics be understood. Analysis of the energy policy-making process itself is important, including identification of who makes energy policy decisions, the timing of such decisions, and the information needs of decision makers. It is also important that improved measures of social costs and benefits be developed and used in energy policy making. Finally, analysis of the roles of various levels of government (federal, state, local) for development and implementation of energy policy is needed.

Table 7-4. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: POLITICAL, SOCIAL, AND ECONOMIC PROCESSES

Research	Priority
1. Investigation of the factors that influence the rate and pattern of diffusion of new technologies (i.e., market penetration).	<u>Crucial</u>
2. Analysis of the implications of a major shift towards a decentralized energy economy for the social system and for social values.	<u>Crucial</u>
3. Impact of conventional energy supply economics on the introduction of renewable energy technologies.	<u>Crucial</u>
4. Measurement and use of social cost and benefit information in energy policy making.	<u>Important</u>

Table 7-4. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: POLITICAL, SOCIAL, AND ECONOMIC PROCESSES (concluded)

Research	Priority
5. Analysis of the energy policy-making process, with emphasis on who makes energy policy decisions, the timing of such decisions, and the information needs of the decision makers.	<u>Important</u>
6. Analysis of the roles of various levels of government (federal, state, and local) for development and implementation of energy policy.	<u>Needed</u>

7.5 SOCIAL AND ECONOMIC IMPACTS

Research in this area would improve public policy outcomes by increasing the accuracy of assessments of raw material demands, environmental impacts, level and skill mix of labor requirements, and other social and economic impacts of particular energy technologies. Crucially needed research would assess, on a disaggregated basis (e.g., regionally), the social and economic impacts of developing alternative energy sources. Important research would assess the environmental impacts of solar energy versus conventional energy sources, while needed research would identify existing end-use requirements for energy and potential applications for solar technologies.

Table 7-5. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: SOCIAL AND ECONOMIC IMPACTS

Research	Priority
1. Assessment of the social and economic regional impacts of developing alternative energy sources.	<u>Crucial</u>
2. Assessment of the environmental impacts of solar energy versus conventional energy sources.	<u>Important</u>
3. Identification of existing end-use requirements for energy and potential applications for solar technologies.	<u>Needed</u>

7.6 POLICY ANALYSIS

This area of research focuses on assessment of alternative federal, state, and local government actions intended to influence the development and application of solar technologies. Research topics should expand our knowledge of the consequences of different courses of government action and develop improved analytical methods for assessing their costs and benefits. It is crucial that assessments of the effectiveness of different mixes of policy instruments and practices such as taxation, regulation, procurement, demonstration, R&D, and information dissemination be conducted. It is also crucial that the effects of public utility commission regulatory practices on solar technology

utilization be assessed. Research is needed that would analyze the influence of policy implementation on the effectiveness of solar energy policies, and that would evaluate specific programs intended to influence the development and application of solar energy.

Table 7-6. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: POLICY ANALYSIS

Research	Priority
1. Analysis of the actual and potential government role in the development and application of new energy technologies.	<u>Crucial</u>
2. Assessment of the impact of public utility commission regulatory practices on solar technology utilization.	<u>Crucial</u>
3. Analysis of the influence of policy implementation, in contrast to policy design, on the effectiveness of solar energy policies.	<u>Needed</u>
4. Increased evaluation of specific programs intended to influence development and application of solar energy.	<u>Needed</u>

7.7 RESEARCH METHODS AND CONCEPTUAL BASES FOR RESEARCH

This category of research calls for the development of improved analytical and methodological tools to address the research needs outlined in earlier sections. A proportion of the BES research budget should be allocated to such studies as an investment in the quality and utility of future research products. It is important that efforts be undertaken to improve the theory and methods of existing energy-economy analyses and models, and to incorporate new energy technologies into these models. Research methods are needed that would improve the evaluation of energy development and application programs, social impact assessments, and the understanding of relationships between individual attitudes and opinions and subsequent behavior. There is also a need to increase the multidisciplinary character of existing socioeconomic databases and models.

Table 7-7. SUMMARY OF RESEARCH NEEDS AND PRIORITIES: RESEARCH METHODS AND CONCEPTUAL BASES FOR RESEARCH

Research	Priority
1. Improved analysis of energy-economy interactions and incorporation of new energy technologies.	<u>Important</u>
2. Development of improved research methods for evaluating energy development and application programs and for depicting more accurately relationships between individual opinions and attitudes and subsequent behavior.	<u>Needed</u>
3. Increased multidisciplinary character of existing socioeconomic databases and models.	<u>Needed</u>

SECTION 8.0

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APPENDIX A

DESCRIPTION OF SOCIAL SCIENCE DISCIPLINES

The following description of the five central social science disciplines is taken from Knowledge Into Action: Improving the Nation's Use of the Social Sciences (NSF 1969).

What Are the Social Sciences?

The social sciences are intellectual disciplines that study man as a social being by means of the scientific method. It is their focus on man as a member of society, and on the groups and societies that he forms, that distinguishes the social sciences from the physical and biological sciences.

Historically, five social sciences have been regarded as central: anthropology, economics, political science, psychology, and sociology. Other important fields that deal with social phenomena are: demography, history, human geography, linguistics, and social statistics.*

Anthropology and sociology are somewhat difficult to distinguish from each other. Both study the societies in which man lives; that is, the social forms and structures within which individual and group behavior takes place. Anthropology (which includes social anthropology, archaeology, physical anthropology, and the linguistics of preliterate cultures) studies the varied physical and cultural characteristics of man throughout the world. Traditionally, its attention has been directed to primitive cultures. But a number of anthropologists now study the cultures of industrialized societies including, of course, the United States; and anthropologists have produced fruitful work on such important contemporary problems as poverty, ghetto life, minority groups, and mental health.

Sociology is often called the science of society. In contrast to anthropology, sociology has always concentrated on the structure and functioning of groups within literate societies. Sociologists study such features of society as the family, rural and urban life, race relations, crime, and occupational groupings.**

Economics is the study of the allocation of scarce productive resources among competing uses. Within this framework, economists engage in theoretical and empirical research on both macroeconomic subjects (reaching and maintaining full employment, avoiding inflation and deflation, understanding and promoting economic

*Branches of psychology and anthropology often fall in the biological sciences as well as the social sciences. Similarly, parts of historical inquiry properly belong in the humanities. We refer the reader to the forthcoming report of the Behavioral and Social Survey Committee for an exposition of the nature of these disciplines, their development, and the kind of work that each does. We also leave to that report the tasks (1) of describing the hybrid fields that exist within the social sciences, and between the social sciences and the natural sciences; and (2) of distinguishing between behavioral sciences and social sciences.

**Social psychology is an important subfield that sociology shares with psychology. Social psychology studies the behavior of man as influenced by the groups to which he belongs.

growth, analyzing fiscal and monetary policies, defining balance and imbalance in international payments) and on microeconomic subjects (market pricing, monopolies, manpower, labor markets, union movements, farm issues, and problems resulting from inequalities in income distribution and poverty).

Psychology studies the nature and organization of mental processes in man. Psychologists deal with man's mental abilities and aptitudes: his capacities for learning, for thinking, for emotional expression, and for motivation. Psychologists have developed intelligence and aptitude tests for a great variety of uses. They work on problems of learning in education, personnel selection in industry, and clinical assessment in mental illness, among many others.

Political Science investigates the ways in which men govern themselves. It is concerned with the goals of the political system, the structural relationships in that system, the patterns of individual and group behavior which help explain how that system functions, and the policy outputs as well as behavioral consequences of that system. Political scientists study a variety of phenomena involved in the process of government, including political parties, interest groups, public opinion and communication, bureaucracy, international relations, and administration.

APPENDIX B

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16. Abstract (Limit: 200 words) This report identifies, describes, and recommends priorities for basic research important to the future development of solar energy. In response to a request from the U.S. Department of Energy, SERI surveyed more than 120 leading scientists who were engaged in or knowledgeable of solar-related research. SERI scientists relied heavily on the opinions of scientists polled, but weighted their own recommendations and opinions equally. The result is an amalgam of national scientific opinion representing the views of key researchers in relevant disciplines and of SERI staff members. The scientific disciplines included in the report are: chemistry, biology, materials sciences, engineering and mathematics, and the social and behavioral sciences. Each discipline is subdivided into two to five topical areas and, within each topical area, research needs are described and ranked according to the priorities suggested in the survey. Three categories of priority were established: "crucial," "important," and "needed." A narrative accompanying the description of research needs in each topical area discusses the importance of research in the area for solar energy development and presents the bases for the priority rankings recommended.			
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