Commercial facilities will not be privately constructed until the economic incentive for these processes is great enough to justify the large capital expense required. The sheer magnitude of billion dollar investments also severely limits the number of companies capable of financing a venture. This possibly means that formation of multicompany groups sharing in costs and the resulting energy and feedstock products will be needed.

5.3.5 Environmental Factors

One of the major differences between natural gas/petroleum and coal/oil shale is that the former are considered clean feedstocks. Natural gas is low in sulfur content and does not produce particulates. Liquid petroleum fractions can be high in sulfur, but the ash content is low. However, coal and oil shale processes must contend with high sulfur content and with ash materials. These resources produce dust in the solids handling facilities and leave solids contained in the liquid products. Oil shale retorting and coal gasification processes require particulate removal from the product gas streams. Oil shale has a high nitrogen content which can complicate processing. All of the coal and oil shale processes require the disposal of either ash or spent shale.

Consequently, coal and oil shale conversion processes require more cleanup facilities than natural gas and petroleum feedstocks. For example, in addition to the dust from the coal handling facilities, the product gas stream from the K-T gasification process has to be treated for particulate removal as well as for sulfur compounds. This typical cleanup procedure produces an ash-water slurry waste that is not produced in natural gas or petroleum-based synthesis gas plants. The H-Coal liquefaction products contain unreacted coal, ash and catalyst which must be

removed. These solids and slurries then require disposal in an environmentally acceptable manner with problems of the fate of trace elements, leaching and stability to be considered. Oil shale retorting processes also contain particulates in the product gas and liquid streams. In addition, large volumes of spent shale are produced which require disposal, all of this at the expense of capital investment and operating costs.

The mining of coal and oil shale deposits also have a much greater environmental impact than the production of natural gas and petroleum. Care will have to be taken in the development of the coal and oil shale deposits to minimize the effects on the environment. This increases the cost of production of coal and oil shale and consequently inhibits the rate of commercial utilization of these resources.

5.3.6 Transportation Costs

All of the oil shale deposits and a significant part of the coal deposits in the U.S. are located in sparsely populated areas long distances from industrial chemical complexes. Therefore, if existing chemical plants are to use chemicals from coal and oil shale conversion processes, a large portion of either the fossil fuel or the conversion products must be transported. A third option would be to build new chemical plants at the conversion plant site and transport the finished products. Petroleum and natural gas have transportation systems already in place, and the development of any new transportation system for coal or oil shale will be very expensive. Synthesis fuels will probably be produced at sites close to where the energy is needed. The lighter fractions of the synthetic fuels will be the chemical feedstocks. Thus, for transportation costs not to be a factor inhibiting chemical production from coal and oil shale, the

facilities that produce these lighter cuts will need to be logistically close to the sites that presently consume the chemical feedstocks.

The sites that produce the chemical rich streams may or may not be at the conversion site itself. The H-Coal and similar processes produce a heavy liquid product. The site of the distillation separation of this product will be determined for the main part of fuel usage requirements. It is these sites that need to coincide with present chemical feedstock production sites in order to minimize any chemicals from coal or oil shale transportation costs increases.

5.3.7 Technological Development

Much of the present technology concerning coal conversion processing was developed thirty and forty years ago when coal played a major role in providing energy and chemical feedstocks. Only in recent years with the decrease in availability and increase in price of natural gas and petroleum has research and development of coal and oil shale conversion processes begun anew in the U.S.

With the exception of coke manufacturing, there is no commercial coal or oil shale conversion process being used presently in the U.S. to manufacture chemical feedstocks. Commercial scale technology for the manufacture of chemicals from coal exists, as is shown in South Africa, but the prices of natural gas and petroleum in the U.S. are not high enough to provide a sufficient economic incentive to use coal conversion processes for chemical production. This picture is in the process of changing as fuels vie with chemical feedstocks for the remaining available oil and gas.

All of the developing conversion processes must address each technical problem area anew with each advancing stage of development. These technical areas, as presented in Section 5.2 include:

- Processing Innovation
- Catalysis
- Reactor Technology
- Process Control Technology
- Materials of Construction
- Environmental and Safety Factors

and also:

- Transportation Advances
- New Product Development

It is anticipated that the first three areas listed will have the greatest effect on the technical feasibility of producing chemicals from coal and oil shale. They are discussed in greater detail below. Advances in processing innovation and catalysis cannot be predicted, so that any effort in these areas will have a questionable return. This still does not change the fact that advances must be made in these areas in order to lower the feedstock production costs and make chemicals recovery from coal and oil shale conversion viable.

Processing Innovation

Processing innovation comes about from ideas and techniques normally fostered through experience and applications of sound engineering judgment. Heat recovery is presently in an area where innovative steps are being taken in a readjustment to the higher energy prices. Areas for process improvement that normally escape detection are being focused on. The new processing carried out in an innovative manner will become more reliable or more efficient or easier, and thereby cheaper. Thus,

processing innovation will overcome many of the price considerations which presently inhibit coal and oil shale-based chemical production.

Catalysis

Chemical production from coal and oil shale conversion would be greatly enhanced if desirable chemicals were more selectively formed and separated from the conversion products. Coal conversion products are being processed using conventional petroleum processing technology in an ERDA funded study (PE-206), and the products characterized for their chemical production potential. Petroleum crudes are different from synthetic crudes, though, so while much of the necessary catalytic processing may be similar, work must be undertaken to try and find new and better ways of synthetic crude processing.

The processability of synthetic crudes in each step of conventional processing technology must also be verified. The trace elements, heteroatoms and other differences in composition of the new processing liquids could have a major effect on catalyst activity and, therefore, chemical processing and suitability for end use.

Reactor Technology

The reactor is the heart of any process, and with each new stage of development the reactor configuration must be verified, modified and improved. It is imperative to have an operating process of at least demonstration size to conclude that a reactor can be designed and constructed for the commercial production of chemical feedstocks. Lack of a proven reactor design is a major factor inhibiting any chemical processing, including the production of chemicals from coal and oil shale.

6.0 REVIEW OF EXISTING RESEARCH PROGRAMS

As pointed out earlier in this report, the coal and oil shale conversion processes that are being developed to produce fuels can also supply chemicals and chemical feedstocks. Thus, all of the invested effort and all of the programs to make the processes commercially viable will still be required, regardless of the product end use. If chemical feedstock production from these processes becomes an objective, the process optimization may simply require a different set of operating conditions or in the case of gasification further processing will be required, but the same basic technology development is still needed.

In this section, ERDA programs which most directly relate to factors associated with producing chemicals from coal and oil shale are reviewed. This review of ERDA programs is in the context of the factors identified as critical to the development and use of technology for producing chemicals from coal and oil shale, and provides the basis for the program suggestions presented in Section 2.

ERDA is currently the sponsor of several programs that directly or indirectly address the feasibility of producing chemical feedstocks from coal and oil shale. The programs vary from those directly applicable, such as the study by Dow Chemical Company to process and characterize coal derived liquids, to several programs concerned with desulfurization and hydrogenation of various coal liquefaction products.

The ERDA programs are organized into four major research areas that impact the question of chemical feedstocks from coal and oil shale. The research areas are:

- Chemical Feedstocks
- Catalysis

- Characterization of Syncrudes
- Liquid Processing

The last three areas are currently aimed at fuel production but these efforts will contribute to the general knowledge needed for a chemicals from coal program. The ERDA programs in these areas are discussed below to put into perspective their impact on the issue of chemical feedstocks from coal and oil shale.

Programs That Address Chemical Feedstocks From Coal and Oil Shale

The following two ERDA programs address the issue of chemical feedstocks from coal.

- CHEMICALS FROM COAL - DOW CHEMICAL COMPANY

  This research program is directed at conducting petrochemical processing operations on COED, SRC, Synthoil and H-Coal products. The processing for the COED and H-Coal samples include distillation, hydrocracking, hydrotreating and steam coil cracking. In general, the program is directed toward defining technology for use of coal liquefaction products for the production of useful aliphatic and aromatic compounds. The data generated are to be used to develop preliminary flow sheets, materials balances, and cost estimates for commercial scale facilities.

- CONCEPTUAL DESIGN OF A COAL TO METHANOL COMMERCIAL PLANT - BADGER PLANTS

  While this project is only in the conceptual design phase, it is directly applying coal gasification technology to existing petrochemical processing and production. Several gasifiers will be matched with several synthesis processes in order to determine the optimum processing and estimated cost for methanol production from coal. The production of ammonia and urea are also being addressed. The final design will be in sufficient detail to assess the potential for commercial production by this route, and recommendations for a demonstration plant are to be prepared.

Both these programs address the question of producing chemicals or chemical feedstocks from coal. The Dow study ties the processing of coal liquids into preliminary design and economics, while the Badger study uses gasification as the conversion process. These programs are defining processing routes to increase chemical yield from coal conversion while still utilizing existing technology downstream of the conversion process.

One recently completed program is directly applicable to chemical production.

- CHEMICALS FROM COAL LIQUIDS - PITTSBURGH ENERGY RESEARCH CENTER

  This research effort is directed toward examining coal liquids from ERDA sponsored liquefaction processes like Synthoil, SRC, and COED as potential sources of low molecular weight organic chemicals. Solvent fractions from those processes have been separated and characterized and the potential as a chemical feedstock assessed.

The PERC study is somewhat more limited as compared to the Dow study but does investigate an additional point - the suitability of different solvent fractions as chemical feedstocks. Only conventional processing is employed.

Development of Selective Catalysts

The development of catalysts for producing chemicals from synthesis gas streams and for upgrading liquid product streams is currently underway in several programs. The production of synthesis gas from coal is the most advanced of the coal conversion technologies. Catalysis of synthesis gas to produce chemicals is a proven technology (Fischer-Tropsch) and is in commercial production for synthesis fuels in South Africa. Other methods of producing chemicals from synthesis gas could provide an important advancement for a chemicals from coal industry.

- PETROCHEMICALS FROM SYNTHESIS GAS - PITTSBURGH ENERGY RESEARCH CENTER

  The objective of this study is to develop catalytic processes for conversion of synthesis gas to olefins, low molecular weight n-alkanes for conversion to olefins and aromatic high octane gasoline. The development of catalyst and processing conditions selective to these chemical groups is primarily a technological development.

- CATALYSTS FOR UPGRADING COAL DERIVED LIQUIDS - OKLAHOMA STATE UNIVERSITY

  The objective of the study is to investigate catalysts for upgrading liquids from coal to oil processes and to remove sulfur, nitrogen and other heteroatoms. Tests will be made on products of various ERDA sponsored coal to liquids processes.

- HOMOGENEOUS CATALYTIC REACTIONS OF H_2 + CO - PITTSBURGH ENERGY RESEARCH CENTER

  The objectives of this study are to develop the chemistry and catalysts of reacting hydrogen and carbon monoxide via homogeneous systems to produce low molecular weight organic chemicals which can be converted to chemicals or fuels.

- CATALYTIC SYNTHESIS OF GASEOUS HYDROCARBONS - CARNEGIE-MELLON UNIVERSITY

  The objectives of this study include the development of improved methanation catalysts, the investigation of intermediates formed on the catalyst during methanation, and development of combined shift conversion and methanation reactions. The results could provide an alternative catalytic process for producing low molecular weight hydrocarbons (C_2 - C_4) by modification of Fischer-Tropsch process.

The research efforts in development of more selective catalysts could dramatically impact the cost of producing chemicals from coal derived synthesis gas and liquids.

RADIAN CORPORATION

Characterization of Syncrudes

There are several existing programs for characterizing synthetic crudes from coal liquefaction processes in an attempt to lay the groundwork for upgrading these materials to useful products, including chemical feedstocks.

- DEVELOP METHODS TO CHARACTERIZE HEAVY LIQUIDS FROM FOSSIL FUEL ENERGY SOURCES - LARAMIE ENERGY RESEARCH CENTER

  The objective of this study is to develop analytical methods for obtaining chemical data for the purpose of evaluating processing and utilization of fuels. The design of efficient refining processes and the efficient utilization of fuel energy sources requires a knowledge of their composition.

- CHARACTERIZATION OF SYNCRUDES FROM COAL - BARTLESVILLE ENERGY RESEARCH CENTER

  The objectives of this study include the determination of composition data for syncrudes derived from various liquefaction processes; the evaluation of physical and chemical characteristics of samples prepared under different conditions of temperature, pressure, catalyst and flow; the characterization of these syncrudes in terms of refining and suitability for upgrading; and the development of improved procedures for characterizing the materials.

These studies basically address the issue of characterizing coal derived syncrudes in order to select processing techniques for converting them to useful products. Such procedures are a necessary step in the development of processing coal derived liquids into chemical feedstocks in the most economical manner.

Processing Techniques for Heavy Liquids

The fourth area of current research that impacts the feasibility of producing chemical feedstocks from coal and oil

shale is the development of processing techniques for the heavy oils. These techniques cover a wide range of processes to both upgrade these materials and to separate them into individual products.

- CHEMICAL CHARACTERIZATION, HANDLING, AND REFINING OF SOLVENT REFINED COALS (SRC) TO LIQUID FUELS - AIR PRODUCTS AND CHEMICALS

  The objectives of this study include the determination of chemical and physical properties and handling characteristics of SRC products, and the experimental determination of the applicability of commercial catalysts to the desulfurization, denitrogenation, and hydrocracking of SRC liquids. The study is directed toward fuel production.

- REFINING AND UPGRADING OF SYNFUELS FROM COAL AND OIL SHALE - CHEVRON RESEARCH COMPANY

  The objectives include the determination of the technical and economic feasibility of hydroprocessing four synthetic crude feedstocks to distill fuel fractions with presently available technology. The liquids to be evaluated are a pyrolysis liquid from coal, shale oil, a product of hydroliquefaction and SRC.

- REFINING PROCESS TECHNOLOGY - BARTLESVILLE ENERGY RESEARCH CENTER

  The objectives of the program are to determine the refining characteristics of synthetic crude oils, the composition and quality of finished products potentially obtainable from alternative raw material sources, and evaluation of changes in refining scenes based on syncrude composition and the desired fuel products.

- KINETICS AND MECHANISMS OF DESULFURIZATION AND DENITROGENATION OF COAL DERIVED LIQUIDS - UNIVERSITY OF DELAWARE

  The objectives of this study are to determine the reactor kinetics and mechanisms for catalytic hydrodesulfurization and hydrodenitrogenation of compounds found or believed to be present in coal derived liquids.

These programs are aimed primarily at the application of existing processing and refining technologies developed by the petroleum refining industry to syncrudes from coal liquefaction and oil shale processing. Some efforts are also being directed toward development of new processing techniques for converting these heavy oil streams to useful products, but these efforts are very rudimentary at present.

The programs reviewed in this section cover major areas considered to be of importance to the development of a chemical from coal industry. The summary does not include all the ERDA programs that could have a secondary impact but does include those judged to be of primary importance.

In general, only a few programs address the question of chemicals from coal and oil shale directly. The current level of effort can only be considered a starting point. Most of the efforts do not address the production of chemicals from coal conversion and oil shale processing as the primary focal point. These programs basically look at products from processes designed for fuel production to see what impact they might have on chemicals. They do not look into the optimization of chemical rich streams that would be needed for a chemicals from coal and oil shale industry. Suggestions for future ERDA research programs addressing aspects critical to the utilization of chemicals from coal and oil shale technology have been previously presented in Section 2.

RADIAN CORPORATION

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