RADIAN CORPORATION

1.0 INTRODUCTION

The petrochemical industry is currently facing major changes in the sources of supply for hydrocarbon feedstocks. Present feedstocks, predominantly derived from natural gas, natural gas liquids, and petroleum fractions, are becoming increasingly less available and less reliable on a long term basis. This trend may be expected to continue as reserves of these premium fossil fuel resources decline and the gap between supply and demand widens. Due to this situation it is apparent that the future status of the petrochemical industry is dependent upon securing a reliable feedstock supply and maintaining a flexible position in regard to potential feedstock sources.

Coal and oil shale, as domestic fossil fuels with relatively abundant reserves, represent an obvious alternative to the feedstock problem. Historically, coal has been a major source of hydrocarbon based chemicals, although coal derived compounds provide only a small portion of the petrochemical feedstocks used presently. However, coal and oil shale processing data indicate that a larger petrochemical feedstock production from coal and oil shale is technically possible.

Besides feedstock availability/reliability needs, incentives for producing chemicals from coal and oil shale exists because of: 1) the competitive relationship of feedstock and fuel demands, and 2) the possibility that chemical production from coal and oil shale might enhance the economic attractiveness of conversion technology, particularly when considered in conjunction with the production of basic fuels. The considerations behind 1) and 2) above are as follows:

- The production of chemical feedstocks is accomplished at the loss of an equivalent amount of fuel production. Since it is projected that the petrochemical feedstock demand will increase

at a rate greater than petroleum production, petrochemical demands will seek a greater portion of the available fuel at a time when the fuel supply is becoming increasingly inadequate to meet the nation's energy requirements.

- Due to a high unit value, chemical production might represent a strong economic incentive for the use of coal and oil shale. Also, the development of combined purpose facilities that co-produce chemicals and fuels might in some cases enhance the overall economic viability of producing fuel from coal and oil shale.

In view of these factors, the ERDA Fossil Energy Office of Program Planning and Analysis retained Radian Corporation through Oak Ridge National Laboratory to undertake a scoping study addressing the subject of chemical production from coal and oil shale. The purpose of this project is to provide ERDA/OPPA with a planning document identifying items for future ERDA research programs based on the factors presently impeding the use of coal and oil shale for chemical production and current ERDA program efforts. This report presents the results of that study.

The approach used in this program consists of the following steps:

- Development of base case projections to estimate the future relationship between chemical feedstock demands and fossil fuel production. This relationship is examined to determine if chemical production from coal and oil shale is an area with which ERDA should be concerned.
- Examination of the processing routes for producing chemicals from coal and oil shale, and the technologies available, to verify the technical feasibility of producing chemicals from these resources.

- Review of historical developments in the chemical industry to identify factors instrumental to the successful introduction of new feedstocks or processes, and, therefore, to help identify factors impeding the switch to coal and oil shale derived feedstocks.
- Review of current ERDA programs that are potentially related to production of chemicals from coal and oil shale, such that the extent to which ERDA is addressing these critical factors can be identified.
- Identification of items concerning the production of chemicals from coal and oil shale which should be considered for ERDA research programs.

The results of the study and the suggestions for future ERDA research programs are described in the following section (Section 2). The remainder of the report, Sections 3-6, correspond respectively to the first four steps of the technical approach which culminated in the identification of the items presented in Section 2.

2.0 CONCLUSION AND PROGRAM SUGGESTIONS

The conclusion of this study is that chemical production from coal and oil shale possesses sufficient merit that ERDA should develop and maintain research programs addressing factors critical to the production of chemicals from these resources. This conclusion is based on the following considerations:

- Petrochemical demand and premium fossil fuel production are in direct conflict and this conflict is projected to intensify as both uses compete for a limited amount of petroleum stocks (Section 3). Any achievement in using abundant resources such as coal or oil shale to supply petrochemical or fuel demands will help alleviate the problem.
- Coal has historically provided feedstocks to the petrochemical industry and presently a small portion of petrochemical feedstocks are derived from coal.
- The production of chemical feedstocks from coal and oil shale is technically feasible (Section 4.); however, factors associated with these technologies such as low straight run yields, and high cost of conversion and downstream processing are inhibiting commercial application (Section 5).
- In the absence of any preeminent procedure for supplying hydrocarbon stocks from coal and oil shale, it would appear beneficial to explore and attempt to facilitate development of alternate methods for utilizing these fossil fuel sources.

On the basis of these considerations, facilitating the production of chemical feedstocks from coal and oil shale is seen as a desirable national goal, and the program suggestions were developed for ERDA to consider.

The suggestions for possible ERDA sponsored programs have been organized into five major areas. These areas are:

- Economics
- Catalyst Development
- Processing Techniques
- Characterization of Liquids
- Environment, Safety and Health

Economics

The primary driving force behind any decision on chemical feedstocks will be economics, as explained in Section 5 of this report. There are, therefore, numerous areas of potential study under the general heading of economics. The important economic studies that would facilitate the production of chemicals from coal and oil shale are listed below.

- An investigation of the economics of producing chemicals from the major technologies already developed for fuel production.
- A study of comparative economics for competing technologies such as different liquefaction processes for specific chemicals (i.e., benzene, toluene, etc.), also a comparison of radically different methods such as olefins from cracking of syncrude versus olefins via synthesis gas.
- A study of the economics of primary products and by-products and the impact of marketing these on the overall economics of the process. This should determine the flexibility in marketing by-products as a method of improving economic viability. The impact of by-product sales on potential markets for these by-product materials should also be examined.
- A study to define the likely impact of increased coal demand, as might be brought about by a large chemicals from coal industry, on the price and availability of coal. This study should include an assessment of capacity of transportation modes to accommodate coal movement to processing centers.

One further economic consideration in the commercialization of any fossil fuel conversion technology is the high initial capital investment. A study should be made to identify the barriers and feasibility of multicompany (utility, refinery, chemical company) funding of commercial facilities.

Catalyst Development

The most important area of technological development for the near term is the area of catalyst development. This general technological area encompasses many program areas that should be evaluated. Catalysts are needed to improve processing techniques for creating and upgrading products from both coal gasification and liquefaction processes. Potential programs to provide data and expertise that would allow the increased production of more useful products from a coal or oil shale conversion process.

- Development of more selective Fischer-Tropsch-type catalysts to produce desired hydrocarbons from synthesis gas with a minimum of by-products. Low molecular weight hydrocarbons (C_2- C_4) are desirable, and the efficient production of these aliphatic fractions would improve the economics of producing olefin based chemicals from coal gasification products.
- Development of catalysts for hydrogenation of heavy oil fractions commonly produced by liquefaction processes to give higher yields of desired chemicals. Benzene, toluene, xylene and other aromatic chemicals are generally produced in abundance in a liquefaction process. Catalytic processes could increase the recoverable yield of these aromatics or facilitate the production of longer chain aliphatics.

Another major area for catalyst technology would be in the reactor for the basic conversion processes. Selective

catalysts in the reactor coupled with the necessary optimization of process conditions aimed at increasing the yield of desired chemicals would simplify later reforming and processing steps. For example, efforts could be concentrated on catalysts which provide higher yields of straight run BTX fractions from coal liquefaction processes.

Processing Techniques

There are many programs currently under ERDA funding to develop processing techniques for the production of fuels from coal liquefaction products. The general areas of processing include upgrading, purification, and separation techniques. The same type of programs currently being conducted in this area for fuels could be undertaken for chemicals. These programs should include:

- Continued work on the applicability of current refining technology to the problems of separating syncrudes into chemical feedstock fractions and subsequent refining and purification of these fractions into chemicals. This would include determining the applicability of current processing for desulfurization and denitrogenation of syncrude streams with emphasis on producing high quality chemical fractions.
- Research and development work into new technologies for syncrude processing with emphasis on providing streams with high concentrations of BTX fractions.
- Development of new technologies for denitrification and demineralization of shale oil.
- Verify processing techniques for purification of chemical streams, particularly aliphatics, from shale oil. (Applicability of procedures such as laboratory separation/purification techniques to reactor effluent processing.)

Characterization of Liquids

Any developments in either reactor technology or liquids upgrading should be examined from the standpoint of liquids characterization. The employment of analytical techniques for the evaluation of physical properties under variations in temperature and pressure should be undertaken, and an analysis of the stream's chemical compositions should also be included. Where applicable, new methods for liquids characterization should be developed. This is a necessary step in defining the upgrading and refining options for these materials.

Environment, Safety and Health

There are several general areas that should be of concern to ERDA from the standpoint of environment, safety and health, should a full-scale chemicals from coal program be instigated. These programs would cover the same range of efforts as those currently underway for fuels. The areas that should be included are:

- Testing and evaluation of products for their toxicity and carcinogenic nature.
- Definition of methods for safe handling of chemical products and by-products depending on hazards identified in the previous step.
- Determination of specific compounds likely to be emitted in chemical-producing coal and oil shale technologies.
- Definition of industrial hygiene procedures appropriate to the specific emissions which could occur from these technologies.

3.0 THE RELATIONSHIP OF PETROCHEMICAL FEEDSTOCKS TO OVERALL U.S. ENERGY SUPPLIES

In the marketplace as it exists today, chemical producers compete directly for petroleum with fuel suppliers. Approximately 7% of the domestic oil and gas resources consumed in the U.S. in 1975 were allocated for chemical use. Future growth in the chemicals industry will depend on a readily available source of feedstocks. If derived entirely from petroleum and natural gas, it is estimated in Section 3.3 that chemical feedstock demand will increase to some 22% of the total available domestic resources by the year 2000. This is a significant displacement from 1975 levels. At the same time, total energy consumption in the U.S. will have approximately doubled, requiring major increases in the use of coal.

This section is intended to provide perspectives on the interrelationships of energy and feedstock supplies and demands.

3.1 Primary Feedstocks for Chemicals Production

A brief description of the petrochemical industry will be helpful in further discussion of the potential for coal based feedstocks. The several thousand products that are outputs of the petrochemical industry can be traced back to a limited number of raw materials. This is illustrated in Figure 3-1 which shows several commodity chemicals traced back to the original hydrocarbon sources. One significant point illustrated by this figure is that the primary chemicals that are used to produce industrial chemicals can, for the most part, be derived from multiple hydrocarbon sources; natural gas, petroleum or coal. The processing that may be employed to convert the raw material to a primary chemical is represented in a simplified form in Figure 3-2. This figure illustrates that the primary chemicals can be represented by three major categories:

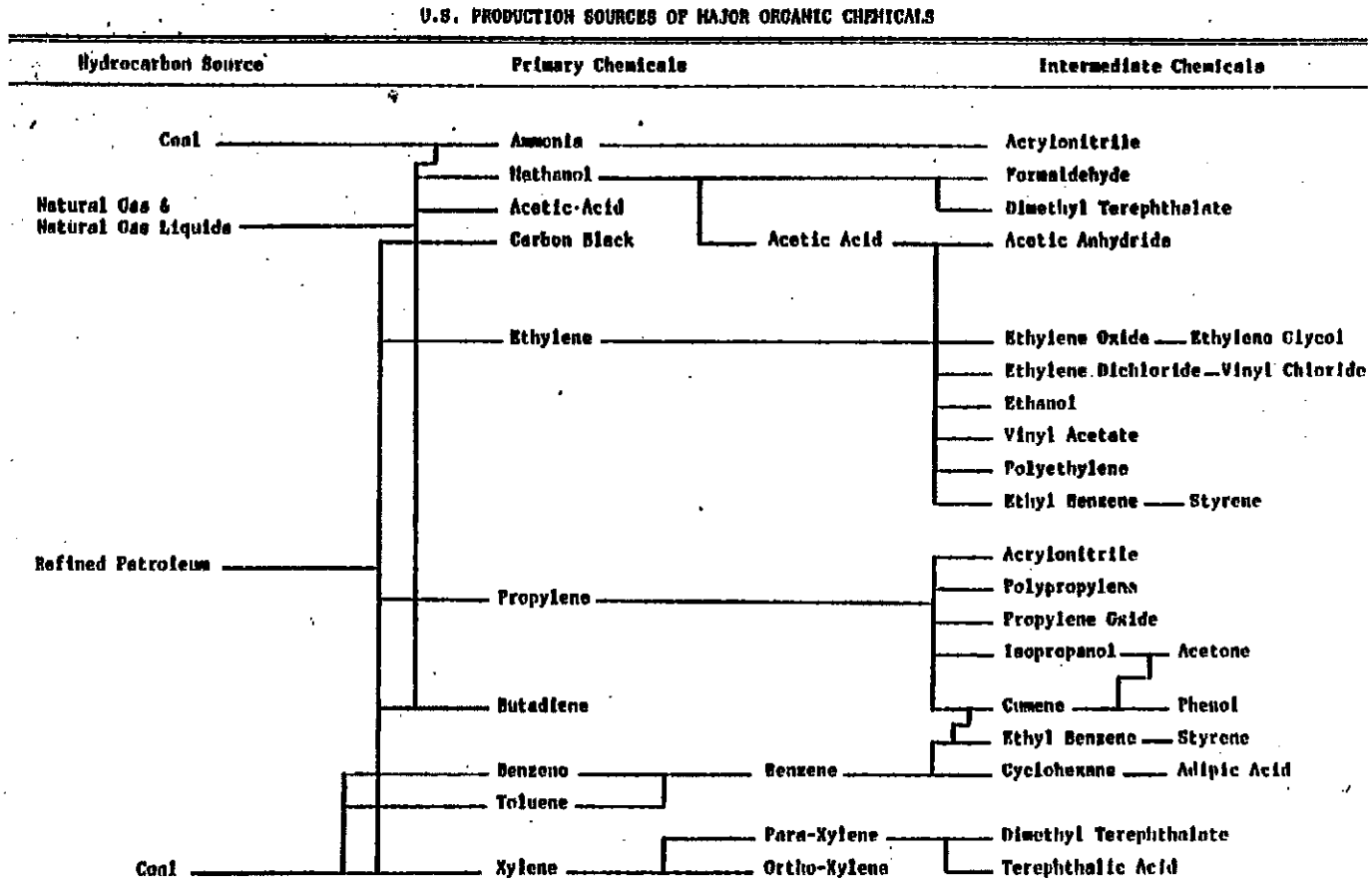

FIGURE 3-1. SOURCES OF MAJOR ORGANIC CHEMICALS

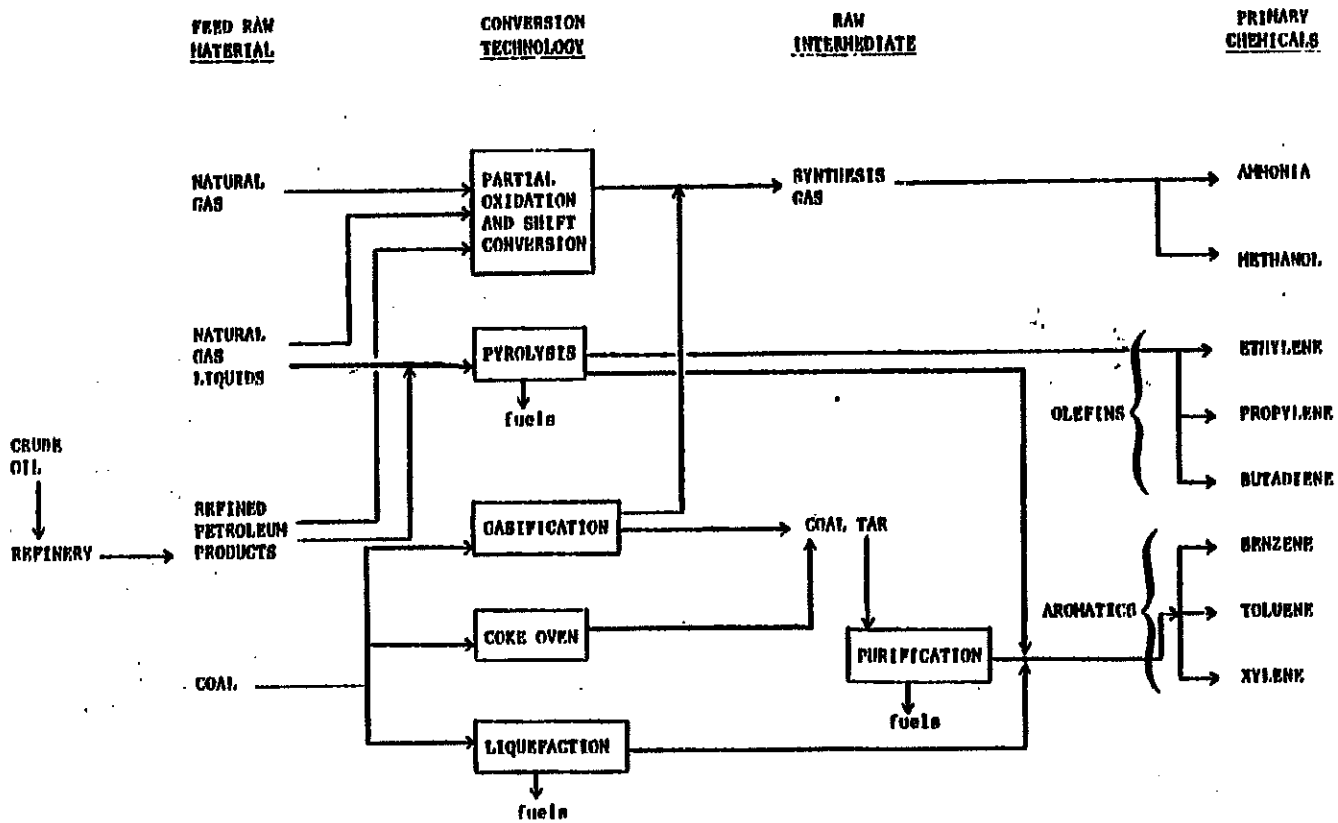

FIGURE 3-2. SIMPLIFIED REPRESENTATIONS OF PROCESSING FOR PRIMARY CHEMICALS OF THE PETROCHEMICAL INDUSTRY

- Synthesis Gas
- Olefins (Aliphatics)
- Aromatics

Carbon black and the primary chemical entry for acetic acid shown in Figure 3-1 are exceptions to this classification. Carbon black is an end use product produced directly from the hydrocarbon source. Acetic acid produced from butane or naphtha (the route qualifying acetic acid as a primary chemical) is not economically viable in today's market.

The salient characteristics of each of the three categories are as follows:

Synthesis Gas

At the present time synthesis gas is primarily produced by partial oxidation of natural gas to form hydrogen and carbon monoxide. Small amounts of synthesis gas are produced directly from petroleum derivatives or from coal by gasification, the latter having particularly found favor outside the United States. Synthesis gas is used to produce ammonia and methanol which in turn are used in the production of such chemicals as as acrylonitrile, acetic acid and formaldehyde. Ammonia is the third biggest volume chemical produced in the United States behind sulfuric acid and lime, and is the largest produced from organic raw materials.* Methanol is the eighteenth largest volume chemical.

Olefins (Aliphatics)

Natural gas liquids have been the major source of olefins such as ethylene, propylene, and butadiene. The remainder of the

*The chemical volume rankings cited in this document are taken from Chemical & Engineering News, May 3, 1976 (AN-175).