

5.0 IDENTIFICATION OF THE CRITICAL FACTORS IN THE UTILIZATION OF CHEMICAL FEEDSTOCKS FROM COAL AND OIL SHALE

Commercial and pilot-size processes for producing chemicals from coal presently exist. These technologies, however, are not being used by the U.S. chemical industry. This situation will certainly change in the relatively near future. Plans are being discussed, for example, for coal gasification units dedicated to ammonia production. The case for production of chemical feedstocks from coal and oil shale is technologically sound, but utilization will require overcoming a variety of barriers or impediments. In this section, the major factors impeding the use of chemical feedstocks from coal and oil shale are presented. In order to derive a listing of possible future impediments, a list of the major impediments as they have impacted the industry in the past is discussed. This appears in Section 5.1. The chemicals that were surveyed to obtain the list of past factors are ammonia, ethylene, acetic acid and phenol. These represent chemicals that are likely to be derived from coal and oil shale conversion processes at some time in the future. These factors are elaborated in Section 5.2. Using this historical basis as a guide, Section 5.3 delineates probable future factors affecting the utilization of coal and oil shale conversion products as chemical feedstocks.

5.1 Historical Factors Responsible for Chemical Industry Feedstock Changes

An initial literature survey for the chemicals that could be produced from coal and oil shale (Table 3-2) was made to determine factors responsible for past chemical feedstock changes. These were found to be:

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- Feedstock Price and Availability
- Capital Investment
- Operating Cost
- Technological Development
- Coproduct Value
- Environmental Factors

The coal and oil shale based feedstocks used in determining these factors were ammonia, ethylene, acetic acid, and phenol. This group of chemicals is representative of the chemical process industry in that they require the three basic feedstocks discussed throughout this report. Aromatic feedstocks are needed for phenols production, aliphatics are required for ethylene and acetic acid, and synthesis gas is the starting point for ammonia production.

### Ammonia

Ammonia is the third largest volume chemical produced in the U.S., and is produced on a commercial scale by catalytically combining nitrogen and hydrogen. Before World War II, ammonia was manufactured in coal-based plants or was produced from coke oven off-gas. Following World War II, natural gas and petroleum fractions were introduced to produce synthesis gas for the manufacture of ammonia. Almost all of the ammonia manufactured in the U.S. is now produced from natural gas rather than from coal or petroleum primarily because of the lower feedstock and production costs. The capital and operating costs required to manufacture ammonia from coal or petroleum are much greater than for natural gas. Operating costs are higher primarily due to the high degree of maintenance required in deriving ammonia from coal.

A number of countries are presently producing ammonia from coal because coal is available at a reasonable cost and

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importation of natural gas or petroleum is not feasible. Now that the availability of inexpensive natural gas and petroleum is decreasing rapidly in the U.S., ammonia manufacturers are considering the use of plentiful U.S. coal deposits to manufacture ammonia. Other ammonia manufacturers are considering the production of ammonia in the Middle East using excess natural gas and transporting liquified ammonia to the U.S.

### Ethylene

Ethylene is the fifth largest volume chemical produced in the U.S. and the biggest volume organic chemical. Ethylene has long been heralded as the backbone of the petrochemical industry (BA-528). Ethylene is a product of coal pyrolysis, thus can be produced directly from coal in limited quantities. Ethylene was almost exclusively manufactured from ethane and propane mixtures recovered from natural gas liquids during the 1960's and early 1970's. However, as the availability of natural gas liquids began to decline in the early 1970's, some ethylene producers started using butanes and naphthas as feedstocks. With the continued decrease in the availability of natural gas liquids and light petroleum fractions, ethylene producers are beginning to use fuel oils as a source. The cracking of heavier materials such as naphtha, fuel oil and coal products to produce ethylene also produces a wide range of coproducts which are potentially marketable.

### Acetic Acid

Acetic acid has been a basic industrial chemical since World War I and is manufactured from a variety of processes and raw material feedstocks. Table 5-1 illustrates the variety of raw material feedstocks and process technologies associated with acetic acid from its initial production to present. This is perhaps

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TABLE 5-1  
CHANGES IN PROCESS, FEEDSTOCKS AND BY-PRODUCTS  
IN THE CREATION OF ACETIC ACID FROM WWI TO PRESENT

ACETIC ACID

<u>PROCESS</u>	<u>YEAR</u>	<u>FEEDSTOCKS</u>	<u>BY-PRODUCTS</u>
OXIDATION OF ACET- ALDEHYDE	WWI	ACETYLENE	NEGLECTIBLE
LIQUID PHASE OXIDATION (LPO)	1952	BUTANE	ESTERS, KETONE, CO, CO <sub>2</sub> , FORMIC ACID, PROPIONIC ACID
WACHER/ ACETALDE- HYDE OXIDATION	1960	ETHYLENE	NEGLECTIBLE
BASF	1960	CO/ METHANOL	NEGLECTIBLE
MONSANTO	1970	CO/ METHANOL	NEGLECTIBLE

SOURCE: LO-184

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the best example of how each of the variable factors influence the use of a chemical production process. The process changes were due to cost and availability of the feedstocks along with capital and operating costs which are not shown. The production of by-products and the attendant separation and marketing requirements is definitely considered a hinderence, such that processes without by-products are favored.

Acetic acid was first manufactured from acetylene, much of which was derived from coal. After World War II the liquid phase oxidation of butane process was introduced commercially in the U.S. The availability of low cost butane and the marketability of the large amount of coproducts made this process commercially economic (LO-134). However, high capital and operating costs are required to separate and market the large quantity of coproducts.

The liquid phase oxidation of ethylene to acetic acid was commercially introduced in the U.S. in 1962. By 1973, 40% of the U.S. capacity was based on this process (LO-184). The oxidation of ethylene is a two-step process that is characterized by high overall yields and mild temperatures and pressures. The mild process temperatures necessitate the use of cooling water for heat dissipation and prevent steam generation for heat recovery. The production of acetic acid from ethylene takes place in two facilities, requiring high capital and operating costs. Even with these disadvantages, the ethylene oxidation process has a lower capital investment and a higher process yield than the butane oxidation process.

Monsanto's low pressure methanol carbonylation process for the manufacture of acetic acid was developed during the late 1960's and the first commercial unit came on stream in 1970. Because of the low process pressures, the very high process yield

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and the simplified purification system, Monsanto claims that the operating costs for this process are the lowest of any known acetic acid process (LO-134). This process is the basis for all new plants constructed since 1970.

Phenol

Phenol has also been a basic industrial feedstock since World War I and was initially extracted from coal tars and petroleum. To keep pace with the increasing demand, phenol was produced synthetically using the benzene sulfonation process. This process now accounts for only 5% of the U.S. synthetic phenol production (ST-414, p. 686.5022B). The benzene sulfonation process has a low capital cost, high material and operating costs, and requires the disposal of a large quantity of byproduct waste which poses a serious environmental problem (BA-507).

The Dow process of phenol manufacturing uses a benzene chlorination step and accounts for 3% of the U.S. synthetic phenol production (ST-414, p. 686.5022D). This process has high capital cost, high operating cost, high material cost and requires the disposal or use of by products (BA-507).

The Raschig process for phenol manufacturing uses benzene oxidative chlorination. This process is characterized by high power requirements for compressing air and high corrosion rates due to high process temperatures and highly acidic conditions. This process has high capital costs and high operating costs (BA-507). The last plant using this process in the U.S. was shutdown in 1971 (ST-414, 686.5022F).

The production of synthetic phenol using the cumene oxidation process has grown from its introduction in the early 1950's to supply 91% of the U.S. demand of synthetic phenol

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(ST-414, 686.5022A). This process uses a low cost feedstock, has relatively low capital and operating costs and produces acetone as a coproduct. The simultaneous production of phenol and acetone from cumene oxidation has led to a 50% reduction in the cost of both products (BA-507). In recent years many non-cumene phenol plants have shutdown as cumene based plants have come on stream (ST-414, 686-5022F).

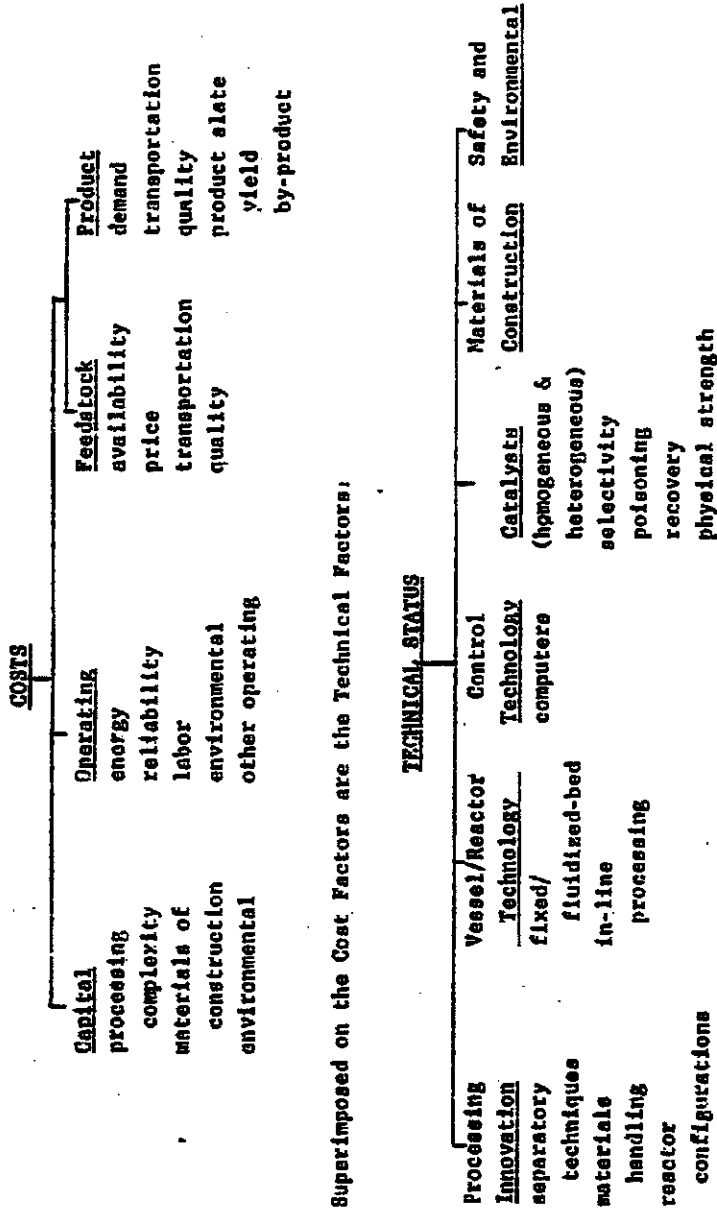
An interesting sidelight on the cumene process is the effect of acetone on another chemical, isopropyl alcohol. As the demand and market price swing, acetone can be converted easily to isopropyl alcohol by hydrogenation. This fact has inhibited the introduction of new fully developed process technology for hydration of propylene to the alcohol.

The major influencing factors on chemical feedstock process development highlighted in this subsection will be discussed further in the next subsection. This discussion will help delineate the key factors in the use of coal or oil shale to produce chemical feedstocks.

### 5.2 Factors Affecting Chemical Processing Choices

The interrelationship between the influencing factors determined in Section 5.1 must yield a significant and economically favorable set of conditions to industrial chemical firms before they can justifiably develop a new process or try a new feedstock on their own accord.

Many inputs contribute to the decision to use one feedstock or one processing route over another. The six factors identified in Section 5.1 are categorized and expanded in Figure 5-1. The figure consists of two parts, the top half "pure" cost factors and the bottom details the technical factors. Direct



Superimposed on the Cost Factors are the Technical Factors:

**FIGURE 5-1. FACTORS WHICH CAN CAUSE CHEMICAL PROCESS CHANGE AND/OR DEVELOPMENT**



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interactions exist among all the factors shown, not only within economics or technology but also crossing over from one to the other.

As an example, assume that a new catalyst was developed so that a high temperature process could be run at a lower temperature. The new lower temperature could lower requirements for materials of construction and might, also, require a less sophisticated, hence less expensive control scheme. The materials of construction and control simplification would lower the capital costs of the process, and the lower reaction temperature would decrease the operating and maintenance costs. On the other hand, the new catalyst might itself be more expensive. All of the technical and cost factors would then be brought together and a decision made on whether to continue with one or the other or possibly both of the processes.

Regardless what the interaction of influencing factors is, the end result must be significant to justify a large capital investment in new process technology by the industrial chemical firms. Also, for a developing process, additional consideration must be given to the risk that problems quite often surface only after a process is in operation, and not during a design or scale-up phase.

5.3 Discussion of Factors Affecting the Use of Chemicals  
from Coal and Oil Shale

In previous sections the types and quantities of chemicals which can potentially be generated from coal and oil shale conversion processes have been identified. In addition, factors which have accounted for changes in feedstock supply in the chemical industry have been discussed. This section presents a discussion of the results of super-imposing these two, thus providing

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a mechanism to identify factors which will strongly impact the production of organic chemicals from coal and oil shale derived feedstocks. The factors discussed in this section includes the historically significant factors pertaining to the organic chemical industry with the addition of transportation costs which are of particular significance in considering coal and oil shale utilization. These factors are:

- Feedstock price and availability
- Coproduct value
- Operating costs
- Capital costs
- Environmental Factors
- Transportation costs
- Technological Development

### 5.3.1 Feedstock Price and Availability

The major factor responsible for altering chemical industry feedstocks is raw material feedstock and availability. It is therefore reasonable to expect that coal and oil shale chemicals must be able to compete with conventional feedstocks on the open market. The factors directly influencing the cost and availability of these new products include:

- Resource cost and availability
- Developmental status of process technology
- Process economics
- Relative cost and availability of competing raw materials feedstocks.

While it is assumed for the purposes of this project that coal and oil shale products will be able to compete cost-wise with conventional raw materials, each of the above factors impacting these economics is reviewed in the following discussion.

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Resource Cost and Availability - Forecasts of coal and oil shale reserves and production indicate that sufficient resources are available to meet market demands, but production itself will have to greatly increase. The estimated economically recoverable reserves of coal are six hundred billion tons, and of oil shale an equivalent of two hundred billion barrels of shale oil (US-215). In energy equivalents, the coal reserves are ten times the oil shale reserves, and, at 1974 energy consumption levels, coal alone would last for over 150 years. The 1975 production level of coal was only 640 million tons. In order to meet the predicted year 2000 energy demands, production will have to increase three-to-four fold (US-409). Thus, the high demand and relatively tight availability of coal could cause coal prices to rise. Any price rise in coal would then be transmitted directly to the cost of chemicals derived from coal.

Developmental Status of Process Technology - The only major manufacturing use of coal in the U.S. at this time is for coke. Coke plants are built solely for the production of this material; by-product chemical recovery is not a major influence in either process design or operation although the technology is available to do so. Coal continues to be the only feedstock used by coke manufacturers because of its low cost, high product yield and superior product quality when compared to other carbon sources.

With the exception of a few coal tar distillation plants, at the present time there are no commercial plants in the U.S. producing chemical feedstocks from coal or oil shale, although the technology is being demonstrated on smaller scales. Commercial processing of coal to produce gasoline and chemical feedstocks is carried out in South Africa, however, where different economic conditions exist.

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Process Economics - Conversion process economics in conjunction with resource cost will have a major impact on the ability of coal and oil shale chemicals to compete with conventional chemical feedstocks. Process economics have been estimated but not yet confirmed for full-scale operation.

The major production costs in the manufacture of chemicals from coal and oil shale are for capital charges and utilities. An excellent example of the cost breakdown for the production of ammonia from coal has been prepared (RO-301), and it showed capital charges constituted 64% of the cost of the product while coal costs were 13% of the total costs. Of course, the manufacturing costs will depend on the specific conversion process employed.

Relative Cost and Availability of Competing Raw Material Feedstocks - A large portion of the worldwide chemical industry feedstocks were obtained from coal before World War I. However, discovery of petroleum and natural gas deposits resulted in rapid development since these resources were economical to recover and process. This development was accompanied by a relative decline in their cost as compared to coal. Consequently, chemical manufacturers turned to petroleum products and natural gas as raw materials for commercial technology development.

The current energy situation brought on in part by the sudden restrictions in the availability of foreign oil and diminishing domestic supplies of both oil and gas has caused a drastic increase in the price of both resources and subsequent increases in the price of conventional feedstocks. Hence, if the cost margin between coal/oil shale and petroleum/natural gas widens, the large coal and oil shale deposits in the U.S. will become more attractive as sources of hydrocarbon feedstocks.

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5.3.2 Coproduct Value

Coal and oil shale derived chemicals will have to achieve initial product equivalency to successfully compete with petroleum. The chemical market can readily assimilate a few new chemical feedstocks and processing shifts, but several major feedstock changes would not be as acceptable to the chemical processing industry. Coproduct value, then, will be an important factor in determining the commercial viability of producing chemicals from coal and oil shale conversion processes.

Many coal and oil shale conversion processes produce a wide range of products. Fuels will, of course, be the predominant product from a liquefaction plant but chemical recovery will be possible from process streams. Exploitation of these streams will help make the conversion processes commercially viable, but the product fractions that will be obtained from processing a synthetically derived crude oil will have a different composition than the products that are now derived from a petroleum crude oil. The uncertainty of this new coproduct slate is a factor inhibiting industry interest in commercial production of organic chemicals from these streams.

The production of coke by pyrolysis of coal converts 25% of the feedstock coal into products other than coke. More recently developed coal pyrolysis techniques, such as the COED process, generated gases, liquids and chars. The product slate from the various coal pyrolysis processes are skewed towards solids such that the production of chemical feedstocks by this route should be considered a small but important by-product recovery. The market value of the major coproducts will significantly affect the commercial feasibility of coal pyrolysis.

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Additional processing will be required if coal liquefaction products are to be used as chemical feedstocks. For example, to produce chemical feedstocks using the H-Coal liquefaction product the following types of processing may be required:

- Distillation
- Hydrotreating
- Reforming
- Hydrocracking, and
- Steam coiling cracking

It is interesting to note that this is going against the trend of the chemical industry which has been to develop one product from one process, and not from several intermediate processes. It should also be pointed out that many or all of these processing steps are used in conventional chemical processing, but when a coal conversion product is to be used as the feedstock, the complexity and degree of processing increases. Assuming minimal changes in feedstock demands, the desired product yields from conventional treatment of a coal conversion feedstock will be lower, and the distillation or separation steps would have higher requirements.

Coal gasification processes will produce a product gas of varying composition, and some gasification processes have liquid products also. Ammonia and  $H_2S$  produced in the gasification reaction will be recovered from the synthesis gas. The ammonia can be marketed, but the  $H_2S$  is an unwanted by-product that usually is converted to sulfur which has little market value. The clean synthesis gas can then be converted to hydrogen, methanol or a variety of hydrocarbons using Fischer-Tropsch technology.

The shale oil produced by the retorting of oil shale will also require a variety of processing to produce chemical feedstocks. These chemicals will be valuable, but large amounts of spent shale will have to be managed.

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A number of chemical feedstocks may be separated and marketed for each coal and oil shale conversion process. The value of these feedstocks will determine whether chemical production from each process will be commercially viable. The desirability of the coproduct as chemical feedstocks will be determined by:

- Market demand
- Product purity
- Product performance characteristics
- Product color and odor
- Product physical characteristics

Thus, any coal or oil shale conversion scheme will have to be viewed with all its coproducts for a fair evaluation.

### 5.3.3 Operating Cost

Operating costs (utility, labor, maintenance, and depreciation) can be a major factor responsible in determining the production of chemicals from coal and oil shale. For coal and oil shale conversion processes, operating costs can be a significant fraction of the total manufacturing cost (RO-301) and can be expected to be higher than for plants using petroleum or natural gas as feedstocks. For example, the operating cost for a 2000 ton per day ammonia plant using the Koppers-Totzek gasifier is twice that of a similar capacity plant using natural gas as the feedstock (RO-301).

The operating costs are high for coal and oil shale conversion processes for many reasons. Solids are much more difficult to convey and process than liquids or gases, and solids handling systems have high utility and maintenance costs. The high temperatures and pressures under which coal and oil shale conversion processes operate also require large amounts of energy

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to heat and pressurize the reactants. Present conversion technology also employs process methods which have higher utility, labor and maintenance costs than do plants using petroleum and natural gas as feedstocks. Thus, coal and oil shale conversion processes have high operating costs which must be balanced by lower raw material costs or higher added value of the products.

5.3.4 Capital Costs

Capital costs for coal and oil shale conversion plants are very high. As an example, the capital cost for the manufacture of ammonia using the K-T coal gasification process is twice that of using steam reforming of natural gas (IA-002, RO-301). The major factors responsible for the high capital investment are:

- Solids handling facilities
- Severe process conditions
- Pollution abatement facilities
- Product processing and cleanup facilities

High capital costs incur maximum capital exposure to the manufacturer and are associated with high operating costs due to increased maintenance.

High capital costs are both an economic handicap and an economic necessity in processes using fossil fuel conversion plants for chemical feedstocks. Any conversion based process will have very high capital costs when compared with conventional processing. One facet, though, of the capital intensive nature of a process utilizing coal or oil shale conversion is the economics of scale. Stated differently, this means the larger the plant, the cheaper the unit cost of the product. These scale economics tend to drive the size of an installation upward within the constraint of an achievable capital outlay.