EXECUTIVE SUMMARY

BACKGROUND

The Office of Program Analysis in the Office of Energy Research of DOE has the responsibility to assess long-term research needs associated with the development of new fossil-fuel technologies. For almost twenty years now, research has been conducted intensively in the U.S. to develop coal liquefaction technologies and processes for the production of transportation fuels. Periodically, this large body of accumulated knowledge and experience needs to be identified, assessed, and applied. In 1980 the Fossil Energy Research Working Group (FERWG) conducted an in-depth evaluation of coal liquefaction research needs and identified a wide range of important research areas and process development activities. FERWG's recommendations were documented in a comprehensive report issued in March 1980 (FERWG-II report).

Since 1980 U.S. research and development efforts in coal liquefaction have undergone major changes in terms of areas of development and project focus. Also since 1980 nine years of fundamental research and development efforts have resulted in an accumulation of new knowledge which needs to be assessed. New and improved coal liquefaction technologies and processes have proliferated, providing alternative approaches and new areas of research opportunities not anticipated in the 1980 FERWG-II report. Research activities have shifted from large, commercial-scale demonstration projects to smaller bench-scale and fundamental research projects.

CURRENT ASSESSMENT

The purpose of this current study was to perform an independent assessment of the research needed to bring coal liquefaction to technical and economic readiness for commercialization. A time frame of 5-20 years

for this research was considered in this assessment, which thus included needs in both the short term and the long term. Short-term research is needed to improve relatively well-developed processes in all technology areas; long-term research is needed both to develop fundamental understanding and to utilize new knowledge and emerging concepts as the basis for better processes. Research priorities were to be established based on each program's perceived importance to reach the objective of commercial readiness.

A twelve-member expert panel was assembled for this assessment to develop and prioritize R&D recommendations in coal liquefaction. The R&D recommendations summarized herein represent the conclusions of an intensive twelve-month effort by the panel involving four days of meetings plus seven site visits by panel members at different locations. Over forty experts made technical presentations of ongoing research and prepared inputs to this study. In addition, independent peer reviews were solicited from ten eminent researchers and research managers to provide proper perspective and comments.

Coal liquefaction to produce liquid transportation fuels now encompasses a number of distinct technologies and processing routes. Specific coal liquefaction technologies include (1) direct conversion of coal by hydrogenation to liquid fuels (direct liquefaction), (2) the conversion of synthesis gas to liquid fuels (indirect liquefaction), (3) pyrolysis and mild gasification to produce liquid fuels from coal, (4) biological conversion of coal to liquid (bioconversion), and (5) production of liquid fuels from combined coal and petroleum feedstocks (coprocessing).

A sixth, emerging technology -- direct conversion of light hydrocarbons -- was also discussed during this assessment, and the panel heard several presentations about this technology, which converts light hydrocarbons such as methane to gasoline directly without involving the production and the conversion of synthesis gas. However, the panel questioned whether this technology, regardless of its potential, is

appropriate for the coal liquefaction program. The research recommendations for this technology are included as a separate list in the project report without evaluation or ranking.

The major themes that have emerged from this study can be summarized as follows: steady and substantial improvements have been made in both the technical reliability and the economics of liquefaction, but current processes are still too costly. More efficient processes must be developed before liquefaction can produce transportation fuels that are cost-competitive with petroleum products. These processes will be based on fundamental understandings of coal structure and chemistry that are now emerging. The recommendations by the COLIRN panel reflect this emphasis on fundamental studies, many of which will apply to more than one liquefaction technology. At the same time, the panel recommended that development programs continue to improve the best of the current processes and build upon the technologies that have evolved as the result of several years of research and development.

STATUS OF LIQUEFACTION TECHNOLOGIES

The following reviews briefly outline the status of each of the five liquefaction technologies and the rationales for the selection of the highest-priority recommendations by the COLIRN panel.

Direct Liquefaction

DOE is funding the development of one process--Catalytic Two-Stage Liquefaction (CTSL)--which is being tested at the proof-of-concept (POC) scale at the Wilsonville PDU, with supporting programs in smaller bench-scale units. No other process is emerging so that improvement of the CTSL process will continue to be the primary development program in the future.

Laboratory tests continue to provide important information on coal structure and liquefaction chemistry. Considerable attention is being

directed toward "preconversion chemistry", attempting to find techniques to liquefy coal that will prevent retrograde reactions and thereby preserve the small-cluster structures of the original coal. If this approach is successful, the efficiency of liquefaction processes may be greatly improved.

Technical advances in recent years have resulted in dramatic increases in the yield and the quality of liquid products. These advances have resulted in a substantial reduction in product cost, which is still about $10-20/bbl above petroleum product prices.

The COLIRN panel recommended that the large-scale development program continue so that the U.S. will improve upon its best process and maintain a position of readiness for large-scale demonstration. This program includes catalyst development and kinetics studies of hydrogenation and cracking reactions at current reaction conditions.

The panel was, however, of the opinion that process improvements will not be of sufficient magnitude to make CTSL economically attractive and that research must lay the foundation of new processes. Thus, most of the high-priority recommendations emphasize research related to coal structure/reactivity, coal dissolution chemistry, pretreatment of coal to enhance reactivity, and the prevention of retrograde reactions. The panel also placed high priority on research to find new catalyst systems and on chemical solubilization techniques which may be the bases of new liquefaction processes.

As always, hydrogen is an important consideration in the economics of direct liquefaction technology. Although this area has been well researched over a number of years, the panel urged continued efforts to find more efficient methods to produce, use, or recover hydrogen in order to reduce process costs.

Indirect Liquefaction

Indirect liquefaction is the reaction of carbon monoxide and hydrogen (syngas) to produce hydrocarbons (Fischer-Tropsch reactions) or oxygenates, such as alcohols and ethers. The syngas is made via gasification of coal. In general, the overall thermal efficiency of the entire process is low, and the product cost is high due principally to the cost of gasification. The DOE indirect liquefaction program is not concerned with gasification or gas clean-up, so that research in this program is focused entirely on improving the syngas reactions.

Fischer-Tropsch reactions make a wide range of hydrocarbons, including methane and other light gases, which reduce liquid yields. Consequently, current research interest is to drive the reaction as far as possible to make middle distillate and wax, and then crack these to transportation fuels. This research was supported by the panel.

Oxygenate syntheses have received considerable attention recently due to the penetration of alcohols and ethers into the motor fuel pool. These research programs are at the laboratory scale. The only process development program is Liquid-Phase Methanol (LPMeOH), which combines several interesting features: the use of syngas with a low hydrogen-to-carbon monoxide ratio that is made from coal via gasification, and the use of a slurry reactor, which uses an inert oil as the reaction medium and heat sink. The LPMeOH process is considered to be applicable to a utility plant that uses an integrated coal gasification combined cycle. The methanol may also find application as a fuel ingredient.

Most of the panel's recommendations were directed to two areas--improved catalyst performance and improved selectivity to desired products. The panel's first recommendation was for the application of several advanced catalyst preparation techniques to produce improved syngas catalysts. Other recommended areas of catalyst research included studies of reaction mechanisms, deactivation, the role of poisons and promoters in product distribution, and reaction kinetics in methanol

synthesis. The panel believed that the most important oxygenates are ethanol and ethers and recommended development of more selective routes to these products. Finally, in recognition of the high concentration of sulfur compounds produced by coal gasification, and the need to shift the syngas to increase the hydrogen content, the panel recommended development of a sulfur-tolerant shift catalyst.

Pyrolysis

Pyrolysis has long been considered to be an inexpensive route to coal liquids. In contrast to direct liquefaction, it requires no hydrogen, catalyst, or high pressure. Results, however, have been disappointing. The tar yield is low and the quality poor, requiring expensive upgrading. The char is the major product, and due to its low volatility and high mineral-matter content, it has less value than the coal feedstock. Consequently, large-scale developments of pyrolysis processes ceased in the early 1980's. However, laboratory research continued, directed toward increasing tar yield. Recently, DOE has shown renewed interest in pyrolysis in its mild gasification program. The processes in mild gasification appear to be the same as those tested before, but additional effort is being expended to convert the tar and char into higher-valued products, such as jet fuel from tar and reactive gasifier fuel from char.

The panel was skeptical that pyrolysis will be able to compete with direct liquefaction. The current mild gasification program is expected to produce relatively minor increases in tar yield; the low-valued char will still be the major product. Consequently, the panel recommended that pyrolysis research adopt a new approach -- catalytic hydropyrolysis -- which has demonstrated high liquid yields and improved product quality. This pyrolysis technique has been tested only in small laboratory units, and considerable research is needed to judge its suitability as a commercial process. The panel was less enthusiastic about other recommendations, which were nevertheless considered to have

the best potential to improve the pyrolysis processes of current interest.

Coprocessing

Coprocessing is a variation of direct liquefaction, with the major difference being that the solvent comes from petroleum. Additionally, the solvent is expected to be used on a once-through basis, so that it is also a reactant and a precursor of liquid products. Coprocessing has been of interest for only a few years, but its development has been so rapid that an 11,700-barrel-per-day plant will be built in Ohio, having received a Clean Coal Technology award on the first round. This plant will be the first commercial application of direct liquefaction technology in the U.S.

Because of this rapid development and its unique features, coprocessing was considered separately from direct liquefaction. The distinguishing feature of coprocessing is the use of reduced petroleum crude oil, which has properties entirely different than those of a coal-derived solvent. The panel therefore recommended that research in coprocessing focus on understanding the fundamental chemistry of coal/oil reactions. Additionally, process studies should be carried out to elucidate the optimum reaction conditions and the effect of a petroleum solvent on coal reactivity and product properties.

Bioliquefaction

Bioliquefaction refers to the biological solubilization of coal or to the biologically catalyzed reaction of synthesis gas. This technology is so new that it is not yet possible to judge whether it will be a commercially viable alternative to the other liquefaction technologies. Certainly, it has appealing features such as low temperature and pressure requirements, and it does not need hydrogen. On the other hand, the possibility exists that the biocatalyst may be too expensive for

production of transportation fuels or that selectivities and reaction rates may fall short of commercial usefulness.

The panel recommended that the most important step in the study of bioliquefaction is to find enzyme systems that catalyze the specific reactions that break down the coal structure, remove heteroatoms or convert synthesis gas to alcohol.

HIGH-PRIORITY RECOMMENDATIONS

Because of the diversity of these liquefaction technologies, the expert panel decided to evaluate R&D recommendations for each of the five technology categories separately to prevent domination by any single technology and possible bias. (Some of the recommendations, notably those pertaining to coal structure and reactivity, cut across technology boundaries.) As a result, a comprehensive detailed list of R&D recommendations was generated for each technology, broken down further by general research needs (areas) and by specific research recommendations. The purpose of the general research needs is to define areas of an overall research program while specific recommendations embody specific programs to be carried out. A total of 178 research recommendations were developed. These recommendations were categorized into 57 general research needs (areas) under fundamental and applied research for the six technologies.

After reviewing the initial panel evaluations and the high-ranking general research need categories, the COLIRN panel made a final prioritization of detailed specific recommendations at the second two-day panel meeting. This prioritization was accomplished for each technology area by having each panel member choose a small number of recommendations and rank them in order. Points were awarded to the recommendation for each mention and each position (five for a first place, three for a second, and one for a third, for example). The recommendation garnering the most points was ranked first in that technology area, the next highest total ranked second, and so on.

This methodology yielded thirty-two (32) specific recommendations which were selected to have the highest priority in liquefaction research. These 32 recommendations are listed in Table ES-1 by technology area in order of priority. The table also shows the percentage of the total points (by technology area) won by each recommendation to show the degree of support for that recommendation by the panel. The panel members did not rank specific recommendations in bioliquefaction but rather endorsed the list of recommendations in this area with an indication of the relative importance of the general research needs.

Table ES-1. Summary of High-Priority R&D Recommendations in Coal Liquefaction

No.	Description	% of Total Score*
Direct Liquefaction		
D1.	Identify structures responsible for retrograde reactions, and determine the mechanism and kinetics of these reactions in order to develop processing strategies that can control them and increase liquid yield. In a broader context, an extensive study is needed of the dissolution and conversion of coal as it is preheated to reactor temperature.	15.8
D2.	Operate a large-scale pilot plant to test engineering and new process concepts, supply samples for other research and upgrading tests, and generate information needed for economic evaluations. The pilot plant must have sufficient flexibility to allow changes in process configuration, operating conditions and feedstocks.	12.0
D3.	Test chemical and low-temperature catalytic pretreatments to enhance coal reactivity, reduce retrograde reactions, or otherwise improve the overall process. These tests must be made in conjunction with the entire process to determine if the cost can be justified by the improvements achieved.	12.0
D4.	Investigate more efficient ways to produce, use, or recover hydrogen.	10.7
D5.	Develop a coal structure - reactivity relationship. Elucidate coal structure features important to liquefaction, e.g., aromatic ring number distribution, "cluster" size, cluster linking groups, population and identity of good hydrogen donors, physical structure, population of bonds capable of thermolysis and cleavage by chain processes, functional group analyses and distribution.	10.1
D6.	Investigate potential homogeneous catalysts for liquefaction. Such catalysts may effect hydrogen addition at significantly lower temperatures, leading to completely new processes.	7.2

*Based on 100% for each technology area

Table ES-1. (Continued)

No.	Description	% of Total Score*
Direct Liquefaction		
D7.	Develop kinetic models of liquefaction that include the processes of bond breaking, crosslinking, hydrogen donation, mass transport, and the effects of solvent.	5.9
D8.	Develop chemical techniques to solubilize coal, based on new information of coal chemistry. Major breakthroughs in processing are likely to require departure from high pressure hydrogenation. Many solubilization techniques have been developed, particularly for analytical purposes, but are uneconomical on a commercial scale. Efforts are needed to develop economically competitive processes based on such new solubilization chemistry.	5.9
D9.	Determine the role of mineral matter on initial reactions of coal. This is especially pertinent with recent emphasis on deep coal cleaning and "ashy" recycle solvent in current process developments.	5.1
D10.	Develop intrinsic quantitative rate expressions for conversion of individual components and ensembles of components as a basis for understanding initial reaction paths during coal dissolution.	5.0
D11.	Develop new catalysts for liquefaction. Current technology has used standard Co-Mo or Ni-Mo supported catalysts that seem to perform similarly and require substantial thermal severity to perform effectively. Unconventional or novel catalysts and supports have been considered in fundamental and model compound studies. The development of new catalyst systems should be related to new liquefaction processing.	5.0
D12.	Study the mechanism of catalytic hydrogenation and cracking functions to establish their interaction and to determine the effects of thermal reaction on these functions.	4.8

*Based on 100% for each technology area

Table ES-1. (Continued)

No.	Description	% of Total Score*
Indirect Liquefaction		
I1.	Apply new advances in materials science to catalyst preparation for Fischer-Tropsch and alcohol synthesis reactions. The preparation techniques may include production of novel supports, co-precipitation of catalyst precursors, novel ways of surface doping, chemical vapor deposition, and plasma doping. This work should also include new methods of catalyst characterization by chemical chemisorption, x-ray diffraction, electron microscopy and spectroscopies. These new techniques offer major opportunities for the scientific design of greatly improved catalysts -- catalysts which would not be achieved by trial-and-error methods.	22.0
I2.	Analyze structure, reactivity, function and role of supported organometallic complexes to elucidate the mechanisms of heterogeneous catalysis in F-T and alcohol syntheses.	21.5
I3.	For the conversion of syngas to alcohols, develop routes to maximize ethanol selectivity, minimizing hydrocarbon yield. Ethanol is already becoming an important motor fuel or additive.	14.8
I4.	Find new catalyzed paths to produce octane-enhancing ethers. Ether production may have to be increased substantially to increase gasoline octane while reducing auto emissions.	13.3
I5.	Investigate maximizing middle distillate yield from syngas, with low methane yield. Develop catalysts for high selectivity to long-chain hydrocarbons that can be cracked selectively to naphtha and distillate fuels.	7.1
I6.	Develop sulfur-tolerant, low-temperature water-gas shift catalysts. Gases made from coal have sulfur compounds that will be costly to remove to the <ppm concentration required by current catalysts.	6.6

*Based on 100% for each technology area

Table ES-1. (Continued)

No.	Description	% of Total Score*
Indirect Liquefaction (Continued)		
I7.	Study the reaction kinetics and develop alternative catalysts for methanol syntheses to improve process economics. New catalysts are needed that have good activity with syngas streams but do not require the expensive cleanup needed for current catalysts.	5.1
I8.	Determine the carbon form that leads to deactivation of F-T catalysts. Define the factors that are important in generating the active carbon from CO, and the catalyst properties which determine the reactivity of this carbon.	4.6
I9.	In F-T and related syntheses, use probe molecules to understand and modify product composition. Analyze role of poisons and promoters in determining product composition. Analyze the possibility of homogeneous reactions occurring in F-T.	4.6
Pyrolysis		
P1.	Study the chemistry and mechanism of catalytic hydropyrolysis. A catalytic hydropyrolysis process that produces >50 percent distillable liquids may be an economically viable alternative to direct liquefaction. Variables, including catalyst composition and form, temperature, pressure, and residence time must be investigated, and a detailed mechanistic understanding of the chemistry involved must be formulated. A number of coals must be tested to define the generality of this approach.	33.3
P2.	Characterize coal functional groups and their relationship to pyrolysis/hydropyrolysis reactivity under different temperatures, pressures and residence time conditions. Functional groups in this context include heteroatom forms and distribution, aromatic ring size distribution, molecular weight between crosslinks, and definition of bridging links in terms of structure and distribution.	13.9

*Based on 100% for each technology area

Table ES-1. (Continued)

No.	Description	% of Total Score*
Pyrolysis (Continued)		
P3.	Compare pyrolysis yields and products with and without reactive atmospheres (CO, CO_2, H_2O, H_2) to understand the roles of these gases in the devolatilization of coal, and seek to understand the chemistry and the mechanisms involved.	13.4
P4.	Conduct systems analysis of pyrolysis/hydropyrolysis coupled with gasification/combustion to determine the technical feasibility and economic incentive for char utilization as fuel for combustion or as a gasifier feed.	9.1
P5.	Study staged catalytic hydropyrolysis. The tar made in the first catalytic reaction stage is hydrotreated/ hydrocracked to reduce heteroatom content and produce an acceptable refinery feed.	8.6
P6.	Study chemistry and reaction networks in pyrolysis reactions to establish optimum operating conditions. Perform fundamental studies of the reactions of coal under actual pyrolysis conditions in order to establish pathways for production of methane, ethane, other key hydrocarbons, CO_x, hydrogen cyanide, and sulfur compounds.	8.1
P7.	Define the chemistry and mechanism of steam-enhanced pyrolysis, under both subcritical and supercritical conditions for steam. Steam-enhanced pyrolysis may lead to increased liquid yields.	6.9
P8.	Study the effects of moisture in coal on pyrolysis and the physicochemical changes that occur during drying or rewetting of coal.	6.4
Coprocessing		
C1.	Study the fundamental chemistry of coal/oil reactions under both catalytic and thermal conditions. Elucidate the role of the residuum. In addition, an innovative approach needs to be undertaken to explore new chemical entities to achieve hydrogen donation.	51.6

*Based on 100% for each technology area

Table ES-1 (Continued)

No.	Description	% of Total Score*
Coprocessing (Continued)		
C2.	Conduct process studies in coprocessing, including the effects of different feeds on reactivities and product quality. The substitution of a petroleum residuum in place of a coal-derived solvent may result in optimum reaction conditions, catalysts, and coal reactivities that are different than for direct liquefaction, and these conditions must be determined.	17.2
Bioliquefaction		
B1.	Look for new enzyme systems that will produce new biocatalysts for specific reactions to facilitate the breakdown of the coal structure, removal of heteroatoms, or conversion of syngas to alcohols.	76.9

*Based on 100% for each technology area

CHAPTER 1

INTRODUCTION

1.1 BACKGROUND

The fossil fuel technologies being researched and developed for converting U.S. fossil resources into liquid transportation fuels have been, and are, facing tough economic competition from foreign oil. For nearly twenty years, research has been conducted intensively in the U.S. to develop coal liquefaction technologies to reduce the long-term dependency on imported oil. This large body of accumulated knowledge and experience needs to be assessed to determine the technology status and the readiness of coal liquefaction technologies.

The Office of Program Analysis in the Office of Energy Research of the U.S. DOE (DOE/OER/OPA) has the responsibility to assess long-term research needs associated with the development of new fossil-fuel technologies. In 1980 this office assembled a Fossil Energy Research Working Group (FERWG) to conduct an in-depth assessment of coal liquefaction research needs aimed at commercializing technologies to produce synthetic coal liquids. At that time, the U.S. was in the midst of an energy crisis, described by President Carter as the "moral equivalent of war". Imported oil prices had escalated from $2.50 per barrel in 1972 to $34/bbl, and spot prices had reached $40/bbl. This sudden rise in energy costs, its destabilizing effect on the economy, and the apparent vulnerability of the economy to foreign pressures galvanized an ambitious program by the Federal government and private industry to commercialize technologies to produce synthetic transportation fuels. As the result, the FERWG-II report (1) identified a wide range of important research areas and commercial process development activities (Appendix A summarizes FERWG's most important recommendations.).

However, since 1980 the energy crisis has abated temporarily, and imported oil prices have dropped drastically. Interest in synfuels has

waned. This lull in National interest has resulted in a significant reduction in Federal funds and an almost complete suspension of industrially funded research and development. Since 1980 the majority of Federally funded research activities has shifted from large, commercial-scale demonstration projects to smaller-scale and applied research areas. Also, the absence of commercialization activities has afforded the research community time and resources to address more fundamental research areas. Several years of fundamental efforts have resulted in an accumulation of new knowledge which needs to be assessed. New and improved coal liquefaction technologies have proliferated, providing alternative approaches and new areas of research opportunities not anticipated in the 1980 FERWG-II report.

After nearly a decade of the current oil glut, imports are increasing steadily and are expected to reach 50 percent of total consumption within 2-3 years. This timetable may be accelerated by the current low oil prices, which are forcing cutbacks in domestic exploration and production, and increased reliance on foreign oil. Growing dependency on foreign oil and its potential effect on the U.S. economy make it increasingly important to identify, explore, and implement coal liquefaction technologies to insulate the U.S. from long-term economic shocks from increases in imported oil prices.

In 1987 Science Applications International Corporation (SAIC) assembled a Coal Liquefaction Research Needs (COLIRN) Assessment Panel composed of multidisciplinary researchers from Government laboratories, industry, and universities and others with experience in identifying, developing, and evaluating coal liquefaction research activities. This assessment conducted by SAIC is the first carried out on coal liquefaction since the FERWG-II report issued in March 1980. This current assessment addresses new areas of coal liquefaction research and contains recommendations that will be critical to bring coal liquefaction to technical and economic readiness in the next 5-20 years.

1.2 ASSESSMENT OBJECTIVES

The overall purpose of this study was to perform an independent assessment of the research needed to bring coal liquefaction to technical and economic readiness for commercialization. A time frame of 5-20 years for this research was considered in this assessment, which thus included needs in both the short term and the long term. Short-term research is needed to improve relatively well-developed processes in all technology areas; long-term research is needed both to develop fundamental understanding and to utilize new knowledge and emerging concepts as the basis for better processes. Research priorities were to be established based on each program's perceived importance to reach the objective of commercial readiness.

To meet these overall goals, the assessment had a number of specific objectives as follows:

- Identify and describe the most technically and economically promising coal liquefaction approaches.
- Identify and describe those process areas and operations which have potential for effecting significant and meaningful process cost reductions.
- Identify and describe present major problems and concerns with current coal liquefaction processes, and the research needed to address these concerns.
- Establish a priority for the research needs identified during the assessment.
- Estimate the degree of risk for the research needs identified during the assessment.

In meeting these objectives this assessment of long-term coal liquefaction research needs addressed the critical issues and alternative approaches to coal liquefaction by emphasizing the following aspects:

- The understanding of new fundamental and applied research that has emerged in recent years
- The emergence of potentially technically and economically promising approaches
- Process areas and operations with potential for significant cost reduction
- Identification of the scientific and technical base necessary to produce technology improvements
- Identification of major problems with and unknowns of coal liquefaction processes
- The technical and economic reasons for changing certain research directions
- The need to develop innovative approaches to coal liquefaction.

The assessment methodology was designed to emphasize the development of recommendations based upon new fundamental knowledge and innovative approaches. The COLIRN panel then prioritized these recommendations on the basis of perceived risks and benefits.

1.3 DEFINITION OF COAL LIQUEFACTION TECHNOLOGIES

Coal liquefaction technologies have undergone significant changes and technical improvements in recent years. In the past there were three different routes to produce liquids from coal: (1) direct conversion of coal to liquid fuels (direct liquefaction), (2) the conversion of synthesis gas from coal to liquid fuels (indirect liquefaction), and (3) thermal treatment of coal (pyrolysis and so-called mild gasification). Recent developments have expanded this list to five, with the addition of (4) production of liquid fuels from combined coal and petroleum feedstocks (coprocessing) and (5) biological conversion of coal or synthesis gas to liquids (bioconversion).

Additionally, indirect liquefaction has taken two routes -- the traditional Fischer-Tropsch method to make a wide range of hydrocarbons, and emerging oxygenate processes to make alcohols and ethers. This interest in oxygenates has been spurred by their growing use as octane enhancers in gasoline and as clean burning fuels to reduce air pollution.

Another liquefaction technology -- the direct conversion of light hydrocarbons to liquid fuels without involving the production and conversion of synthesis gas -- is also emerging, although there may be some question about whether this should be classified as a coal liquefaction technology.

Another recent development in coal liquefaction technologies has been the sharpened focus on the desired product mix, which was brought about by the realities of liquefaction economics. Liquefaction is too expensive to be used as a source of solid or liquid boiler fuels or of coke. The current liquefaction technologies, therefore, produce exclusively transportation fuels, either directly or after refining of the coal liquids. The one major exception is pyrolysis, from which the principal product is char.

1.4 REPORT ORGANIZATION

This chapter presents an introduction to this coal liquefaction R&D needs assessment including (1) the background to the study, (2) the assessment objectives, (3) a description of coal liquefaction technologies, and (4) a description of this report.

Chapter 2 contains a brief description of the methodology used for the assessment. Additional information about assessment methodology is included in the Appendix, including the members of the expert panel (Appendix C), panel meeting reports (Appendix D), and database development and recommendation prioritization (Appendix E).

Chapter 3 discusses the conclusions and recommendations reached as the result of this assessment. Included in this discussion is a description of the status and the important features of each coal liquefaction technology. The research recommendations found to have high priority by the expert panel are described in detail, including their background and supporting rationale. Other conclusions and recommendations developed by the panel regarding future directions for coal liquefaction R&D are also found in this chapter.

Brief reviews of the different coal liquefaction technologies then follow in Chapters 4 to 8. These reviews are not meant to be encyclopedic; several outstanding reviews of liquefaction have appeared in recent years and the reader is referred to these, wherever applicable. Instead, these chapters contain reviews of selected topics that serve to support the panel's recommendations or to illustrate recent accomplishments, work in progress, or areas of major research interest. Each of these review chapters contains a summary section which summarizes the most important research recommendations brought out in the panel discussions and supported by the material presented in the review.

REFERENCE FOR CHAPTER 1

1. Fossil Energy Research Working Group (S.S. Penner, Chairman), "Assessment of Long-Term Research Needs for Coal Liquefaction Technologies," Report for DOE Contract No. DE-AC01-79ER10007, March 1980.

CHAPTER 2

ASSESSMENT METHODOLOGY

2.1 TECHNICAL APPROACH

SAIC used the following overall technical approach for conducting this independent assessment of long-term coal liquefaction research needs:

- Selection of an SAIC principal investigator who is technically competent, familiar with coal liquefaction R&D issues, and experienced in organizing a project team to conduct various assessment activities.
- Selection of members for an expert panel whose collective expertise covers all facets of the significant coal liquefaction R&D areas.
- Identification of the most technically and economically promising coal liquefaction approaches and research activities through inputs obtained from the expert panel members.
- Conduct of site visits by the expert panel members to important coal liquefaction research facilities to verify and update information regarding current and future proposed activities.
- Meetings of the expert panel to assess priorities and risks for research needs.
- Documentation of the final findings, including prioritization of R&D needs and development of technical rationale to support the findings.
- Peer review of draft findings, and incorporation of these comments and minority opinion in the final report.

This approach is depicted in Figure 2-1.

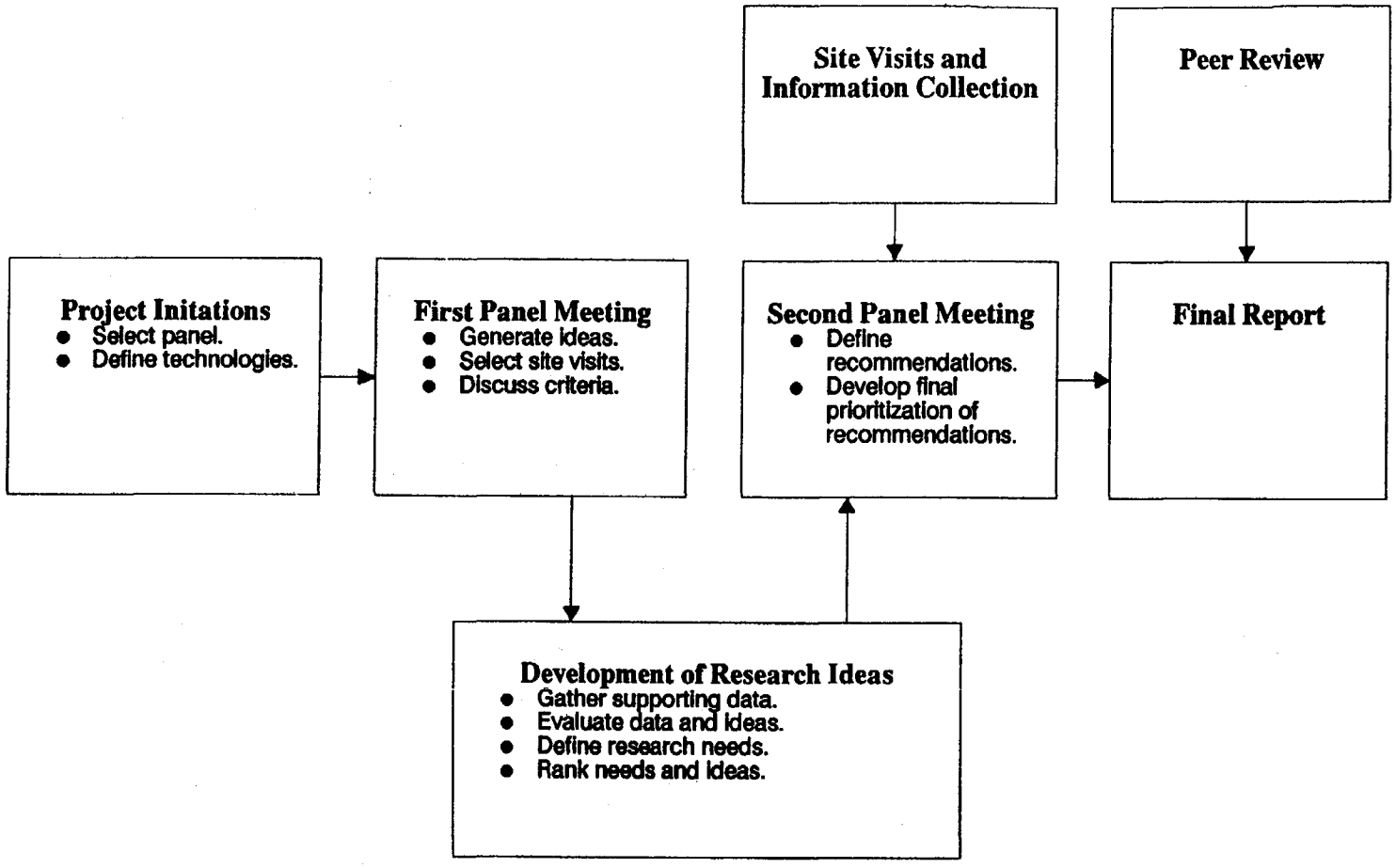

Figure 2-1. Overall Technical Approach for Conducting R&D Needs Assessment in Coal Liquefaction.

2.2 SELECTION AND ROLE OF THE COLIRN PANEL

2.2.1 Selection

In keeping with the changed environment for DOE-sponsored R&D in coal liquefaction, SAIC selected a panel made up of experts who are knowledgeable about the recently developed basic information and oriented towards the basic and applied research in coal liquefaction. However, the panel members' experience spanned the scientific, technical, economic, environmental, and application areas of coal liquefaction. The panel members are all currently active in coal liquefaction R&D and have demonstrated up-to-date technical competency and expertise directly related to coal liquefaction. The COLIRN panel consisted of 12 members, including the SAIC principal investigator. The panel members were:

- Dr. Harvey Schindler, Principal Investigator and Panel Chairman, SAIC
- Dr. Francis Burke, Consolidation Coal Company
- Professor Kwang Chao, Purdue University
- Dr. Burtron Davis, Kentucky Energy Cabinet Laboratory
- Dr. Martin Gorbaty, Exxon Research and Engineering Company
- Professor Kamil Klier, Lehigh University
- Dr. Carl Kruse, Illinois State Geological Survey
- Professor John Larsen, Lehigh University
- Dr. Robert Lumpkin, Amoco Corporation
- Dr. Michael McIlwain, Idaho National Engineering Laboratory
- Mr. Norman Stewart, Electric Power Research Institute (EPRI)
- Professor Irving Wender, University of Pittsburgh.

The technical qualifications and the experience of the panel members are summarized in Appendix C. The technical strengths and the diversity

of experience represented by this team included fundamental coal structure and science, applied technology research, process development, and product application in all coal liquefaction technologies. The diversity of experience of the panel members also provided a spectrum of viewpoints to the assessment.

2.2.2 Role

In this assessment of coal liquefaction R&D needs, the COLIRN expert panel played the central role and, representing the coal liquefaction community as a whole, provided a technically competent review. As expert researchers with extensive hands-on experience in coal liquefaction, panel members were responsible for providing up-to-date information on the status of liquefaction research, identifying R&D goals, and defining the activities required to reach the goals. The panel was also responsible for assessing all of this information and developing a set of recommendations and research priorities. In summary, the role of the COLIRN panel was to provide a balanced and objective analysis of research needs and opportunities in coal liquefaction.

Specifically, the expert panel reviewed available information, directed SAIC's efforts to fill information gaps, assessed R&D risks, recommended R&D initiatives, evaluated the recommendations, and set R&D priorities. The expert panel developed recommendations in two meetings. The first meeting was preliminary, but focused the panel on information gaps, necessary analyses, and information gathering activities needed to prepare a final comprehensive set of R&D priorities and recommendations. After conducting selected site visits and other information collection and analysis activities, the panel reconvened at a second meeting to arrive at a final set of recommendations.

2.3 SITE VISITS AND OTHER EXPERT INPUTS

This assessment included a number of activities aimed at collecting current information on coal liquefaction R&D. Both the expert panel and the SAIC support team conducted activities in this task. The panel contacted researchers, visited research sites, and gathered data. The principal investigator notified panelists of the dates of each site visit, established the format and the agenda for each visit, and disseminated gathered information to all panel members. The principal investigator also informed DOE/OER/OPA of the sites to be visited and the schedule.

The approach for each site visit included:

- Contacting the site to schedule the visit.
- Conducting the visit to gather the information.
- Preparing a trip report and circulating it to the panel, site representatives visited, and DOE/OER/OPA.

For each site visit SAIC invited nearby organizations working in coal liquefaction to attend and make presentations about their work. During each site visit the SAIC team collected information from presenters and recorded the meeting proceedings for the site visit report. R&D recommendations developed as a result of the visit were incorporated into the project database. These site visit reports were then distributed to all the panel members to keep them updated on project progress.

The following site visits were made by the expert panel during the course of this assessment.

Site	Date
Pittsburgh Energy Technology Center	January 7, 1988
Wilsonville PDU, Wilsonville, AL	March 9, 1988
SAIC, Paramus, NJ	March 14, 1988

AMOCO, Naperville, IL	March 22, 1988
ARCO Chemical, Newtown Square, PA	April 12, 1988
Morgantown Energy Technology Center	April 27, 1988
EPRI, Palo Alto, CA	May 17, 1988

2.4 COLIRN PANEL MEETINGS

An important element of the methodology used in conducting this assessment of coal liquefaction R&D needs was holding two formal meetings of the whole COLIRN expert panel. The initial two-day panel meeting at the beginning of the project was held to conduct a preliminary evaluation of R&D needs and to define the information needed for the assessment. The second full panel meeting was held to finalize the recommendations of the study. The panel meetings were organized and chaired by the principal investigator and structured to give the experts the primary role in making R&D recommendations and guiding study efforts.

2.4.1 First Panel Meeting

Prior to the first panel meeting, each panel member was sent a set of briefing materials for the meeting. The purpose of these briefing materials was to bring the panel members up to speed on the study objectives, background for the assessment, procedures, and methodology, as well as to stimulate their thinking about the project. In this way the panel members were fully briefed prior to the first panel meeting so that they were ready to begin their discussions of coal liquefaction R&D, and the time during the panel meeting was utilized in an optimum way.

Specific activities during the meeting included:

- Holding a session of the full panel to review and revise criteria for selecting R&D directions, agree on ground rules, identify technology cost and performance goals, and refine SAIC's outline of the study final report.
- Breaking up into three subpanels organized by technology area--direct liquefaction, pyrolysis, and indirect liquefaction--to conduct a preliminary evaluation of R&D needs in each area.
- Reconvening the full panel to review subpanel findings and agree on the next steps, including site visits, other information-gathering efforts, and panel member assignments.

The first panel session produced preliminary R&D recommendations and identified information gaps and requirements. The conclusions of the panel meeting were summarized in a report. One part of the report focused on the activities of the meeting itself and reported on the procedures and the conduct of the meeting. The major part of the report was concerned with the preliminary R&D recommendations and other information developed during the meeting. Also included in this report were the presentations and other material from the panelists. A summary of this report on the first panel meeting is included in Appendix D to document the methodology of the assessment.

2.4.2 Second Panel Meeting

A second two-day session of the panel was held to finalize R&D recommendations and priorities.

Prior to this meeting, each panel member received briefing materials, which included a copy of the complete database of research recommendations, the accumulated information on supporting rationales for the recommendations, and the scoring data on the recommendations.

Briefly, the meeting consisted of:

- A session to review evaluation criteria and suggest issues to consider in presenting the final results of the study.
- Sessions organized by technology area -- direct liquefaction, coprocessing, bioliquefaction, pyrolysis, indirect liquefaction, and direct conversion of methane -- to review technology status, discuss the research recommendations, and do ranking and prioritization.
- A final session to review the findings and discuss the remainder of the project activities and schedule.

A meeting report similar to the report on the first meeting was prepared. The report focused on the activities of the meeting and

reported on the discussion which took place. Comments and opinions were also included in this report on a number of issues. The final recommendations and the results of the evaluation and prioritization are discussed in Chapter 3. A summary of the report of the second panel meeting is included in Appendix D.

The complete database of research recommendations developed and discussed during this assessment is included in Appendix E.