THE HYBRID PLANT CONCEPT: COMBINING DIRECT AND INDIRECT COAL LIQUEFACTION PROCESSES

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OBJECTIVE:

The objective of this study is to assess the technical and economic impacts of siting direct two-stage coal liquefaction and indirect liquefaction, using slurry Fischer-Tropsch (F-T) reactors, at the same location. The incentives for this cositing include the sharing of the large number of common unit process operations and the potential blending of the very different, but complementary, products from the two processes, thereby reducing the refining required to produce specification transportation fuels. Both direct and indirect coal liquefaction share a large number of unit operations. These include coal handling and preparation, coal gasification to produce synthesis gas or hydrogen, gas purification, ammonia, and sulfur recovery. Common offsites include an oxygen plant, waste water treatment facility, power generation equipment, fuel gas supply, cooling water towers, and other facilities.

The raw liquid products from two-stage direct liquefaction are predominantly aromatic in character, contain heteroatoms, and require substantial upgrading or refining to meet current transportation fuel specifications. The aromatic naphtha portion from direct liquefaction produces a high octane, high aromatic gasoline after hydrotreatment and reforming. The percentage of aromatics in this gasoline is high and would require blending with other feedstocks to be environmentally acceptable for possible future gasoline specifications. The middle distillate or diesel fraction from direct liquefaction requires substantial hydrotreatment to remove heteroatoms, especially nitrogen. The resulting hydrotreated product is predominantly naphthenic in character and can be hydrocracked to lower its end point to be compatible with diesel or jet fuel specifications.

For the raw indirect liquefaction products produced from slurry-phase F-T synthesis, the naphtha range material, after hydrotreatment to remove olefins, is almost totally paraffinic. Because of this, it is a poor feedstock for reforming and requires very severe reforming with low product yield of high octane gasoline. The diesel fraction from indirect, because of its total paraffinic character, produces an excellent diesel range material with a cetane number of over 70.

Thus, these raw materials from direct and indirect liquefaction have the potential to produce specification fuels with proper blending thereby greatly reducing the severity and amount of upgrading required.

This paper reports on the results of a study that attempts to quantify the extent of these potential synergisms by estimating the costs of transportation fuels produced by direct liquefaction, indirect liquefaction, and by a combined direct and indirect hybrid plant configuration under comparable conditions.

TECHNICAL APPROACH:

The technical approach used to accomplish the above objective was to combine the MITRE computer simulated coal liquefaction models for the direct and indirect systems into one integrated model. An analysis of refining and blending of the raw product streams to produce specification diesel and gasoline fuels was included in the direct, indirect, and hybrid models so that comparable product slates could be developed.

The components of the MITRE two-stage direct coal liquefaction model are shown in figure 1. This computerized simulation model has been under development for several years, and has undergone continual improvement and updating as additional data become available. As part of this improvement, the overall plant configuration has been significantly altered since its initial documentation.(1) The original UOP/SDC integrated two-stage plant design(2) initially used in the MITRE model has been updated to include Shell gasification for hydrogen production, Kerr-McGee ROSE-SR units for deashing, and a combined-cycle facility for on-site electric power generation. In addition, the two-stage coal liquefaction section of the model has been improved by simulating the coal dissolution and resid upgrading reactors using first-order lumped kinetics. These kinetics are used to determine the required space velocities and resulting reactor volumes for the required coal conversions to specific product distributions. For the purpose of this hybrid plant analysis, the direct model has been extended to include naphtha hydrotreatment, distillate hydrotreatment and hydrocracking, and naphtha reforming.

The components of the indirect model are shown in figure 2. The development and use of this model to investigate the economics of a base case plant have been previously documented.(3) In summary, the indirect plant conceptualized in the model is totally integrated from coal to products, and all power and energy requirements are generated within the plant. For the purpose of explanation, the plant can be considered as being divided into three main sections, although there is complete integration among these sections with respect to mass and energy flows. The first section simulates the preparation of clean synthesis gas. This is accomplished using Shell gasification of coal followed by shift of raw product gas, gas cooling and cleaning, and sulfur and ammonia recovery. The second section simulates the F-T synthesis. Slurry-phase synthesis units are used to produce the raw products. This section also simulates the raw F-T product separation, carbon dioxide removal, and hydrogen recovery. The third section simulates the raw F-T product refining to produce diesel, gasoline, and liquified petroleum gas (LPG). This section includes a refinery that alkylates light ends, hydrotreats the raw product, hydrocracks the F-T wax, and recovers the alcohols.

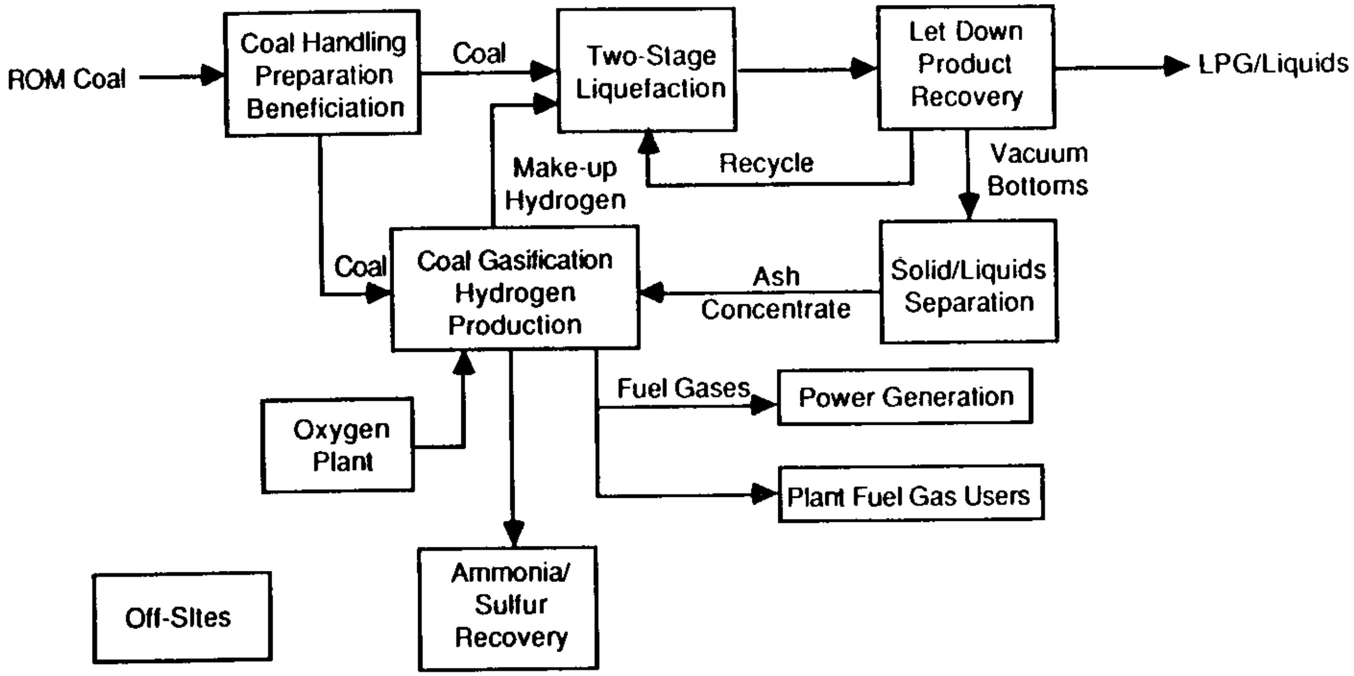


Figure 1
Components of MITRE
Direct Coal Liquefaction Model

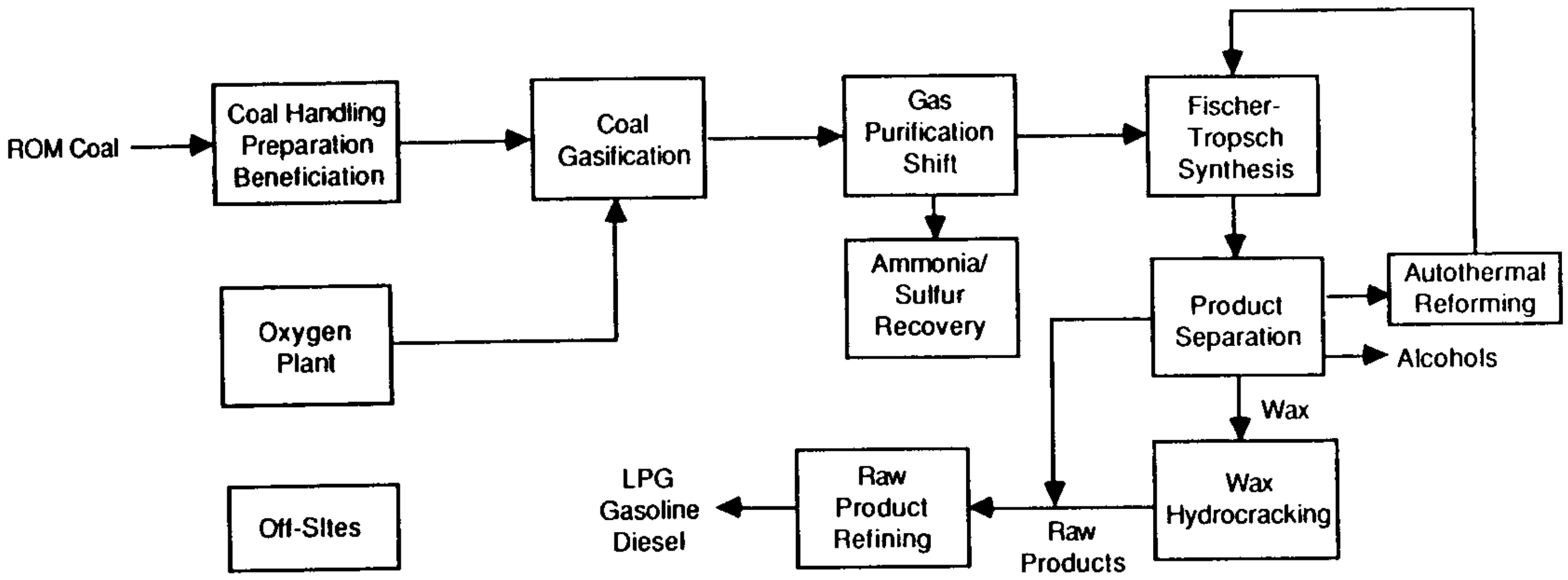


Figure 2
Components of MITRE
Indirect Coal Liquefaction Model

A complete utility balance is performed for all the unit operations in the indirect plant. Both high- and medium-pressure steam are generated from waste heat from the gasification, autothermal reforming, and F-T sections. The steam produced in these plant areas is more than sufficient to power the turbines for oxygen and electricity production, and for steam users throughout the plant.

In addition to the three main sections described above, the indirect model includes the necessary off-site supporting units. The major units are the oxygen plant for the gasification section, coal handling and drying, the cooling and boiler feed water systems, waste water treatment, power generation and distribution, F-T catalyst preparation, refrigeration, storage, and infrastructure.

The economic sections of both models provide estimates of the plant construction cost, total plant capital required, operating and maintenance costs, annual revenue required, and required selling prices (RSP) of the products. Total plant construction cost is estimated by using cost data of unit operations obtained from various open literature sources. The unit operation cost data are scaled based on capacity, adjusted to the reference calendar year, and summed to give the total cost of construction. Total capital is calculated from the construction cost by adding engineering design and contingency costs, and funds used during construction. Addition of the non-depreciable capital (start-up cost, working capital, and initial catalyst and chemical cost) gives the total capital required. Gross annual operating costs are calculated as the operating and maintenance expenses minus the by-product credits. The annual revenue required is the sum of the capital and operating cost components. The capital component is calculated from a discounted cash flow (DCF) analysis using specified financial parameters. The RSPs of the products are then calculated from the total plant product outputs and the annual revenue requirement.

To develop the hybrid plant simulation, the MITRE direct two-stage and indirect models were combined into an integrated plant configuration. There are many possible hybrid plant configurations that could be investigated. Figure 3 shows simple block schematics of two of these. In the upper schematic, the hydrogen required for the direct liquefaction process is recovered before the indirect F-T synthesis section. The lower schematic shows a configuration where the direct liquefaction hydrogen is recovered after F-T synthesis. The latter configuration has the advantage that a once-through F-T approach can be used with hydrogen being recovered from the F-T tail gas. This eliminates the need for recycle in the F-T synthesis loop. This paper reports on the detailed analysis of this latter type of configuration; detailed analysis of the former type will be undertaken at a later date.

Figure 4 shows a detailed block flow diagram of the hybrid plant configuration selected for detailed study in this analysis. In this configuration, 11 percent mineral matter Illinois #6 coal is used as feedstock to the plant. This coal is fed both to the direct liquefaction section and to the gasification section of the plant such that the resultant F-T tail gases contain sufficient hydrogen after synthesis to satisfy the two-stage liquefaction requirement and the total hydrogen requirement for the refinery. This coal split can be varied to produce a final product mix containing different

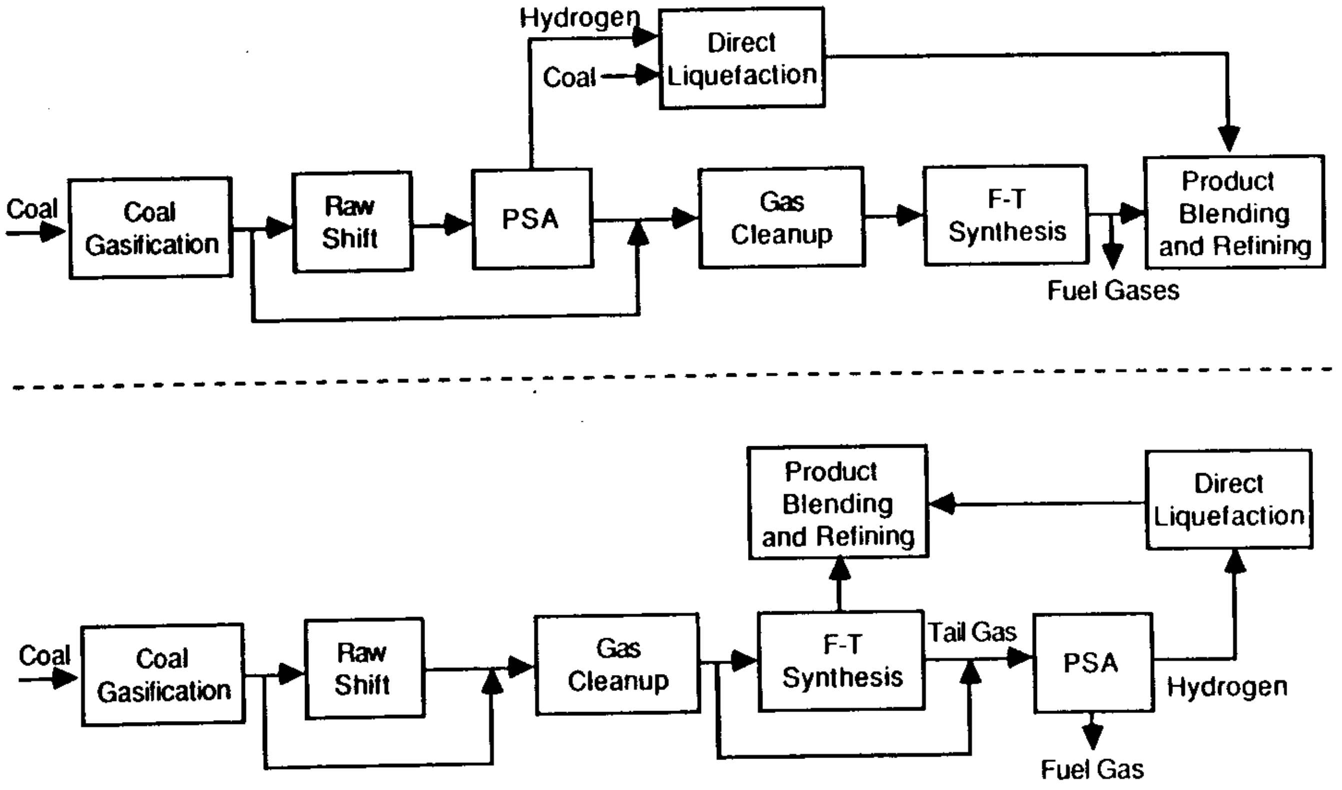


Figure 3
Possible Hybrid Plant Configurations

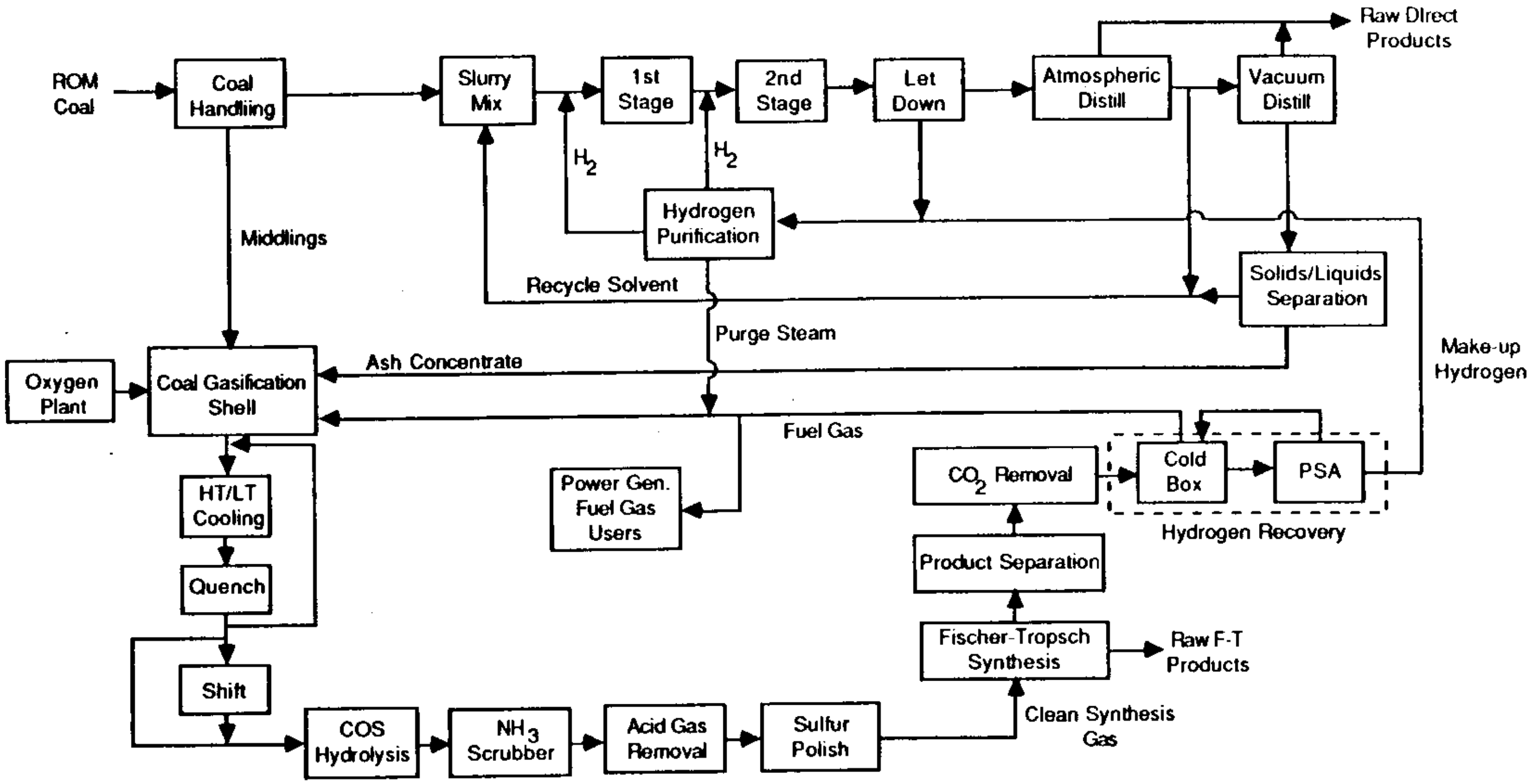


Figure 4
The Hybrid Plant Configuration
Block Flow Diagram

proportions of direct and indirect liquids. The hybrid case selected produces approximately 50 percent direct and 50 percent indirect products.

The Shell gasification section of the plant uses coal and ash concentrate from the ROSE-SR unit as feedstock, and sour fuel gas is used as transport gas for coal injection. The raw synthesis gas is cooled with recycle gas and enters waste heat boilers before quenching. High temperature and high pressure steam is raised from the exit gas sensible heat, and this steam is used to power the air and oxygen compressors. After shift and cleaning, the gas containing 0.06 ppm total sulfur is passed once through the slurry F-T reactors at a space velocity that results in a synthesis gas conversion of about 64 percent. This conversion level provides the correct product mix and residual hydrogen for direct liquefaction and refining. After product separation and carbon dioxide removal, the tail gas is passed to the hydrogen recovery system that consists of a cold box and pressure swing absorption (PSA) unit in tandem. This recovery system provides a 97 percent recovery of almost 100 percent pure hydrogen with less than 1 ppm carbon monoxide. The purge stream from hydrogen recovery is used as plant fuel gas and could be combusted in gas turbines for electric power generation in other hybrid plant configurations, if necessary. In this hybrid case, gas turbine generators are not necessary because of the large quantity of steam available in the plant from process waste heat sources.

The F-T section consists of slurry phase reactors containing precipitated iron catalysts. The activity of the catalyst is based on experimental data obtained by Kuo at Mobil during testing in their bubble column reactor.(4) The hydrocarbon selectivity produces approximately 50 weight percent wax. The details of this section have been described in an earlier MITRE report.(3)

The performance of the two-stage direct liquefaction portion of the hybrid plant is based on data obtained from Wilsonville run 257 using Illinois #6 coal. The performance is shown in figure 5 based on 100 lbs of MAF coal. Total C_4 - 850°F liquid yield is 71.15 percent of MAF coal with a soluble reject plus unconverted coal of 16.33 weight percent MAF coal.

The raw products from both direct and indirect liquefaction sections of the plant are further upgraded and blended to produce transportation fuels. A block flow schematic of this refinery scheme is shown in figure 6. For the direct product, the whole liquid is fractionated to produce a naphtha (C_4 - 350°F) fraction and a 350°F$^+$ distillate fraction. The naphtha fraction is hydrotreated to reduce heteratoms to acceptable levels for subsequent gasoline blending or reforming. Typically the resultant heteratom levels after hydrotreatment are nitrogen 0.6 ppm, sulfur 0.5 ppm, and oxygen 30 ppm.(5,6) This hydrotreated naphtha is then sent to the gasoline blending pool. The approximate chemical component analysis of this material is as follows: aromatics 17 volume percent, naphthenes 64 volume percent, and paraffins 19 volume percent.

The 350°F$^+$ distillate material from the two-stage direct liquefaction section is also hydrotreated to lower nitrogen to an acceptable level for hydrocracking (~0.5 ppm). After hydrotreatment, the distillate is hydrocracked to a recycle cut point of 450°F. The hydrocracked

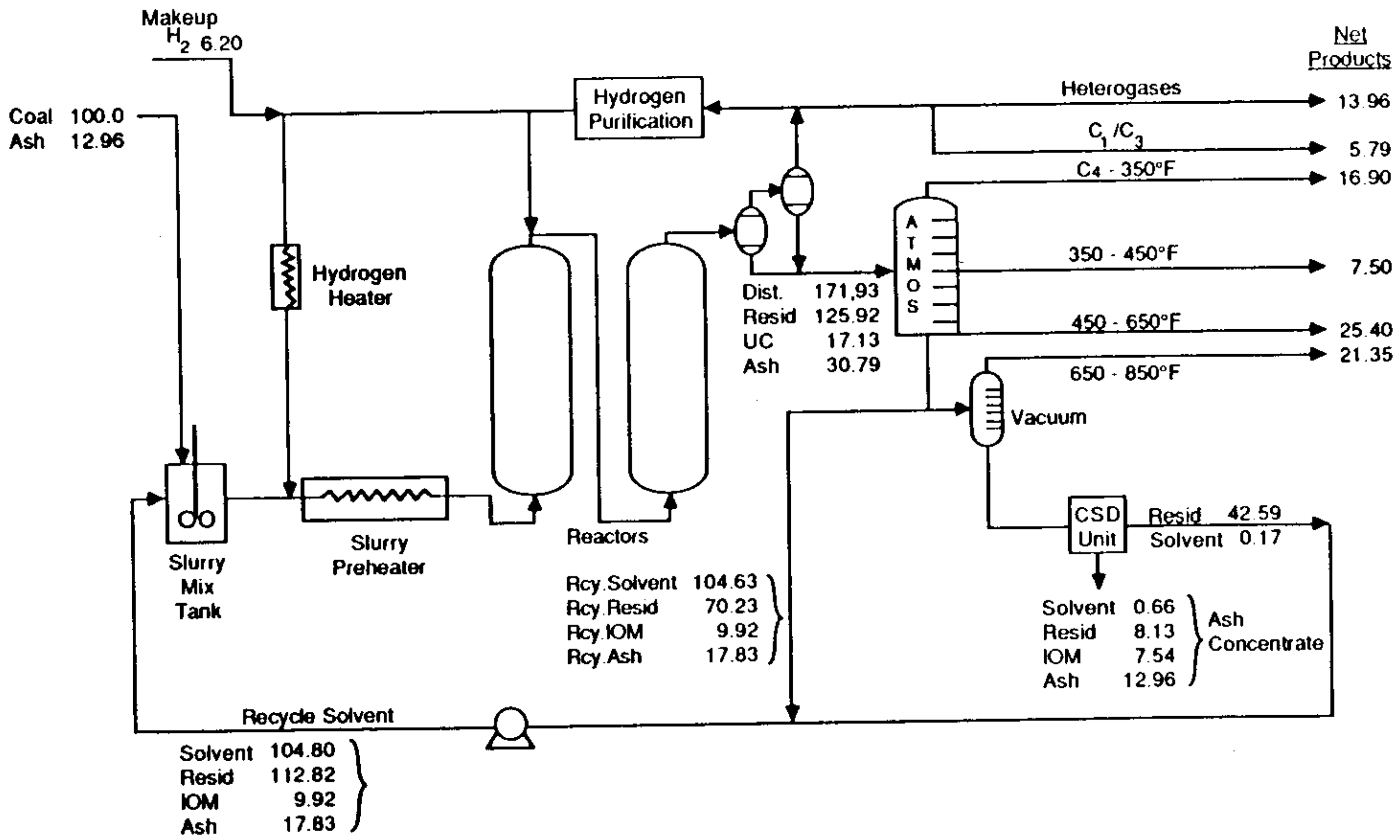


Figure 5
Hybrid Plant: Direct Liquefaction Section

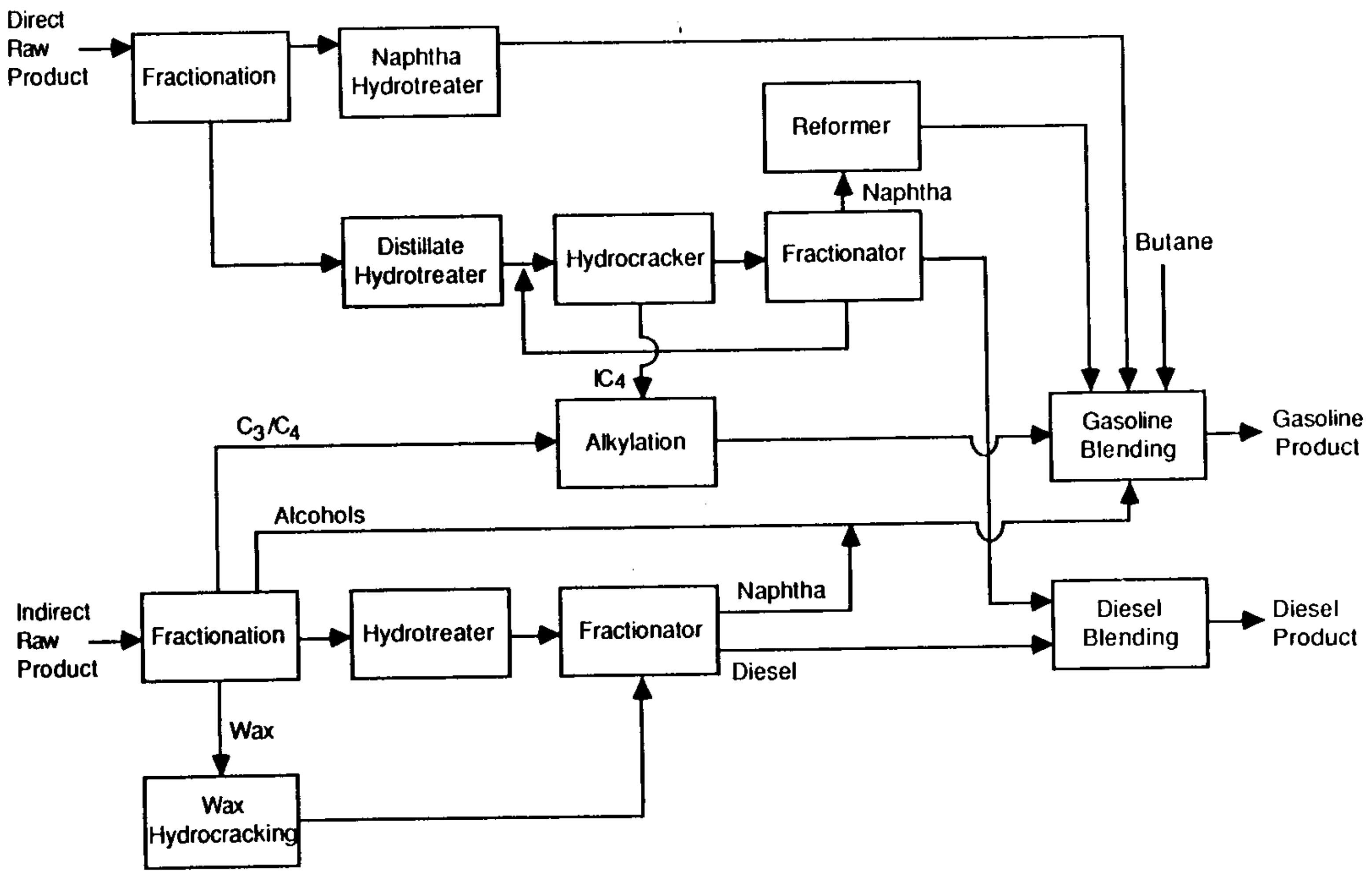


Figure 6
Hybrid Plant Product Refining

naphtha fraction is then reformed at low severity(6) and the reformate sent to gasoline blending. The 350 - 450°F diesel cut from the hydrocracker is sent to the diesel blending pool.

For the indirect raw products, the following refining scheme is used. The raw F-T liquid product is hydrotreated to remove olefins; it is then fractionated to produce a naphtha fraction that is directly blended into the gasoline pool and a distillate fraction for the diesel product. The F-T wax product is hydrocracked to produce naphtha and distillate. Yields and operating data for this operation were based on actual experimental runs performed by UOP on F-T wax.(7) This naphtha is blended directly as straight run material in the gasoline pool. The distillate is excellent high cetane paraffinic diesel and is blended in the diesel pool. Propane and butanes are sent to the alkylation unit together with isobutane from the direct distillate hydrocracker. The alkylate is sent to gasoline blending along with butanes and F-T alcohols to make the final gasoline blend product.

SIGNIFICANT ACCOMPLISHMENTS:

MITRE has totally integrated the direct and indirect liquefaction plant simulations and developed one hybrid plant configuration as illustrated in figure 4. A summary of this resulting configuration is shown in simple block flow schematic in figure 7. The total plant size is based on 100,000 barrels per stream day (BPSD) of total refined gasoline and diesel fuel. The coal input is 38,423 TPD moisture-free (MF) basis, and this coal is split so that 30 percent of it is sent to the direct liquefaction section. The remaining coal and ash concentrate is sent to the gasification section. The resulting clean synthesis gas is passed once through the slurry phase F-T reactors to produce raw F-T liquids, gases, and wax, and the tail gas is processed to recover make-up hydrogen for direct liquefaction. Figure 7 shows the rate of production of both raw and refined products from the plant. The raw products are refined as shown previously in figure 6. The configuration shown in figure 7 is essentially balanced with respect to plant fuel gas and hydrogen needs and only exports a small quantity of excess electric power for sale.

Table 1 shows the component blending for the final refined gasoline and diesel fuels from the hybrid plant. For the gasoline product, the blend is composed of six streams, two from the direct section of the plant and four from the indirect. The direct reformate, containing approximately 65 volume percent aromatics, accounts for 39 volume percent of the product. The direct straight run naphtha (from the naphtha hydrotreater), containing approximately 15 percent aromatics and 75 percent naphthenes, makes up 19 volume percent. The indirect contributions include the paraffinic straight run F-T naphtha that comes from both wax hydrocracking and raw product hydrotreatment, the alkylate from alkylation of the C_3/C_4 olefins and isobutane, the alcohols, and some of the butane. The diesel product consists of the direct hydrocracked distillate containing about 5 percent aromatics, and the paraffinic indirect distillate. This consists of a C_{12} - C_{18} fraction and a heavier C_{19}^+ fraction from the wax hydrocracker. The total aromatics content of the blended gasoline is estimated to be about 32 percent and only about 2 percent for the blended diesel.

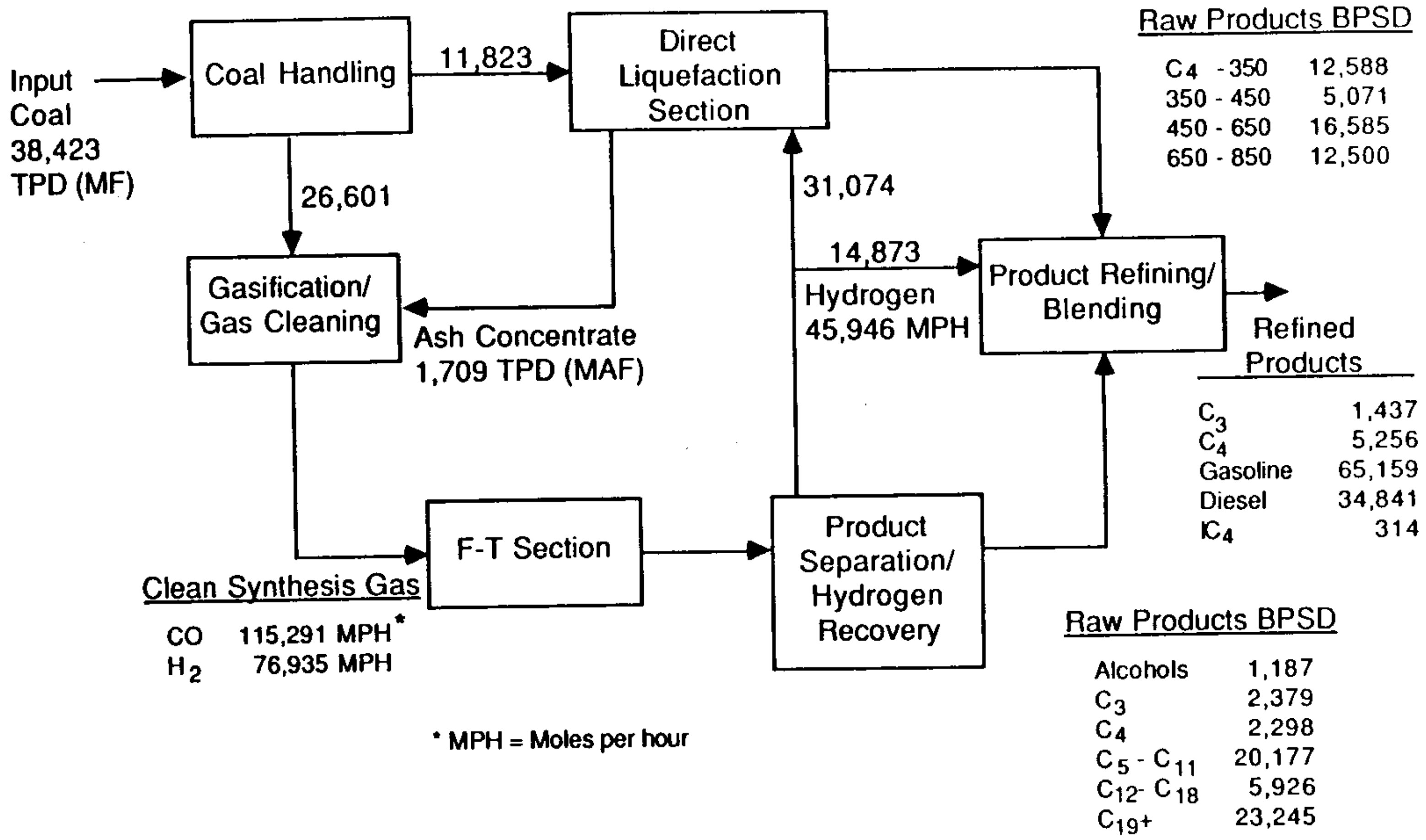


Figure 7
The Hybrid Plant Configuration
Block Flow Schematic

Table 1
Hybrid Plant: Product Components

Gasoline Blending Pool

	BPSD	Volume Percent
Direct Reformate	25,710	39.5
Direct Stream Naphtha	12,610	19.4
Straight Run F-T	20,510	31.5
Alkylate	4,220	6.5
Alcohols	1,190	1.8
Butanes	930	1.4

Diesel Blending Pool

	BPSD	Volume Percent
Direct Diesel	10,860	31.2
Indirect C_{12} - C_{18}	16,760	48.1
Indirect C_{19}^{+}	7,220	20.7

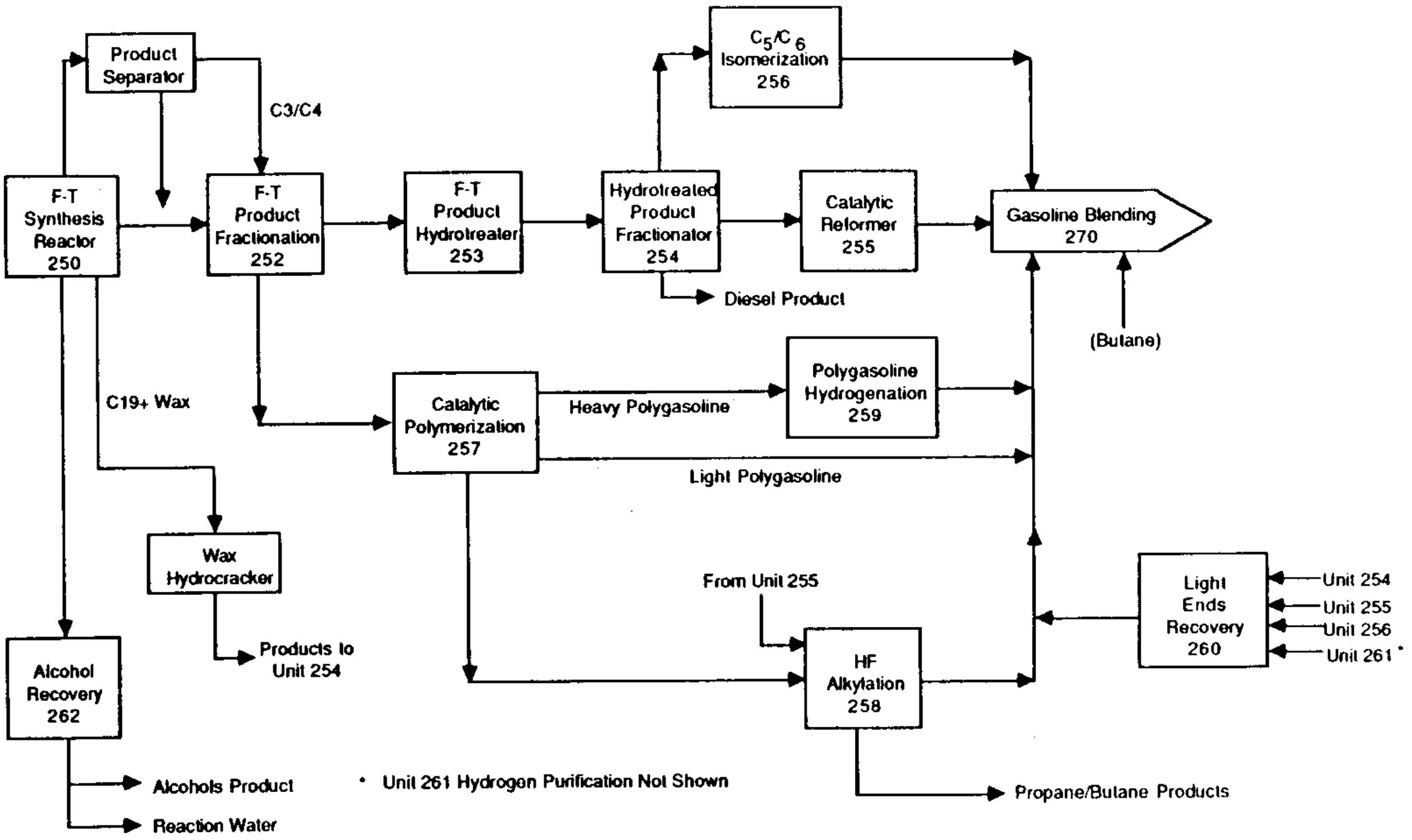
For comparative purposes, a direct liquefaction-only plant of comparable size was also analyzed for the same coal feedstock. This direct plant produced 100,000 BPSD of gasoline and diesel fuel from 39,171 TPD (MF basis) of Illinois #6 coal. The liquefaction performance was also based on Wilsonville run 257, just as in the hybrid plant case. This conceptual plant included the identical upgrading of raw products as used in the hybrid plant for the direct liquids. The resulting gasoline was estimated to contain approximately 33 volume percent aromatics and the diesel fraction approximately 5 volume percent.

An indirect-only F-T plant that produced 100,000 BPSD of gasoline, diesel, and alcohols from 45,207 TPD (MF basis) of Illinos #6 coal was also simulated. This plant produced raw F-T products that were refined as shown in figure 8. This refining scheme was used by Mobil(8) in their F-T plant study and by MITRE(3) in the development of their indirect liquefaction base case plant. This additional refining of the raw F-T products was necessary to produce specification gasoline and diesel fuels. The resulting gasoline contained approximately 29 percent aromatics.(8)

The comparative results of the analyses of these three plants are summarized in table 2. Capital costs for the plants, including refining, vary by about 12 percent; operating costs vary by about the same percentage. The RSPs of products were calculated from the annual revenue required by assuming identical financial assumptions of 75 : 25 debt to equity, 15 percent return on equity, 8 percent interest on debt, 3 percent general inflation, and an income tax rate of 34 percent. The RSP of gasoline and diesel (assumed to be equal in price on a volume basis) for the hybrid plant is about the same as for the direct plant. The hybrid plant results in a 7 percent decrease in gasoline and diesel cost compared to the stand-alone indirect plant. Equipment costs for gasifiers, F-T reactors, and direct liquefaction ebullated bed reactors were scaled using a 0.9 exponent factor, while other equipment and offsites were scaled using a 0.7 exponent. Because of the low single pass conversion required for the F-T section of the hybrid plant, the number of slurry reactors has been reduced by about 60 percent compared to the indirect stand-alone case.

Although the hybrid plant does not appear to result in any substantial cost savings with respect to the final cost of gasoline and diesel compared to a stand-alone direct liquefaction plant, it can produce products more cheaply than a stand-alone indirect plant and does allow an enormous flexibility in product slate and product characteristics that cannot be achieved by each technology separately. In addition, the hybrid plant has the potential to produce fungible, high-quality transportation fuels by refining and blending on-site. This is more difficult to achieve by direct liquefaction alone because of the high aromatic character of the products. For indirect liquefaction, specification fuels can be produced after extensive refining. Thus, the hybrid plant has the potential to produce transportation fuels that can probably meet or exceed the environmentally-driven specifications of the future.

An important aspect of the overall utility of the hybrid plant concept is the potential to blend the products after minimal refining. This analysis has relied on refining data of direct coal liquids that were performed many years ago on feedstocks that are different in quality from those currently



* Unit 261 Hydrogen Purification Not Shown

Figure 8
Raw Fishcher-Tropsch Product Refining

Table 2
Overall Summary of Results

	Hybrid	Direct	Indirect
Coal Input TPD MF			
Liquefaction	11,823	22,708	0
Gasification	26,601	16,463	45,207
Total	38,424	39,171	45,207
Refined Products BPSD			
Propane	1,437	2,076	5,777
Butane	5,256	0	7,635
I-Butane	314	4,569	2,680 (Alcohols)
Gasoline	65,159	79,200	45,280
Diesel	34,841	20,800	52,035
Estimated Product Characteristics*			
Percent Aromatics	32/2	33/5	29/0
Percent Alcohols	1.86/0	0/0	0/0
Percent Butanes	1.14/0	3.0/0	3/0
Density Lbs/Bbl	269/272	279/289	249/275
Overall Thermal Efficiency HHV Basis	65.0	63.2	56.4
Economic Data ($1989)			
Total Capital (MM)	5,987	5,808	6,592
Coal Cost (MM)	324	330	376
Other Operating (MM)	355	388	396
Required Selling Price $/bbl			
LPG/I-Butane	18.07	18.19	19.79
Gasoline	47.56	47.87	51.25
Diesel	47.56	47.87	51.25
Equivalent Crude	37.56	37.85	41.07

*The first number refers to gasoline and the second to diesel.

produced at Wilsonville and Hydrocarbon Research Inc. (HRI). This earlier refining work performed by Chevron and UOP demonstrated that direct coal liquids could be upgraded to specification transportation fuels under fairly severe conditions of space velocity and hydrogen pressure (2,000 - 2,500 psi). The heavier fractions (700°F$^+$) of the liquids did present difficulties, but upgrading tests were often performed after the liquids had been stored for long periods. Current liquids may be easier to upgrade using lower pressures.

In these earlier upgrading studies, some important data on the characteristics of the refined products are missing. These are properties that determine engine performance, like octane and cetane numbers. Also, no attempts have been made experimentally to blend direct and indirect liquids to produce specification fuels. Therefore the blend characteristics in this study are based on volumetric percentages of chemical compound types when the characteristics of the blend components are known. Although this study attempts to simulate blends that are suitable for gasoline and diesel applications, in the absence of experimental data, it is not feasible to estimate specific octane and cetane values, and thus how these blends will perform in actual engines.

Because of these important data gaps, it is recommended that research on the refining and blending of current direct and indirect liquids be pursued to determine the optimum upgrading required for production of fuels. Also, characterization of these refined blends should include determination of properties that effect actual engine performance and suitability as fuels. An experimental program to determine the refining requirements and compatibilities of these blends is essential to demonstrate that coal-derived fuels have an important role to play in providing future high-quality transportation fuels.

PUBLICATIONS AND PRESENTATIONS:

A presentation describing the methodology used to investigate the hybrid plant and its potential technical impact was given at the AIChE Summer National Meeting, August 19-22, 1990, in San Diego, CA.

ACKNOWLEDGEMENT:

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