SECTION 1
INTRODUCTION

SECTION 1

INTRODUCTION

This report describes the results of an investigation of coal liquefaction processes that are under development. The main objectives of the investigation were to:

- Survey coal liquefaction processes being developed;
- Review the status of development;
- Make comparative technical and economic evaluations of high potential processes.

The survey was conducted under Subcontract No. 7186 with the Oak Ridge National Laboratory operated by Union Carbide Corporation, Nuclear Division (UCC-ND) under the Principal Contract No. W-7405-eng-26 with the Department of Energy (DOE), Fossil Energy Division of Program Control and Support. Their support and guidance are gratefully acknowledged.

The survey was a limited effort assignment relative to the broad scope of the objectives and the number of candidate coal liquefaction processes. It used the experience gained, previously and concurrently, in the development of seven comprehensive conceptual designs/economic evaluations plus reviews of design, construction and operation of several pilot plants. The conceptual designs included candidates from all generic liquefaction classifications, i.e., hydroliquefaction, donor solvent, pyrolysis and indirect.

Information used in the survey and evaluation was, in general, that available from published sources, provided by DOE, or obtained by nonproprietary consultation with process developers. Proprietary information is not included.

At the beginning of the survey more than 60 candidate processes were defined. From these candidates, a list of 33 were judged worthy of more extensive review. Approximately 30 processes were deleted from further consideration at this stage for various reasons. To illustrate, some were judged to have limited potential for commercialization, some appeared too similar to processes which were more advanced in their development cycle to warrant separate study, for some there was insufficient data available to us to permit detailed evaluation, and in some cases development work had been terminated by the developers.

The 33 processes reviewed represented an effective overview of the current state of coal liquefaction art. A summary of the characteristics of these processes was compiled and published; this "Data Source Book"[1] served as a starting point, as well as a reference, for the work reported here.

The survey results summarized in the following pages represent the equivalent of a "photograph," at a point in time (July, 1978), of judgements regarding the relative commercial potential for liquefaction processes. The judgements were based on analysis of information available to us within the limits of time and resources available.

SECTION 2
SUMMARY

SECTION 2

SUMMARY

A survey of coal liquefaction technology and analysis of projected relative performance of high potential candidates has been completed and the results are reported here.

The key objectives of the study included preparation of a broad survey of the status of liquefaction processes under development, selection of a limited number of high potential process candidates for further study, and an analysis of the relative commercial potential of these candidates.

Other objectives which contributed to successful achievement of the above key goals included definition of the characteristics and development status of known major liquefaction process candidates, development of standardized procedures for assessing technical, environmental, economic and product characteristics for the separate candidates, and development of procedures for selecting and comparing high potential processes. The comparisons were made for three production areas and four marketing areas of the U.S.

The survey was a limited effort in view of the broad scope of the objectives. It used the experience gained during preparation of seven comprehensive conceptual designs/economic evaluations plus comprehensive reviews of the designs, construction and operation of several pilot plants. Results and conclusions must be viewed in the perspective of the information that was available for use in the study, how this information was treated, and the full context of the economic comparison results.

Comparative economics are presented as ratios; they are not intended to be predictors of absolute values. Because the true cost of constructing and operating large coal conversion facilities will be known only after commercialization, the relative values are considered to be more significant to achieve the objectives of this study.

There are many logic patterns that may be used for a technology assessment of this scope. As an overview prior to summarizing the results and conclusions, the particular logic pattern used here consisted of:

- Completion of a broad survey of coal liquefaction processes that are under development or have been operated commercially; more than 60 processes were defined.

- Selection of processes justifying further review; 33 of the 60-plus were selected.

- Development of a "Data Source Book" containing process characteristics and development status for the 33 processes; this served as a reference during the subsequent portions of the assessment program.

- Development of criteria for selection of high potential processes for more detailed study:

  - development status factors
  - technical factors
  - economic factors
  - other

- Selection of high potential processes; four were selected using the selection criteria described above plus other relevant criteria described later. Importantly, because of high interest, and potential for defined conditions, characteristics of one configuration of the Mobil-M process for production of gasoline are summarized here.

- Development of process configurations including predicted heat and material balances, product yields and thermal efficiencies, environmental control procedures, product quantities/characteristics, and economics for the four high potential processes.

- Comparison of the economics for the four high potential processes:

  - Fixed Capital Investment

  - Total Capital Investment

  - Operating Costs

  - Required Product Selling Price (RPSP) at a 12% Discounted Cash Flow (DCF) profitability level for a defined project structure

  - Possible product market values

  - A benefit/cost (B/C) ratio, representing the ratio of possible market value to RPSP; this is a direct function of projected profitability.

- Retrospective Analysis of the results including:

  - Comparison of relative economics developed for this study with results from comprehensive conceptual designs/economic evaluations prepared by major contractors.

  - Economic impact of differences in product compositions, i.e., as more highly refined products are produced, what is the added cost?

- Development of conclusions and recommendations.

The contract required client agreement with the procedures used for technical and economic assessment; also agreement on the high potential processes selected for more detailed study.

The process configurations for all high potential candidates produced marketable products. Of key importance in a comparative assessment is to either make the comparisons based on virtually identical products or, alternatively, to adjust the comparison to quantitatively rationalize the economic impacts of differences in products generated by the candidate processes. In general, processes which produce heavy fuel products will require low capital investments and yield low annual revenues; the full profitability analysis envelope must be viewed to provide a meaningful comparison.

The information assembled for the 33 processes and published as a Data Source Book,[1] in conjunction with background from comprehensive conceptual designs/economic analyses and pilot plant performance reviews provided a portion of the basis for selection of high potential processes. Key elements of the selection criteria included:

- The development status; emphasis on the ability to permit commercialization by 1990.
- Capability of producing a product slate responsive to the historical energy consumption requirements for the producing area.
- Maximum profitability.
- Ecologically acceptable.
- A limited number of processes to be defined as "high potential" after assessing multiple techincal, economic, product characteristics and development status factors; see Appendix A for details.

The preliminary assessment of 33 processes was completed using the above criteria guidelines. As a result, the following four high potential processes were selected:

- H-Coal based; a catalytic hydroliquefaction process.
- SRC II based; a pseudocatalytic hydroliquefaction process.
- Consolidation Synthetic Fuel (CSF) based; a donor solvent process.
- Fischer-Tropsch based using a flame sprayed catalyst system; an indirect process.

In conjunction with DOE, it was agreed that adequate detailed information was not available to us at the time (in 1977) to permit detailed objective inclusion of the Exxon Donor Solvent (EDS) process as a candidate. Additional information has subsequently become available and future assessments should include EDS.

Also, as indicated earlier, by virtue of special interest in the M-Gasoline and the high rating it obtained, the results of an independent evaluation of one configuration of the process is summarized in some detail in Appendix C. The information on this process available to us at that time contained what might be termed conservative technology for the gasification and methanol synthesis steps and therefore requires separate interpretation. Subsequently more detailed design and analysis would place it on a more comparable basis with the four high potential candidates.

A preliminary process package was developed for each of the candidates; this consisted of a block flow diagram, heat and material balances, product yields/characterizations, thermal efficiencies and environmental facility design. Each plant had the capacity to produce fuels with an energy content of 600 billion Btu per day, equal to 100,000 barrels per day of fuel based on a nominal 6 million Btu per barrel reference value. The amount of feed coal required varied and was a function of the projected thermal efficiency.

Facilities were included in the design to upgrade and refine the coal liquids produced in the candidate process coal liquefaction step; product classifications included SNG, LPGs, gasoline, distillate fuel oils and residual fuel oils. These upgrading/refining additions caused us to introduce the terms "SRC II based," "H-Coal based," etc. to emphasize that while the basic coal liquefaction process to produce coal liquids was based on referenced data from the process developer, the added refining facilities were, in general, our design inputs.

The separate processes produced products in the SNG, LPG, gasoline, distillate fuel oil and residual fuel oil classifications, but they differed in quantities and characterization. Table 2-1 summarizes the product slates, feed coal quantity and other characteristics projected when processing Illinois No. 6 seam coal at an Eastern Region of the Interior Coal Province plant site; these results are considered typical of this Coal Province which include Kentucky, Indiana and Illinois. Table 2-1 shows: the SRC II based plant configuration used here would produce the greatest amount of residual fuel oil and least amount of gasoline; the H-Coal based plant would produce less resid and more gasoline; the CSF based plant would produce no residual fuel oil, a significant amount of distillate fuel oil, and about the same amount of gasoline as the H-Coal based plant; the Fischer-Tropsch based plant produced primarily gasoline and SNG with lesser amounts of LPG and distillate fuel oils. The SRC II based, H-Coal based and CSF based configurations all produce approximately the same amount of SNG, equivalent to 25-30% of total fuels produced on a Btu basis, while the Fischer-Tropsch based plant produces approximately twice as much SNG. Therefore, while the configurations used, in general, produced fuels in the target product categories, they tend to be lighter products and more highly refined as you move from left to right in Table 2-1. This should be kept in mind as the summary of relative economics unfolds.

Estimates of capital investment requirements, operating costs, and RPSP at 12% DCF were prepared for each candidate. All economic factors were developed based on first quarter 1978 dollars. The fixed capital investment (FCI) estimates were based on an estimate specific to the primary coal liquefaction operations as defined by non-proprietary information provided by the process developer plus estimates of coal preparation and coal derived liquids/gas recovery and refining based on prior comprehensive conceptual design results; also experience factors for upgrading/refining operations from the petroleum refining industry. More details of the estimating procedures are presented in Section 7. Operating costs were developed by an analysis of operating labor, catalyst and chemicals, utilities and other requirements; in general, all plants captively produced their steam and electricity needs. The RPSP indicates the equivalent uniform annual revenue required to generate a 12% DCF rate of return, first quarter 1978 dollars, using a 65/35 debt/equity project structure, 9% interest rate, 5-year construction period and 20-year operating period.

The possible product market values were next developed for each candidate process by comparing projected coal derived product characteristics with current petroleum-based product characteristics and market values. In the case of SNG, a judgemental value of $3.25 was selected for the base case analysis; sensitivity of relative economics to SNG market value over the range of $2.25 to $4.25 was also developed. The $3.25 value is intermediate between natural gas pricing and projected cost of SNG from coal and the allowed pricing for incremental SNG from naphtha.

The marketability and market values of coal derived liquid and gaseous fuels requires confirmation. This should be an important goal of the national coal conversion development program.

Finally, a B/C was developed which represents the ratio of possible annual revenue to RPSP at 12% DCF. This ratio is significant since the higher the value the higher the indicated potential profitability.

The results of the comparative economic analysis show the following rankings, where a ranking of 1 represents the most favorable economics and higher numbers successively less favorable.

Process	Benefit/ Cost Ratio (B/C)	Required Product Selling Price @ 12% DCF (RPSP)	Possible Annual Revenue	Capital Investment Requirements	Operating Costs
SRC II Based	1	1	4	1	1
H-Coal Based	1	2	2	2	2
CSF Based	2	3	3	3	3
Fischer-Tropsch Based	1	4	1	4	4

These results indicate that, proceeding from the SRC II based configuration to Fischer-Tropsch in the above table:

- The products tend to become lighter and more highly refined.
- The capital investment and operating costs increase.
- The possible annual revenues and RPSP increase; the inversion of H-Coal based and CSF based is an exception to this generalization.
- The B/C ratio, an indicator of potential profitability, groups SRC II based, H-Coal Based and Fischer-Tropsch based technologies as equivalent, with CSF based having the lowest indicated B/C ratio.

Analysis in retrospect indicates that the Fischer-Tropsch configuration used for this study has the greatest potential for relative improvement among the candidates listed.

The economics of the Fischer-Tropsch based configuration used is most sensitive to SNG market value. At $2.25/MCF, its B/C ratio is lower than H-Coal and SRC II based, at $3.25 the three are equivalent, and at $4.25, Fischer-Tropsch based clearly shows the highest B/C (profitability).

Recognition of the critical effect of product composition on the comparative economics generated the objective to develop a correlation between product compositions and key economic parameters such as fixed capital investment, product market value and required product selling price. The results, considered significant, indicate that each of these parameters correlate well with the hydrogen to carbon (H/C) weight ratio of the products. The logic is that coal liquefaction essentially involves adding hydrogen to coal; coal has a H/C ratio of about 0.07, aromatic liquids such as benzene a ratio of approximately 0.08, aliphatic liquids such as heptane about 0.19, and SNG (methane) about 0.33. The addition of the hydrogen consumes added material such as coal and water plus requires additional equipment.

The correlations of H/C vis-a-vis economic parameters presented in Figures 8-1, 8-2, 8-3, and 8-4 in this report provide a unique contribution to the field of coal liquefaction as a direct result of our contractual work.

The H/C correlations also indicate that there is only a slight difference in the economics of the Fischer-Tropsch based plant and a SNG plant using similar gasification/gas purification procedures. This may be interpreted as confirmation that the costs of producing a purified mixture of carbon monoxide and hydrogen (syngas) dominates the economics of indirect liquefaction processes such as Fischer-Tropsch.

The process designs and economic evaluations developed here were alloted modest effort relative to that applied to more comprehensive conceptual designs by major contractors. In order to shed some light on the question of whether differing conclusions would have been reached if significantly more effort were applied, the results of conceptual designs/economic evaluations for SRC II, H-Coal, CSF and Fischer-Tropsch were compared. In this case, the SRC II based and Fischer-Tropsch based designs/economic evaluations were developed by one major contractor while the H-Coal based and CSF based units were developed by a second major contractor. The trends between designs/economics for the processes, when generated by the same contractor, were similar to those developed in this assessment.

Assessments and comparisons were also developed for two additional production plant sites and four marketing areas. Other production locations were the Appalachian Region of the Eastern Coal Province and the Powder River Region of the Rocky Mountain Province; Pittsburgh No. 8 seam coal and a sub-bituminous coal typical of a Wyoming location were used for feeds to these plants, respectively. To provide a basis for estimating transportation costs, the production plants were arbitrarily sited at New Athens, Illinois; Moundsville, West Virginia and Gillette, Wyoming; some site data was available for each of these locations based on the results of earlier studies. The marketing locations, defined by Oak Ridge National Laboratory, were Delaware, Chicago, Houston and San Francisco.

The most detailed work was done on the plant conceived to be located in Illinois; this is termed the "base case." The base case was then modified for the other two locations based primarily on differences in feed coal composition. The results indicate that the FCIs tend to be slightly lower in the Appalachian Region and 3-15% higher in the Rocky Mountain Region when compared with the base case. The RPSPs were similar for the Appalachian and base cases but were higher for the Rocky Mountain Region. Similar results were indicated for the B/C ratios.

Estimates were developed for transportation costs from the production sites to the indicated marketing areas; for the base case, these amounted to 3-6% of the plant F.O.B. RPSP with the lowest being for CSF and the highest Fischer-Tropsch. In general, transportation costs from the Appalachian Region to Dover, Delaware were approximately twice as great as the Interior Region and for Gillette, Wyoming to San Francisco, two-to-four times as great.

This study has looked closely at high potential candidates which are capable of supplying synfuels by 1990. The importance of development of a viable coal conversion capability in the U.S. requires that the analysis effort exemplified by this survey be continued and updated as new information becomes available.

As improvements are made in the liquefaction technologies, there is an incentive to maintain an active cross-fertilization program to minimize the time required to incorporate the improvements and/or problem solutions generated by one technology to other technologies also under development.

Details of the survey and assessment are contained in the following sections of this report.

Table 2-1 - Coal Feed and Product Summary
Base Case: Eastern Region of Interior Coal Province

Item	SRC II Based			H-Coal Based			CSF Based			F-T Based		
	TPD	BPSD (10^6 SCFD)	10^9 Btu/D	TPD	BPSD (10^6 SCFD)	10^9 Btu/D	TPD	BPSD (10^6 SCFD)	10^9 Btu/D	TPD	BPSD (10^6 SCFD)	10^9 Btu/D
Feed												
Coal	30,627		767.9	32,257		808.8	35,716		896.5	36,341		912.1
Products												
SNG	3,422	(140)	155.1	3,703	(155)	165.6	3,515	(135)	151.6	7,274	(325)	316.0
C_3-LPG	452	5,101	19.6	422	4,793	18.3	1,040	11,721	44.7			
C_4-LPG	218	2,133	9.3	114	1,117	4.9	278	2,476	11.9	1,186	11,751	50.7
Gasoline	1,379	10,337	55.5	2,941	21,965	118.1	2,822	20,973	113.6	4,643	37,536	197.0
Oxygenates										642	3,759	13.6
Distillate Fuel Oil No. 2										413	2,223	15.9
Distillate Fuel Oil No. 4				481	3,005	18.6	4,870	46,983	278.2			
Distillate Heavy Fuel Oil							3,219			168	1,076	6.8
Residual Fuel Oil	10,482	52,309	360.6	7,725	40,151	274.5						
By-Products												
Sulfur	987		7.9	1,074		8.6	1,201		9.6	1,228		9.8
NH_3	97		1.9	128		2.5	182		3.6			
Product Ratios												
Total Fuel Products												
MMM Btu/D		600			600			600			600	
MM Btu/ton of coal		19.6			18.6			16.8			16.5	
Liquid Products												
bbl/D		69,880			71,030			82,155			56,845	
bbl/ton of coal		2.3			2.2			2.3			1.6	

SECTION 3
SELECTION OF HIGH POTENTIAL PROCESSES

SECTION 3

SELECTION OF HIGH POTENTIAL PROCESSES

A prime objective of this study was to select a limited number of high potential coal liquefaction processes and then develop documented opinions regarding their rankings with regard to potential technical performance, pertinent economic factors, and product marketability. The selection of the high potential processes was accomplished by establishing selection criteria plus evaluation procedures to display the projected performance of the separate processes in comparison with the selection criteria. This section will describe the logic pattern used to select four high potential processes for more detailed analysis.

3.1 SELECTION PROCEDURES

Prior work under this contract had defined sixty-plus liquefaction process candidates and had reported the characteristics and development status of thirty-three of what were considered the most promising of the processes.[1] The processes were arbitrarily classified and given process numbers as follows:

1. Hydroliquefaction

  1.1 Direct, Non Catalytic

    1.1.1 Solvent Refined Coal (SRC-I)

    1.1.2 Solvent Refined Coal (SRC-II) (Pseudocatalytic)

    1.1.3 UOP Extraction

1.2 Direct, Catalytic

1.2.1 Gulf Catalytic Coal Liquids (CCL)

1.2.2 SYNTHOIL

1.2.3 H-Coal

1.2.4 Clean Fuel From Coal (CFFC)

1.2.5 CONOCO Zinc Halide Hydrocracking

1.3 Indirect, Donor Solvent

1.3.1 Exxon

1.3.2 ADL Extractive Coking

1.3.3 Consolidation Synthetic Fuel (CSF)

2. <u>Pyrolysis</u>

2.1 Direct

2.1.1 Char-Oil-Energy Development (COED-RMP)

2.1.2 Char-Oil-Energy Development (COED-FMC)

2.1.3 Occidental Research Corp. Coal Flash Pyrolysis

2.1.4 TOSCOAL

2.1.5 Lurgi-Ruhrgas

2.2 Hydrocarbonization

2.2.1 U.S. Steel Clean Coke

2.2.2 Coalcon

2.3 Rapid Hydrogenation

2.3.1 BNL Rotating Fluidized Bed

2.3.2 Short Residue Time (SRT) Hydropyrolysis

2.3.3 Intermediate Coal Hydrogenation

2.3.4 Schroeder's Rapid Hydrogenation

2.3.5 BNL Flash Hydropyrolysis

2.3.6 Rockwell Direct Coal Hydrogenation

3. <u>Indirect</u>

3.1 Fischer-Tropsch

3.1.1 Flame Sprayed Catalyst

3.1.2 ARGE

3.1.3 SYNTHOL

3.2 Indirect, Methanol

3.2.1 High Pressure Methanol

3.2.2 ICI LP/LT Methanol

3.2.3 Lurgi LP/LT Methanol

3.2.4 Three Phase Methanol Synthesis

3.3 Indirect, Other

3.3.1 M-Gasoline (Mobil)

4. <u>Miscellaneous</u>

4.1.1 Supercritical Gas Extraction (SGE)

4.1.2 British National Coal Board

Principle categories of this particular classification system are hydroliquefaction, pyrolysis and indirect liquefaction, with donor solvent processing classified as a subdivision of hydroliquefaction.

The procedure used to achieve the objective of selecting high potential processes from this list of thirty-three candidates is described in the following paragraphs.

A list of selection criteria elements is shown in Table 3-1. Key elements include:

- The successful candidates must be capable of commercialization by 1990.
- The processes are to be tested for their ability to produce a product slate typical of the fuel consumption patterns for each geographical area as shown in Table 3-2 using feed coal to the process plants with typical analyses as summarized in Table 3-3.
- High profitability and ecologically satisfactory.

- Definition of the candidate as a high potential process by assessment of multiple technical, economic, product characteristic and development status factors.

To accomplish the broad range technical/economic/status assessment described in the last criteria listed above, a detailed procedure was developed and implemented; details of the techniques used and the results are presented in Appendix A.

3.2 HIGH POTENTIAL CANDIDATES

Using the above criteria, the selection process was completed and the following four processes were chosen as high potential processes:

- SRC II; a pseudocatalytic hydroliquefaction process
- H-Coal; a catalytic hydroliquefaction process
- CSF; a donor solvent process
- FSC (Fischer-Tropsch using Flame Sprayed Catalyst); an indirect process to produce hydrocarbons.

The M-Gasoline process is not included in the above list of candidates but was however, evaluated because of special interest in the process and the high rating it obtained. The evaluation basis, established for another study, differed from that adapted for the above candidate list. The Mobil-M results are therefore presented separately for reference in Appendix C of this report.

The Exxon Donor Solvent process (EDS) was not included in the more detailed analyses because, as decided mutually with DOE, sufficient information was not available to us at the beginning of our work.

Table 3-1 - Selection Criteria for High Potential Processes

Criteria	Comment
1. Time Frame	Starting a commercial design in 1985 and start up in 1990
2. Product Slate	A product slate is selected based on product and energy profiles for each geographical area shown in Table 3-2
3. Maximum Profitability	—
4. Ecological Acceptability	—

Table 3-2 - Target Product Slate By Geographical Area

Item	Appalachian Region of Eastern Coal Province		Eastern Region of Interior Coal Province		Powder River Region of Rocky Mountain Coal Province	
	Btu/day (Billion)	(%)	Btu/day (Billion)	(%)	Btu/day (Billion)	(%)
SNG	171	28.5	269	44.8	202	33.7
LPG	15	2.5	11	1.8	13	2.2
Gasoline	106	17.7	182	30.3	183	30.4
Distillate Fuel Oil	125	20.9	106	17.7	111	18.5
Residual Fuel Oil	183	30.4	32	5.4	91	15.2
Total	600	100.0	600	100.0	600	100.0

Table 3-3 - Typical Feed Coal Analyses[a] By Coal Source Area

Item	Appalachian Region of Eastern Coal Province	Eastern Region of Interior Coal Province	Powder River Region of Rocky Mountain Coal Province[b]
Proximate Analysis wt (%)			
Volatile Matter	40.5	38.5	44.2
Fixed Carbon	49.5	51.7	45.1
Ash	7.3	7.1	8.0
Moisture	2.7	2.7	2.7
Total	100.0	100.0	100.0
Ultimate Analysis wt (%)			
Carbon	71.6	70.7	66.3
Hydrogen	5.0	4.7	4.7
Oxygen	7.7	10.3	16.3
Sulfur	4.4	3.4	0.8
Nitrogen	1.3	1.1	1.0
Moisture	2.7	2.7	2.7
Ash	7.3	7.1	8.0
Total	100.0	100.0	100.0
Gross Heating Value			
Btu/lb	12,640	12,550	11,211

[a]This is feed coal to Process Plant, cleaned and dried as necessary.
[b]Run of mine subbituminous coal from this area contains approximately 25% water and has a gross heating value of about 8,720 Btu/lb.