1.0 INTRODUCTION

1.1 PURPOSE OF STUDY

For many years the Federal Government has supported the development of processes for converting coal to more desirable solid, liquid and gaseous fuels under the auspices of the Bureau of Mines, Energy Research and Development Administration (ERDA), and recently the Department of Energy (DOE). Current interest is particularly high because of the expressed Federal Government policy to decrease dependence on foreign oil by the increased use of domestic coal. Also, stringent environmental regulations are encouraging utilities to consider clean fuels for compliance.

A considerable amount of R&D support work for many different processes has been partially or fully funded by DOE. This support has included concept designs and cost estimating for industrial operation of many of the processes together with detailed economic studies. In addition to assistance to the private sector for energy planning, many of the studies also assist DOE in budgeting and program planning. Most of the detailed feasibility and economic studies have been done by different private firms and have been based on various economic and technical assumptions. The quality of the engineering input data and engineering designs and thus the quality of the conclusions have varied considerably.

This study starts with adoption of uniform technical and economic assessment methods. These methods are then used with available data and published studies to prepare analytical comparisons for a variety of coal conversion processes.

It is important to note that this study does not recommend the selection of any single process for development or application. There are many different markets to be served and various coals available. Several of the processes under development may be chosen for commercial application at different sites within the United States before the end of the century.

Because of the U.S. reliance on foreign energy sources, the need is greater than ever to develop energy alternatives for the nation. A similar need was voiced at the beginning of this century. The need was again expressed during World War II when Congress passed the Synthetic Liquid Fuels Act of 1944. In each case, a cheaper energy source halted the development of alternatives and lulled the nation back into a complacent attitude.

This study consists of uniform technical and economic comparisons of fourteen processes which convert coal to other energy forms. The major energy media - fuel liquids, fuel gas and electric power - were chosen intentionally to provide a broad comparison on a consistent basis. The techniques used may be easily applied to other processes not included here.

A previous study by C.F. Braun, Inc., (Ref. 1), completed in 1976, compared a number of gasification processes on a consistent basis. As the Braun study was concerned only with pipeline quality gas, reporting cost solely as dollars per million Btu ($\$/10^6$Btu) was completely satisfactory. A cost per Btu basis has also been used for coal-derived liquid products in many preliminary studies. It is a useful approximation for preliminary studies and it also avoids the problem of allocating costs to the variety of liquid products made by coal liquefaction plants. However, simply calculating total product cost as $\$/10^6$Btu is not satisfactory from a realistic market standpoint. Assigning product cost solely on a heating value basis gives relative fuel prices which never have, and probably never will, prevail in the marketplace. Even with Federal price control, gasoline has a wholesale price higher than home heating oil which in turn has a wholesale price higher than residual fuel oil. Even worse, a fixed price per Btu of heating value would invert the price ranking of these three fuels which are sold on a volumetric basis since heating oils have a higher fuel value per gallon than does gasoline.

Because fuel gas, liquids and electricity are traditional fuel competitors, and will continue to compete in the future, it was necessary to develop methods for objective economic comparison. Any method which does not consider inherent differences in values and market preferences for alternative fuels falls short of a realistic appraisal.

An important feature of this report is the use of a product value technique for estimating product prices which provides for the realistic distribution of costs to the various products from multi-product plants and for the meaningful assignment of all costs to the same single reference product for all technologies.

In addition to descriptions and discussions of technical aspects of the processes included, a section of this report is devoted to commercialization prospects for coal conversion plants. This section serves to emphasize that the present barriers to commercialization are not primarily technical. However, the analytical methods developed for this study are limited to technical and economic aspects.

Costs for products are estimated in terms of mid-1979 dollars on private and utility financing bases. No attempts were made to predict results from future inflation nor from price reductions that may occur with technology improvements. Guessing as to long-term inflation is not meaningful; price reductions for technology improvements are not likely to be significant.

1.2 SCOPE

The processes which are included in this study, and the abbreviations used in this report are as follows:

Solid Solvent Refined Coal (SRC-I)
Liquid Solvent Refined Coal (SRC-II)
Exxon Donor Solvent (EDS)
H-Coal, Fuel Oil Mode (H-FO)
H-Coal, Syncrude Mode (H-Syn)
Fischer-Tropsch (FT)
Methanol
M-Gasoline (M)
CO_2 Acceptor, Substitute Natural Gas Mode (CO_2-SNG)
CO_2 Acceptor, Syngas Mode (CO_2-Syn)

Hygas (HyG)
Bigas (BiG)
Synthane (Synth)
Lurgi (Lur)
Westinghouse, Syngas Mode (West-Syn)
Westinghouse, Combined Cycle (West)
Combustion Engineering, Combined Cycle (CE)

To be included in this comparison, it was decided that:

(a) Process must now be under development or considered a candidate for Federal R&D funds in the near future.
(b) Federal funds must be supporting R&D.
(c) Process is not a combination of other established technologies.
(d) Sufficient process data is available.

There are several established coal processes which do not meet this criterion and therefore are not included in this comparison.

However, even though the Lurgi process has never been supported by Federal R&D funds, it is included as a reference standard because it is one of the few gasification processes that has been commercially available for some time.

The COGAS process was not included because it is a combination of other established technologies which have been developed and modified by a private group. In addition, care was taken to avoid directly comparing technologies that were, at the time the report was prepared, before the Federal Energy Regulatory Commission for approval or, like COGAS, were in competition before DOE for commercial demonstration plant approval. The Exxon Catalytic gas process is still in the early development stage so data of sufficient reliability were not available. DOE support of Occidental Flash Pyrolysis has been recently dropped and the data available did not warrant including the process in the comparison. None of the omitted processes are expected to have economics significantly different from the range encompassed by the included technologies.

No separate gasifier units are included because the gasifiers are components within integrated processes. These reactors are important and serve as key operations within Fischer-Tropsch, methanol and most of the other processes studied, either as primary reactors or as sources of hydrogen. Gasifiers warrant thorough study because of their significant contribution to process efficiency. Such studies are best limited to the gasifier only. Electric Power Research Institute has sponsored several good reports on this subject (Ref. 23).

1.3 COAL RESOURCES

Enormous consumption rates for coal are being projected through the end of this century. Projections range from 0.8 to 2.0 Billion Tons/year (19 to 44 Quads*/yr), Ref. 22). Additional production beyond present rates is necessary to partially displace imported oil and to meet new energy demand. Reserves to meet these projections are proven. The location of these reserves is sufficiently well established that it is felt that economic production will be a reality.

Coal, however, is a heterogeneous raw material. This source of variation has existed ever since coal has been in use. A detailed discussion of this subject is given in Appendix 4.

1.4 MECHANICAL UPGRADING

Reducing the unwanted constituents of any particular coal can be accomplished in a number of fundamentally different ways. For coal from some sources, a portion of the ash and sulfur can be removed by relatively simple mechanical procedures, often including relatively simple water washing. Yet there are severe limits to the improvement of coal by these means. A further discussion of this topic is given in Appendix 4.

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* Quad is the abbreviation for a quadrillion British thermal units (10^{15} Btu).

1.5 CHEMICAL PROCESSES

Chemical methods hold the only promise for economic conversion of raw coal into more desirable end products. Coal is a relatively inert material and, while it burns readily, most other reactions proceed slowly. The chemistry of coal conversion is extremely complex and not thoroughly understood. Many mechanisms and intermediate compounds occur. Many reactions involving hydrogen and steam are involved. Some of the reactions are endothermic and others release significant amounts of heat.

When coal is subjected to high temperature, it passes through stagewise changes and decomposition. Volatile compounds are released as vapors and the remaining solid becomes plastic, swells and then resolidifies. The plastic behavior is a function of heat, particle size, pressure and type of coal. As heating continues a second variety of volatile matter is released leaving a semi-coke residue. The volatile matter from both stages consists of gases and condensable liquids. Subbituminous and lower coals behave differently than described above.

Dissolving coal in a solvent was a laboratory technique used more than a hundred years ago to study its structure. The bitumen fraction is first to dissolve. The presence of free hydrogen or use of solvents able to donate hydrogen to the coal molecule was found to increase the fraction of coal liquefied. Hydrogen has the effect of opening ring compounds and cracking long hydrocarbon chains. Liquid solvent may also serve as a transfer medium for hydrogen.

The liquids derived from direct break-down and hydrogenation-fragmentation of the coal molecule are principally aromatic hydrocarbons with naphthenic and aliphatic compounds comprising the remainder. Many of the compounds contain oxygen, nitrogen and/or sulfur atoms.

When gas is the desired product, the liquid may be hydrogasified, which is a pyrolysis aided by hydrogen. Hydrogasification of aromatics gives gas plus coke. Coke reacts to a lesser degree with hydrogen to give more gas plus a residue char.

Whether gas or liquid products are desired, the properties of the products are all important. The scientific tools available to effect and control conversion are pressure and temperature and the use of heat rate, hydrogen, steam and catalyst.

There is an excellent review and discussion of coal conversion reactions in the dissertation by Li. (Ref. 9).

Higher temperature and pressure are known to give a higher degree of conversion to liquids and gases and thereby leave less char residue. Hydrogen is an active reagent for breaking large molecules and forming more gas products. Steam has the effect of contributing hydrogen to react with the coal and supplying oxygen which reacts with carbon. It is the effective amount of hydrogen present in the reactor which is the main factor in determining product slate.

Catalysts are materials which accelerate reaction rates and since they typically affect particular reactions, they can strongly influence product slate in a multi-reaction system. There are problems maintaining catalyst activity since their activity is normally dependent upon surface effect involving adsorption mechanisms. The catalyst surface is subject to two types of interference problems. The first is mechanical, e.g. masking by a coating such as coke or fusion by high temperature. The second is a chemical surface change due to combination with any of many "poisons." Coals contain many potential catalyst poisons including sulfur and most of the heavy metal elements. All of the liquefaction processes involve catalysts in some way to accomplish and accelerate the conversion. Independent research continues to develop catalysts which will improve coal conversion.

Liquefaction technologies are often catagorized as "direct" and "indirect". Indirect liquefaction technologies first convert all coal to a synthesis gas and then convert the gas to desired liquid products. Direct liquefaction technologies use processes that work directly with the solid and liquid phases though they usually add hydrogen as a gas.

Desired results from a successful coal conversion process include:

1. High products efficiency - energy value of products close to input energy.
2. Ability to handle variety of coal types - particularly including caking coals.
3. Preferred product characteristics to replace either present petroleum-derived products or natural gas.
4. Low product cost.

The fact that coal, as a raw material, has increased in price dramatically with increases in petroleum price has confused the outlook for coal conversion processes. (Ref. 26) It is obvious that the end product must always cost more per energy unit than the raw material. The gains because of the conversion processes are decreased pollution and increased convenience due to better handling characteristics of the derived fuels.

2.0 COMPARISON METHODS

The many different coal conversion processes which are currently being developed have significant differences in design concepts and product mixes. Some have limitations with respect to the type of coal which may be used. The general problem here is to develop and apply useful comparison criteria. Because the ultimate objective is commercial use, the criteria which will be most meaningful are those which recognize the market potential for the conversion products.

The convenience of the energy form is effectively dealt with by use of the product value technique for product price estimating which will be discussed in detail later.

All of the processes studied are believed to be capable of meeting existing environmental regulations. All costs used in this study include systems within the process plant needed to achieve legal requirements.

Before comparing the various coal conversion processes, it is necessary to be sure that key standards for comparison are well understood and have the same meanings for all users. Aside from simple costs, the only common standard which applies is efficiency.

2.1 EFFICIENCY

There is a universally recognized definition for thermodynamic efficiency which can be applied to any of the conversion processes considered. The definition, in simplest terms, is total output energy divided by total input energy. This definition includes all utility inputs and credits for temperature and pressure of products above ambient conditions. This definition does not relate to the basic purpose of providing fuel products as well as a modified efficiency definition.

The modified definition which is called "product efficiency" in this report has been in common use by others for years. Others have also called it by other names such as "cold products" or"fuels" efficiency. This definition is the "higher heating value" (HHV) of all fuel products divided by total energy input of coal feed and electric power. As a practical consideration, where electric input is required for the energy balances, this report, and many others, use 10,000 Btu/kWh rather than 3,413 Btu/kWh to allow a realistic conversion loss for electric power generation.

2.2 PROCESS COMPLEXITY

When comparing processes, it is desirable to arrive at some measure of how complicated systems are, relative to each other. If the same product can be made by several processes, it is axiomatic that, given the same feed materials and final products, the simpler the process, the less prone it is to process upsets, the less the plant should cost, and the less the final product should cost. However, it is difficult to provide a simple definition or criterion of process complexity. Process complexity involves many intangible elements which require a careful and realistic appraisal. These include:

- Reaction complexity. A process which requires several consecutive reactions is less desirable than a process involving fewer reactions. The sensitivity of any one reaction to changes in any of the important variables, such as temperature, concentration, etc., may have strong effect on quality control and reliability. Coal is a heterogeneous material and composition from a given mine often varies with time. This further aggravates the reaction problems.
- Operational complexity. A process with many steps which entails multiple handling of solids and fluid streams will be prone to more equipment failures and consequently greater downtime. As detailed in the section on reactor complexity, the methods used for gas/solids contacting and catalytic conversion can also greatly increase process complexity. As a general rule, solids cause more problems than fluids, and liquids are more troublesome than gases.
- Operating regime. The chemistry of coal conversion processes normally involves high operating temperatures and pressures. Very high pressures or temperature involve more difficulties. Special materials and equipment such as high pressure solids feeders and non-standard items must be built and maintained with much higher standards than required for simpler conditions.

- Auxiliary facilities. The number of required support facilities such as catalyst reclaiming, by-product recovery plants and special utility services will make the process more complex. Each auxiliary service brings with it its own complexity factor with an influence on cost and reliability.

A relatively comprehensive system of rating complexity was used by a DOE Energy Technology appraisal group* in mid-1978 to rate several gasification processes. They also identified their system as subjective but their values were produced using the opinions of a number of knowledgeable people. They rated the processes for both Eastern and Western coal and assigned values to each in a technical and also an Operability/Complexity/Flexibility category. Three of the processes they rated are included in this report and there is full agreement with their ranking order.

2.3 ECONOMICS

The final, and usually most important, criterion for selecting one coal conversion process from among a group of proven processes is based on economic projections. This is why cost analyses typically begin while a process is still bench scale and continue to be revised and refined throughout development.

2.3.1 Cost Per Unit of Energy

The simplest cost calculation is the determination of cost per energy unit, typically $\$/10^6$ Btu. This is sufficient for processes producing only SNG but has limited value for the other processes. To make such a calculation, all that are required are estimates of capital investment and some reasonable assumptions for operating cost, fuel cost and product efficiency. This is one of the methods used in this report. Costs are shown for both private and utility financing. This report uses the costing guidelines and recommended financial parameters set forth in the ESCOE "Guidelines for Economic Evaluation of Coal Conversion Processes"(Ref. 27). All data are presented so that calculations on different bases can be made if desired.

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* (The system devised by this group has not yet appeared in a published report.)

2.3.2 Energy Products Market

The problem becomes more difficult when product costs are to be determined for the purpose of comparing processes, each with a variety of products of different properties. For liquid products, assigning cost directly proportional to heating value is entirely unrealistic and cannot be supported by marketplace history. Price for any commercial fuel is dependent upon availability, convenience, environmental suitability, production costs and demand; i.e., value in a competitive market. Gasoline should and does cost more than boiler fuel because of its convenience in the very large transportation market. Natural gas is more valuable than coal because it is clean-burning and now, after many years of extremly low regulated prices, is being priced at a premium value above coal. Fossil fuels have no more reason to be priced the same on an energy content basis than should various foods be priced the same by such an over-simplified system.

Coal-derived fuels are going into an existing market dominated largely by natural gas and petroleum-derived fuels. Initial efforts are to tailor the new products to serve as replacements. So long as petroleum is available as the major energy source, it will tend to control the market.

ESCOE has developed a technique for product cost estimating that recognizes varying product values. This product value technique first calculates a price for a reference fuel. All individual fuel prices are then determined from the reference fuel price. The initial choice of which fuel form to use for the reference product does not affect the final results for individual product prices.

2.3.3 Product Value Technique

The value method of determining estimated costs for individual products is based on the assumption that future energy prices for particular products will maintain a fixed ratio to each other. All prices are normalized relative to a reference product. Although we have used the relative values of products as existed in 1978 as the assumed relative values in the future, any other slate of relative values can be assumed.

Since all plant production costs must be recovered, the sum of all product sales in a particular time period must equal all costs (including profit) attributed to that time period. Thus

$$\Sigma P_i B_i = F + M + kC \tag{2.1}$$

where:
P_i = individual product price in \$/10^6 Btu
B_i = annual production for product i in 10^6 Btu
F = annual coal cost in \$
M = total annual cost for labor and all other operating expenses in \$
k = capital factor which allows for all interest, taxes, return, and recovery of capital investment
C = total invested capital for project in \$

For each individual product, the value factor, f_i, is defined as:

$$f_i = \frac{P_i}{P_r} \tag{2.2}$$

where: P_r = the price of the reference product

substituting P_i from Equation 2.2 into Equation 2.1 yields:

$$P_r \Sigma f_i B_i = F + M + kC$$

or:

$$P_r = \frac{F + M + kC}{\Sigma f_i B_i} \tag{2.3}$$

Thus, the necessary market price for the reference product if the subject technology is to be competitive is, from Equation 2.3, a simple function of annual costs, annual production of the various products, and the relative market values of the various products.

Once the reference product price is calculated, the individual product prices are determined simply, from Equation 2.2, by multiplying the reference product price by the respective value factors, f_i.

For this report, premium gasoline has been chosen as the reference product.

The cost components data and associated calculations are presented and discussed in Appendix 2 and k is explained in Chapter 5 where it is used. The values for k in this report are based on and discussed further in the ESCOE Economic Evaluation Guidelines (Ref. 27).

To calculate value factors, f_i, it is first necessary to select a complete set of market values for all products. This price set is for a particular point in time and the choice of the time is reflected in the value factors. For the present study, f_i for liquid products were determined from mid-1978 published market prices. All liquid fuel products were subject to Federal price controls to some degree in 1978 and this is reflected to the same degree in all value factors.

Because natural gas prices are just now being released from crippling price controls over the last 25 years (the regulated well-head price for new natural gas in the interstate market has increased some eightfold in the last six years and will be deregulated in another six years) it is impossible to measure the value of natural gas in 1978. However, because of its convenience for most stationary uses and its high environmental advantages, we have assumed market value for natural gas equivalent to premium gasoline on a Btu basis. The slopes of recent price curves for oil and natural gas also support this as a reasonable assumption (see Ref. 26). Recent FERC approved prices for supplemental supplies also bracket this value. Since there has been no significant production of lower-Btu fuel gas in recent years in the U.S., there is no market and thus no 1978 market price. We have assumed here that all gas fuels have the same value per Btu regardless of heating value per volume.

There has been no market for SRC-1 clean solids since there are no commercial production facilities.

The solid fuels are priced on their heating value relative to fuel oil. Clean SRC solid fuel is discounted ten percent to allow for the added handling costs. Char is further discounted to allow for higher ash contents. The value shown for char would be too high for a material with a significant sulfur content. The amount of sulfur contained in a char depends strongly on the feed coal analysis and the process used.

Tar oil is a material peculiar to gasifiers. There is a potential for recovery of valuable chemical by-products.

Fuel oil in this report refers to industrial fuel commonly referred to as No. 6, Bunker C or residual fuel. There are variations in the physical properties for the oils sold in this category. It is not uncommon for residual fuels with a higher heating value to sell for less per barrel due to high viscosity and resultant extra handling cost. No. 2 oil is considered synonymous with diesel fuel in this report.

Naphtha is a generic term for a distillate product which is not commonly sold on the open market. It is an intermediate refinery stream which ends up as gasoline, diesel fuel and specialty products. Naphtha physical properties and hence value varies considerably depending upon crude oil source and pretreatment. The naphthas from coal conversion processes also vary both between processes and even from a given process depending upon feed coal and operating conditions. For this report, all naphthas were assigned a single f_i value related to cost necessary to upgrade the product to gasoline.

Liquid petroleum gas (LPG) is a commercial product consisting mostly of propane and butane. It is shown as a lower energy price than the principal components which reflects market conditions and value of the purer materials as feedstocks for higher value chemicals.

The gasoline shown in Table 2.1 is low octane such as obtained from a simple Fischer-Tropsch process. It is lower quality than the regular grade sold in the U.S. market. The premium gasoline is 93 Research Octane Number and the same as sold in the U.S.

Methanol is sold commercially but not on the scale required for the transportation fuels market. Thus the mid-1978 commercial price has no relation to future cost as a major fuel. For this study pure methanol was assigned an energy value equal to premium gasoline since it can be used in the same type engines as an acceptable replacement. Methyl fuel is priced proportional to the heating value for pure methanol. It is discounted to allow for water.

The value factor for electricity was determined from a typical mid-1978 cost to medium size users.

Table 2.1

Value Factors for Energy Products
(Reference to Premium Gasoline)

Product	1978 Price ($)	Heating Value (10^6Btu)	Energy Price ($/$10^6$Btu)	Value Factor f_i
SRC Solid (1)	- /ton	32.0	1.75	.50
Char	26.32/ton	16.0	1.65	.47
Tar Oil	14.88/bbl	5.0	2.98	.85
Fuel Oil	12.35/bbl	6.3	1.95	.56
No. 2 Oil (Diesel Fuel)	14.92/bbl	5.2	2.87	.82
Naphtha	14.92/bbl	5.2	2.87	.82
LPG	12.04/bbl	4.0	3.01	.86
Gasoline	15.75/bbl	5.0	3.15	.90
Premium Gasoline (2)	17.50/bbl	5.0	3.50	1.00
Methanol (3)	- /bbl	2.7	3.50	1.00
Methyl Fuel (4)	- /bbl	2.6	3.36	.96
Butane	13.11/bbl	3.5	3.75	1.07
Propane	12.10/bbl	3.2	3.78	1.08
All Fuel Gases (5)	——	——	3.50	1.00
Electricity	31.06/10^6wh	3.4	9.10	2.60

(1) No sales in 1978. Energy price assumed 10% less than fuel oil.

(2) Premium gasoline is reference fuel. $f_i = 1.00$

(3) No significant market in 1978. Energy value assumed same as premium gasoline.

(4) No market in 1978. Energy price 4% below methanol for water content.

(5) Severe price regulation for natural gas in 1978. Energy value set at 1.00. See text.