APPENDIX A

SUMMARY OF RECOMMENDATIONS FROM THE FERWG-II REPORT[1]

A.1 INTRODUCTION

The starting point for the present assessment of coal liquefaction research needs was the report on Assessment of Long-Term Research Needs for Coal-Liquefaction Technologies prepared by the Fossil Energy Research Working Group in March 1980 (the FERWG-II report). This report contains a number of general and specific recommendations which were developed as a result of evaluating the status of the technologies being developed at that time.

As background for evaluating the results of the present assessment, it may be useful to refer to these FERWG-II recommendations, and many reviewers of the present report will want to do this. By comparing the present recommendations with the results of the FERWG-II study, it should be possible to obtain an understanding of how coal liquefaction technologies and their needs are evolving.

A.2 EXECUTIVE SUMMARY OF FERWG-II

Reproduced in this section is the Executive Summary of the FERWG-II Report. This summary contains what FERWG believed to be their most important recommendations, although no ranking or prioritization methodology was apparently used to arrive at this list. All references are, of course, to parts of the FERWG report.

---

[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.

(From the FERWG-II Report (1))

EXECUTIVE SUMMARY

Funding for basic, applied and exploratory studies on coal-liquefaction systems by the Department of Energy (DOE) is not adequate to support the development of technologies for the efficient production of liquids from coals, using direct or indirect coal-liquefaction processes or pyrolysis. There are three principal problem areas that require long-term and stable research support, viz., problems arising in pilot, demonstration, and commercial plants require solutions; developing coal-liquefaction systems require interactive supporting research; innovative and novel research ideas, including new liquefaction concepts, need to be supported. Improved provisions must be made for integrating R&D support within pilot and demonstration plant programs. Contractors should exercise program flexibility to adjust supporting process research in the light of new findings or unexpected occurrence of unforeseen problems. Coal-liquefaction processes require an integrated systems approach in which all aspects of the technologies (coal preparation, hydrogenation, hydrogen production, bottoms processing, liquid refining, etc.) are properly considered and optimized.

We identify below important R&D areas, each of which we believe requires substantial additional funding (i.e., more than $\$10^6$/year) and the first three of which we regard as especially urgent:

1. Research is needed on each of the following topics: the basic physics and chemistry, structure, composition, and thermochemistry of coals and of model compounds; volatilization; kinetics and mechanisms of bond scission; subsequent free radical and ionic reactions, including reaction steps involving unstable intermediates; transport properties and fluid mechanics of multiphase flows (see Section 2.1).

2. Major opportunities exist for improving direct and indirect coal liquefaction through research in homogeneous and heterogeneous catalysis, using either recoverable or disposable catalysts. Fundamental research should concentrate on mechanisms, kinetics and surface chemistry (see Sections 2.1 and 2.2).

3. Bottoms processing is likely to limit commercialization of direct coal liquefaction processes (see Sections 2.6 and 2.7). An integrated program of R&D is needed, using bench-scale tests and pilot plants processing up to 100 tons of coal per day. These tests should be used to study gasification, combustion, and coking of residues (see Sections 2.4 and 2.5).

4. Scale-up and optimization of coal-liquefaction processes require improved understanding of processing steps, including two- and three-phase flows with heat and mass transfer and chemical reactions (see Section 2.7).

5. A review of environmental and health effects has not been performed by FERWG. We are aware of work in this field. We recognize the need for careful studies on methods of analysis and toxicology in order to assure the definition of adequate environmental and health standards. The emphasis should be on determining health effects of the finished products (see Sections 2.1, 2.8, and 2.9) in parallel with development.

6. Improved instruments must be developed for the measurement and control of all phases of the coal-liquefaction technologies, including the characterization and control of effluents (see Section 2.6).

7. An augmented and integrated effort must be made to solve, control, or avoid the many physical and chemical materials problems that have been encountered in the development of a variety of coal-liquefaction technologies (see Appendix C).

8. Additional research is needed on the characterization of a wide range of individual coals for different coal-liquefaction processes and for optimizing the designs of coal-liquefaction processes for particular coals (see Section 2.1 and Appendix C). These studies will require the creation of a carefully selected coal-sample bank.

9. Research on rapid pyrolysis of coal (at low and high pressures) and on coke utilization may lead to attractive alternative routes to coal liquids (see Chapter 3). Fundamental research is needed on the escape of pyrolysis products from a coal particle and on their subsequent chemical reactions, both within the particle and in the vapor phase (see Section 2.1 and Chapter 3).

10. Basic research is needed on mechanisms to control regressive reactions that lead to high viscosity of vacuum bottoms and to formation of sticky reactor residues. These studies are needed to assure system operability, good product recovery, and long catalyst life (see Section 2.3).

11. Fundamental and applied research should be pursued on separations of liquid streams and solids from the reaction products formed during coal liquefaction. These studies are needed in order to improve recycle systems to reduce processing costs. Vapor/liquid equilibria should be better defined, especially in regions near the critical points (see Sections 2.3, 2.4, and 2.5 as well as Appendix C).

12. Down-stream refining facilities should be leased or built for experimental refining of coal-derived oils to produce commercially usable liquids for engine development and also for use in turbines and boilers (see Section 2.9 and Appendix C).

A.3 DISPOSITION OF FERWG-II RECOMMENDATIONS

The Executive Summary of the FERWG-II Report (1) contains twelve high-priority recommendations, which, for the most part, are directed toward general areas of interest in liquefaction. Recommendation No. 9 is specific for pyrolysis, No. 3 is specific for direct liquefaction, and No. 2 for direct and indirect liquefaction. The recommendations are to do research in the following areas:

- Coal structure and coal chemistry
- Catalysis
- Bottoms processing
- Multi-phase flow
- Environmental concerns
- Coal characterization
- Retrograde reactions
- Product recovery
- Product refining

A number of other recommendations appear throughout the report. These are more process- or technology-specific, although only one other is for indirect liquefaction because the FERWG-II report emphasized pyrolysis and direct liquefaction.

In reviewing these recommendations, the reader must keep in mind that the largest liquefaction plant in operation at the time of FERWG-II was the 50 ton-per-day SRC-I and SRC-II pilot plant in Fort Lewis, Washington. A major concern was the need for larger-scale integrated operations to provide the information needed for reliable scale-up and design of commercial plants. This is seen in Recommendations 3, 4, 6, and 7.

Since that time, two 100-200 tons-per-day direct liquefaction pilot plants have been operated, a 200 ton-per-day plant was operated in Bottrup, Germany, and a 150 ton-per-day bituminous coal pilot plant is being designed and will be built in Japan. Many of the larger-scale tests have, therefore, been performed. Of greater significance is that the Great Plains Gasification Plant in Beulah, North Dakota, produces 137

million cubic feet per day of synthetic natural gas from 14,000 tons of lignite. Although the final product is natural gas, most of the operations are identical to those of an indirect liquefaction plant. In the planning stage is a coprocessing plant that will produce 11,700 barrels per day of distillable liquids from 800 tons per day of Ohio bituminous coal and 8000 barrels per day of Cold Lake reduced crude. Despite the relatively small coal feed rate, the large petroleum feed will require that this plant contain one train of a commercial-sized plant.

Although each process and each plant design will have its particular scale-up problems, these two commercial plants will resolve many of the scale-up and design uncertainties addressed by these FERWG-II recommendations.

Recommendation No. 5 is for the study of the toxicity of finished products. This work was performed by Battelle Pacific Northwest Laboratory, which concluded that coal liquids with a boiling point below 650°F and with a H/C atomic ratio of at least 1.5 has a toxicity no greater than petroleum liquids (Section 4.3.5). Thus, product toxicity is no longer a major research concern.

Recommendation No. 12 is for downstream refining of coal liquids. The tests by Chevron that concluded in 1985 (Section 4.3.3) showed that coal liquids can be refined by conventional refinery processes and catalysts. Thus, this is another liquefaction concern that has been resolved.

Some of the FERWG-II recommendations are still applicable today. Recommendation No. 1 on coal structure and chemistry is reiterated in direct liquefaction recommendations 1.1.2, 1.1.4, 1.3.4, and 1.3.5 (see Table F-2 in Appendix F). Sections 4.2.1 and 4.2.2 show that we know more about coal structure and chemistry. However, more research is needed to develop the desired coal structure-reactivity relationship that will lead to more efficient liquefaction processing.

Catalysis (FERWG Recommendation No. 2) continues to be an area of research interest for both direct liquefaction (1.8.1 and 1.8.2) and indirect liquefaction (1.1.2, 1.1.1, 1.4.1, 1.5.1, 1.2.1), although the process improvements that can be attributed to catalyst development have been modest.

Recommendation No. 3 was to test liquefaction bottoms as a feed to gasification, combustion, and coking. This has been done, most extensively by Exxon's fluid coking tests. These operations are not considered to be problems for commercialization, although performance depends on the bottoms properties, which will vary with each process.

Finally, Recommendation No. 2 is for a study of the control of regressive reactions. This recommendation refers to the stability of liquid products in reactors, and during product recovery and distillation. The stability of these products has improved considerably as the result of more extensive catalytic hydrogenation in the liquefaction reactors (Section 4.3.2) and product stability during processing is no longer considered to be a major problem.