

## USE OF A REFINERY LP MODEL TO DETERMINE VALUE OF COAL DERIVED LIQUID

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### INTRODUCTION

Conversion of coal to a synthetic liquid product has been studied experimentally for a number of years. Because such processes appear to be moving closer to commercial reality, the economics of these processes have received more emphasis in recent years. One of the major problems in determining the economics of coal conversion processes involves settling on a value for the coal-derived liquid. In some economic studies a price has been estimated for this liquid based solely on the cost of producing it, including an arbitrary profit. Other studies, on the other hand, have tried to estimate a value for the coal-derived liquid on the basis of one or more inherent properties, or have used a somewhat arbitrary value.

In actual practice, however, the value of a feed stock to a refinery depends primarily upon the value of the products which can be made from it and the costs of processing to make such products. In the case of coal-derived materials, which have unusual characteristics compared to most crude oils, this is believed to be the most realistic method of estimating its value. This paper reports the results of such calculations made for a liquid produced in a conceptual coal conversion complex utilizing several experimental processes now being developed under sponsorship of the Office of Coal Research, U.S. Department of the Interior.

### SOURCE OF COAL DERIVED LIQUID

This complex which produces the coal-derived liquid has been designated a COG (Coal, Oil, Gas) Refinery, since the two major products it produces from coal are the liquid feedstock to a petroleum refinery and a high BTU synthetic natural gas. The primary conversion step of this complex utilizes the Pittsburg & Midway Coal Mining Co's Solvent Refined Coal (SRC) process. Chem Systems has recently completed an economic evaluation of this complex for P&M.

An overall flowsheet for the COG Refinery is shown in Figure 1. The following processing steps are included:

- **SRC Process** - This is the primary coal conversion step where coal is dissolved in the presence of a process solvent and hydrogen at high temperatures (~825°F) and pressures (~1000 psia). The reaction product is filtered to yield solvent refined coal, a low sulfur de-ashed product. Filter cake, containing undissolved coal and ash is sent to the gasification section. A light oil, C<sub>5</sub>-450°F and gases, C<sub>1</sub>-C<sub>4</sub>, are also produced in the SRC process.

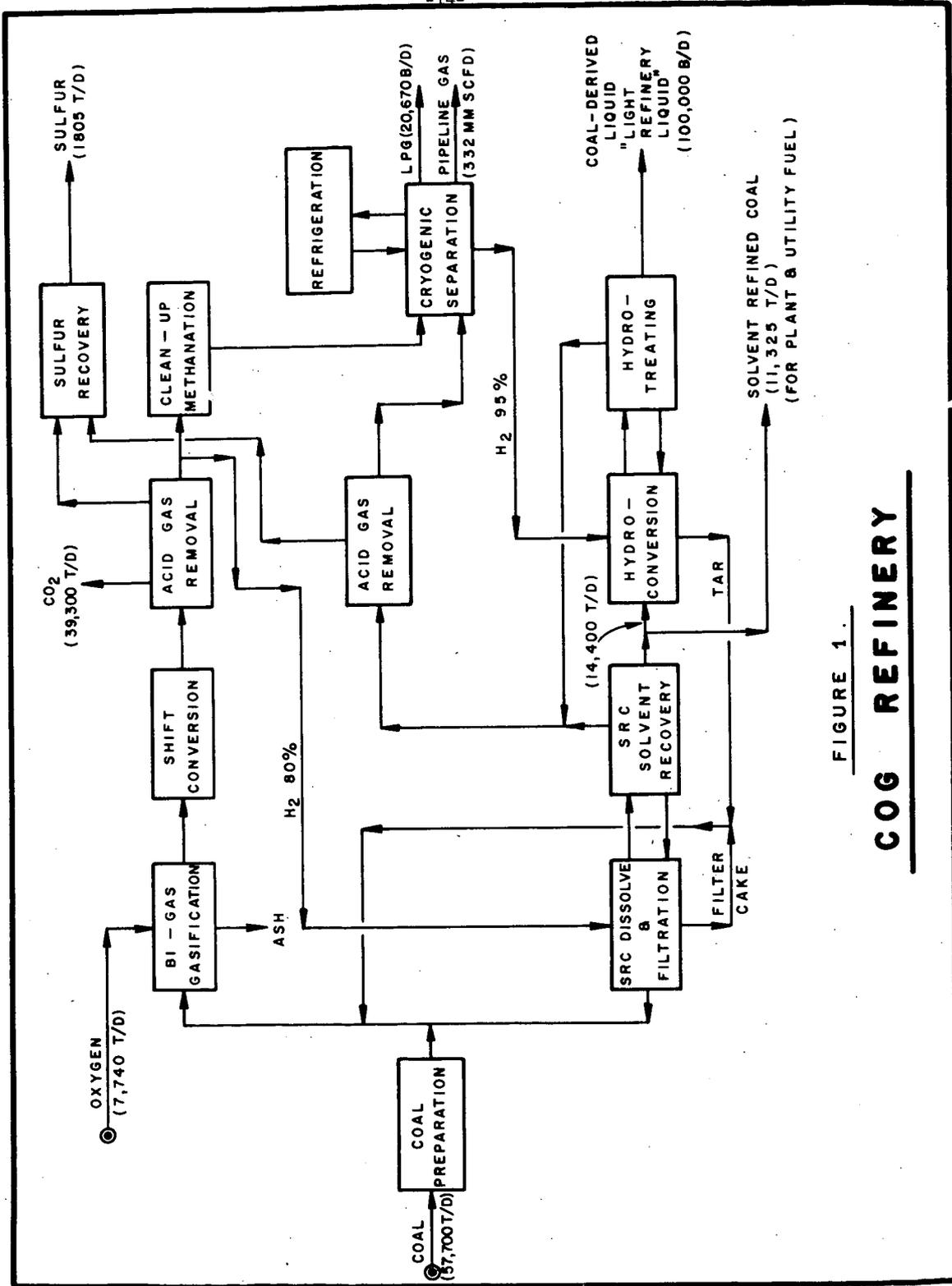


FIGURE 1.

# COG REFINERY

- Hydroconversion and Hydrotreating - These processes upgrade the solvent refined coal and light oil produced in the SRC process to the coal-derived liquid product.
- Bi-Gas Process - This is Bituminous Coal Research's coal gasification process and produces synthesis gas and methane directly from coal. This stream, after downstream purification steps, supplies the hydrogen requirements of the COG Refinery.
- Shift Conversion - This process shifts the CO in the Bi-Gas reactor effluent with steam to produce hydrogen.
- Acid Gas Absorption - Conventional hot potassium carbonate processes are employed to remove CO<sub>2</sub> and H<sub>2</sub>S from both the Bi-Gas effluent and the off-gases recovered from other sections of the COG Refinery. The bulk of the CO<sub>2</sub>, containing less than 5 ppm H<sub>2</sub>S, is vented to the atmosphere. All the hydrogen sulfide with the rest of the CO<sub>2</sub> is sent to a sulfur recovery unit. A portion of this purified stream (approximately 80% H<sub>2</sub>) is sent directly to the SRC process.
- Clean-Up Methanation - This process removes the residual CO from shift conversion to meet pipeline gas specifications.
- Cryogenic Separation - This low temperature separation is required to produce a 95% H<sub>2</sub> stream for hydroconversion and hydrotreating. Methane is recovered here as the pipeline gas product. LPG produced in various sections of the COG Refinery is also recovered in this section.

As seen from Figure 1, the high BTU pipeline gas consists of methane generated in the Bi-Gas and SRC processes and methane made in subsequent downstream processing steps.

The hydrotreated liquid product represents the material that will be fed to a petroleum refinery. Approximately 70% comes from hydrocracking and hydrotreating the solvent refined coal, while the remaining 30% comes from hydrotreating the light oil produced in the SRC process. The SRC process has been evaluated in the laboratory and plans are underway for a pilot plant. The design bases for the hydrocracking and hydrotreating steps have been estimated based on previous work on similar materials. The liquid product from the hydroconversion section is a 750°F end point material. The product obtained after hydrotreating is a C<sub>5</sub>-650°F distillate with an 35° API gravity. This hydrotreated liquid product obtained from the COG Refinery represents a relatively light material for feed to a petroleum refinery. Because of these properties, this coal-derived liquid has been designated as "light refinery liquid".

The above describes how this liquid has been derived from the coal conversion processes making up the COG Refinery. The conceptual nature of the COG Refinery has been described and will be referred to later when the properties of the light refinery liquid and the way in which it will be treated in a refinery will be discussed in more detail. Before getting to that, however, it is appropriate now to discuss the approach used in the evaluation of this liquid as refinery feedstock.

#### APPROACH

The approach used in this study has been to determine the parity value of the light refinery liquid to a refiner compared to a standard crude. Since the objective of a refiner is to make profit, he would be willing to buy and process coal liquid as long as the properties of the coal liquid allowed him to operate as profitably as he could by processing crude oil. By determining the return on investment for a crude oil refinery, and fixing that return for a coal liquid refinery, the value of the light refinery liquid can be calculated.

In addition to comparing all crude oil and all coal liquid refineries, the evaluation also determined the effect of running mixtures of natural crude and coal liquid. This was done to see if there might be synergistic effects when processing mixtures.

### LP MODEL

The analysis was performed using Chem Systems' refinery linear program (LP) computer model. The model considers the investment and operating costs associated with each of the process units which can be included in a new refinery. It makes the economic decision as to which units are to be included in the refinery, the raw material allocation among all of the process units and product blends, the operating severity of each process unit, and the optimum market slate from the refinery. The model performs an objective analysis of each problem, determining the most profitable solution available within the constraints placed on the problem.

A linear program is a technique for finding the optimum solution to a series of linear equations for which there are more variables than equations e.g., an infinite set of possible solutions. In this case, the optimum solution is the one which yields the most profitable operation for a specified set of marketing, feedstock and economic conditions. Certain variables are specified, such as capacity or feedstock, and other variables, such as operating severity levels, allocation of intermediate process streams, etc. are examined to find the solution which produces the maximum profit.

The refinery situation chosen for the evaluation is typical for the U.S. The total refinery throughput was fixed at 100,000 BPCD to avoid problems with plant size and investment factors and to match the total coal liquid output from the COG Refinery. The process units, raw materials and product specifications considered by the refinery LP for each case are indicated in Table 1.

TABLE 1  
PROCESS UNITS CONSIDERED FOR THE REFINERY

Atmospheric Crude Distillation  
Vacuum Crude Distillation  
Naphtha Unifiner  
Catalytic Reformer  
Catalytic Cracker  
Distillate Hydrocracker  
Alkylation  
Isomerization  
Gas Oil Desulfurization  
Kerosine Desulfurization  
Hydrogen Generation

### RAW MATERIAL SPECIFICATIONS

Southwest Louisiana Crude Oil	\$3.50/Bbl.
Light Refinery Liquid	Price to be Determined
Normal Butane	\$3.00/Bbl.
Iso Butane	\$3.25/Bbl.

Total quantity of crude and coal liquid, 100,000 BPCD, Mixture varied in steps from All Crude to All Light Refinery Liquid

PRODUCT SPECIFICATIONS

	<u>Quantity</u>	<u>Value</u> <u>\$/Bbl.</u>
Gasoline Pool - 93 RON Unleaded	50,000 Min, 60,000 Max.	5.50
LPG	Unrestricted	2.83
Number 2 Heating Oil	Unrestricted	4.75
Number 6 Heating Oil	Unrestricted	3.50
Refinery Fuel Gas (FOE)	Unrestricted	3.80

The product specifications applied equally to all cases, and the reason for the limits on gasoline production was to avoid the possibility of results so widely different as to prevent meaningful comparison. The 93 RON clear specification on the gasoline pool is typical of what might be expected by 1980 when the COG Refinery would be constructed. All feed and product prices, investment, etc. are on a 1971 basis.

Before proceeding with the computer runs, certain decisions had to be made concerning the processing options available for the light refinery liquid.

PROPERTIES AND DISPOSITION OF LIGHT REFINERY LIQUID

Figure 2 shows a typical refinery configuration for feeding the coal liquid. Basically three cuts would be taken from the crude distillation unit:

- A C<sub>5</sub>-180°F cut would go either to an isomerization unit or directly to gasoline blending.
- A 180-375°F cut would go to a catalytic reforming unit for upgrading into high octane gasoline.
- A 375-650°F cut would go either to a distillate hydrocracking unit or directly to the No. 2 fuel oil pool. The hydrocracking unit would produce a light naphtha for gasoline blending and a heavy naphtha for additional feed to the catalytic reformer. Previous work<sup>(1)</sup> on treating coal derived liquid in a refinery has indicated that hydrocracking rather than catalytic cracking should be employed to process this gas-oil cut.

Properties of each of the above cuts have been estimated and are shown in Table 2.

TABLE 2

INSPECTIONS ON LIGHT REFINERY LIQUID

	<u>C<sub>5</sub>-180°F</u>	<u>Fraction</u> <u>180-375°F</u>	<u>375-650°F</u>
Vol %	7.1	37.7	55.2
Wt. %	5.4	36.3	58.3
Gravity, °API	90	43	28
Sulfur, ppm	Nil	10	100
Nitrogen, ppm	100	200	700
Oxygen, ppm	50	200	400
P	50	20	6
O	-	-	-
N	47	65	57
A	3	15	37

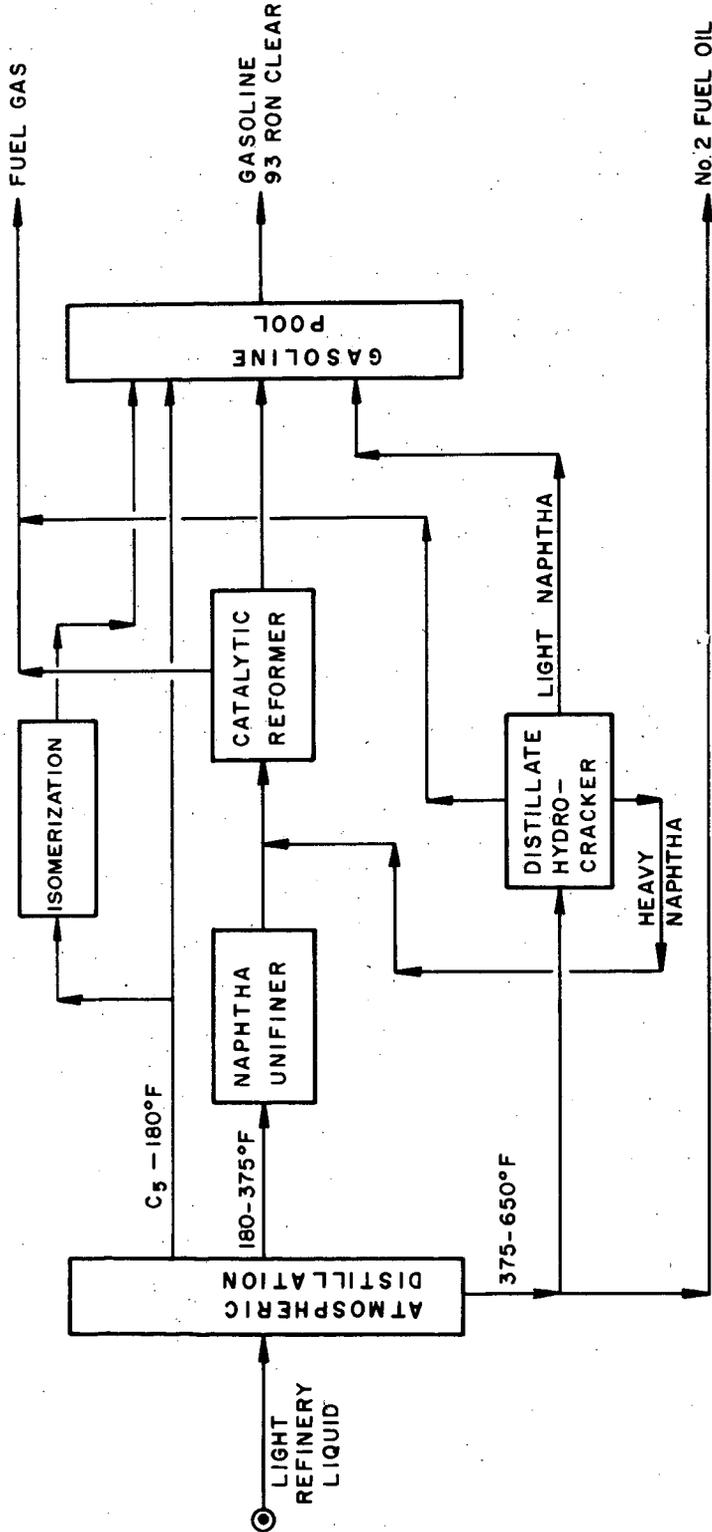


FIGURE 2.

# REFINERY PROCESSING COAL LIQUID

For comparison purposes, a typical refinery flowsheet for the all crude oil case is shown in Figure 3. As mentioned previously, cases have been considered for various mixtures of the two feeds. In those situations, the LP model has the option of selecting the optimum flowsheet configuration considering all the processing units shown in Figures 2 and 3.

### DEVELOPMENT OF DATA

In order for the LP model to function, certain basic process data had to be generated, such as yields, investments and operating costs as a function of capacity for the catalytic reforming and hydrocracking units operating on the cuts from the light refinery liquid. Once developed, this data was incorporated into the basic LP data package so that the model could use it as required in determining the optimum configuration for each case considered.

Since the COG Refinery is a conceptual design, light refinery liquid has not been produced. Therefore, there is no commercial or even laboratory data available for conventional processes feeding this liquid. However, previous work has been done on similar coal-derived liquids. Chem Systems reviewed the work done by UOP on the synthetic crude produced from the bench scale research program on the Consol Synthetic Fuel Process. Additionally licensors of commercial reforming and hydrocracking processes were sent the feed properties denoted in Table 2 for their evaluation. These sources together with Chem Systems background on refinery operations have been used to estimate the necessary data for the individual processing units.

#### Catalytic Reforming

As seen from Table 2 the 180-375°F feed to this unit is highly naphthenic, ca. 65%. To attain high unleaded octane levels (95-102) simple dehydrogenation of the naphthenes to aromatics is sufficient. Very little cyclization or hydrocracking of paraffins would be required. This results in both a relatively simple plant and high C<sub>5</sub><sup>+</sup> reformate yield. Yields, investments and operating costs have been estimated for various severity levels of reformer operation, ranging from octane numbers of 95 to 102 for the C<sub>5</sub><sup>+</sup> reformate. Because the heteroatom content of the 180-375°F cut is relatively high, a pre-hydro-treating step is necessary for reforming processes that employ a noble metal catalyst. This is accomplished in the Naphtha Unifier as shown in Figure 2.

#### Hydrocracking

This is a conventional petroleum refining process that converts low quality middle and heavy distillates into gasoline, jet fuel and high quality middle distillates. There has been some experimental work done by UOP in a pilot scale Isomax unit utilizing a feedstock obtained from Consol's bench-scale extract hydro operations<sup>(2)</sup>. The properties of Consol's feedstock are comparable to the properties of the 375-650°F cut obtained from the light refinery liquid. Their results have been used as a guide in estimating yields and operating costs for the hydrocracking unit.

The light naphtha product (C<sub>5</sub>-180°F) from the hydrocracker has a clear octane number of approximately 82 and is sent directly to the gasoline pool. The heavy naphtha product, 180 to 375°F, has a clear octane rating of approximately 63 and therefore must be further up-graded before entering the gasoline pool. It is sent directly to the Catalytic Reformer, bypassing the Naphtha Unifier since the heteroatoms have been removed in the hydro-cracking operation.

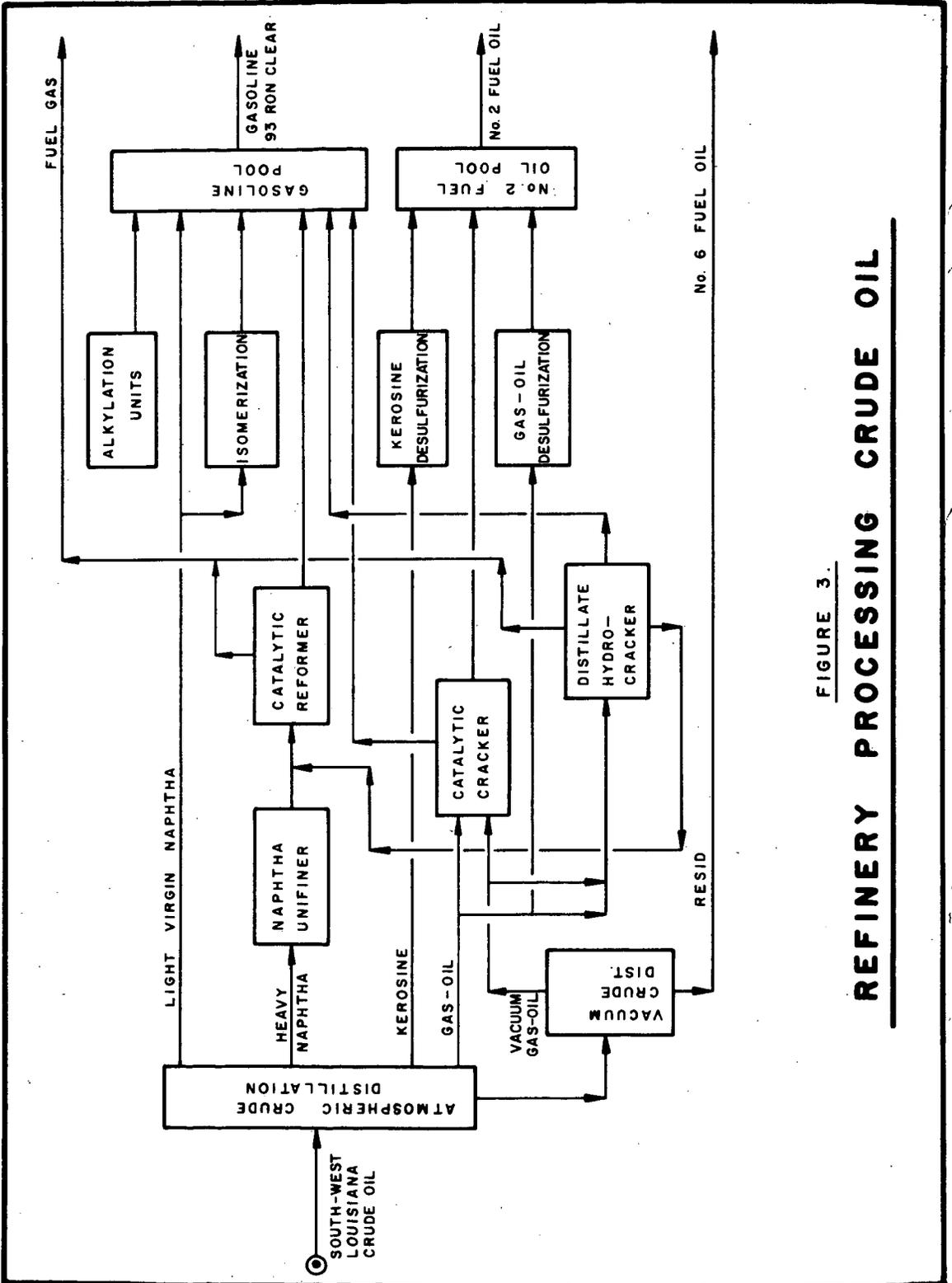


FIGURE 3.

# REFINERY PROCESSING CRUDE OIL

### CALCULATED VALUE OF COAL LIQUID

The value of the coal-derived liquid has been determined for four different ratios of coal liquid to Southwest Louisiana crude. From the basic refinery LP model the return on investment has been calculated for feeding 100% Southwest Louisiana crude at \$3.50/Bbl. The value of the coal liquid then was determined which would give the same profitability as the basic crude case. Coal liquid is used to supplement Southwest Louisiana crude in percentages of 25%, 50%, 80% and 100%.

The results are summarized in Table 3. As seen, the value of the coal liquid ranges from \$4.30-\$5.07 per barrel with the highest value at 25% coal liquid. The value of the coal liquid as a function of feedstock ratio is shown in Figure 4. This chart indicates that the coal liquid has a higher value as a supplement to crude than when refined alone.

It can also be observed that one of the major effects of adding a coal liquid is to decrease the overall investment required for the refinery. The investment decreases from \$92,100,000 for the 100% crude to only \$66,100,000 for the 100% coal liquid. This reduction in investment results since there are fewer processing units required for the all coal liquid case than with the all crude oil case. Since the coal liquid has no fraction suitable for catalytic cracking, the capacity of this unit decreases to zero as the quantity of light refinery liquid is increased to 100%. The same is true for vacuum distillation since the coal liquid contains no residue. The yield of No. 6 fuel oil is decreased substantially, of course, but at the same time the more valuable No. 2 fuel oil yield is increased. Furthermore, the high octane of the coal liquid reformat means that alkylation and isomerization units are not required to satisfy the gasoline pool octane requirement as more light refinery liquid is fed to the refinery. The overall effect of these changes is to increase the overall yield of products from the refinery and to decrease both the investment and operating costs. These advantages explain why the coal liquid has a higher value than that of Southwest Louisiana crude.

### SYNERGISTIC EFFECTS

The dramatic change in the value of light refinery liquid with the changing mix of crude oil and coal liquid can be explained by examining the gasoline pool. For the all crude case it is costly to the refiner to make 93 RON unleaded gasoline, and anything which relieves the difficulty is valuable to the refinery. Since the light refinery liquid is highly naphthenic, it produces a high octane reformat which is desirable for blending into the gasoline pool. Case II, (25% coal liquid) takes full advantage of this material by blending off the high octane components with reformat from the Southwest Louisiana naphtha. Since this minimizes yield losses from reforming of the straight run naphtha, the value of the coal liquid is increased proportionately. There is a definite economic advantage in converting most of the coal liquid to gasoline. With only a small amount of coal liquid in the crude mix, essentially all of it is converted to gasoline. Cases III, IV, and V fail to take full advantage of the tremendous potential of the coal liquid to produce gasoline since more and more of it must be used in No. 2 fuel oil to fulfill the product requirements. Since this is a less attractive use for it, the calculated value of the coal liquid decreases.

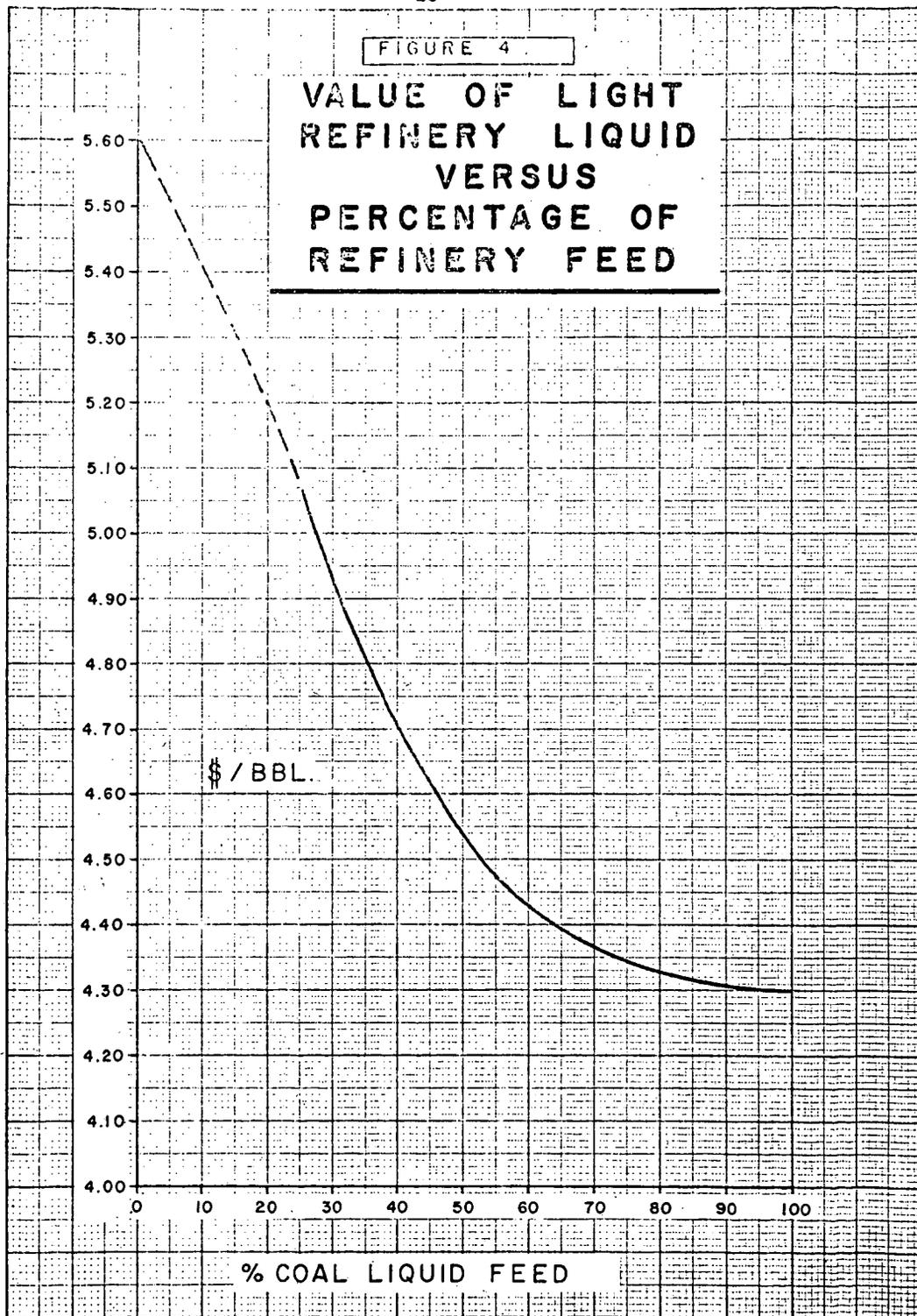
**TABLE 3**  
**Light Refinery Liquid Evaluation**  
**Summary of Results - 100,000 BPCD - Feedrate**

Refinery Investment	Value	Case I		Case II		Case III		Case IV		Case V	
		MB/CD	M\$/CD	MB/CD	M\$/CD	MB/CD	M\$/CD	MB/CD	M\$/CD	MB/CD	M\$/CD
			\$92,100,000		\$82,400,000		\$81,400,000		\$72,200,000		\$66,100,000
Raw Materials											
Southwest Louisiana Crude	\$3.50/BBL.	100.0	\$350.0	75.0	\$262.5	50.0	\$175.0	20.0	\$ 70.0	-	-
Light Refinery Liquid	calc.	-	-	25.0	126.5 <sup>(1)</sup>	50.0	226.56 <sup>(1)</sup>	80.0	346.56 <sup>(1)</sup>	100.0	\$429.65 <sup>(1)</sup>
N-Butane	\$3.00/BBL.	2.0	6.5	2.74	8.2	3.5	10.62	4.1	12.30	4.6	13.88
Total Raw Material Costs			356.5		397.2		412.18		428.86		443.53
Other Operating Costs			51.16		44.83		45.13		43.08		41.70
Total Production Cost			\$407.66		\$442.03		\$457.31		\$472.04		\$485.23
Products											
Refinery Fuel Gas, FOE	\$3.80/BBL.	4.15	15.78	4.15	15.78	3.82	14.53	1.87	7.09	0.28	1.05
LPG	2.83/BBL.	6.43	18.20	4.72	13.36	4.64	13.12	4.44	12.56	3.92	11.10
Unleaded Gasoline	5.50/BBL.	60.00	330.00	60.00	330.00	60.00	330.00	60.00	330.00	60.00	330.00
Heating Oil No. 2	4.75/BBL.	17.54	83.32	30.74	146.02	36.67	174.21	39.69	188.54	43.03	214.48
Heating Oil No. 6	3.50/BBL.	13.11	45.90	3.81	13.35	0.27	0.96	0.96	0.80	-	-
Product Revenues			\$493.20		\$518.51		\$532.82		\$538.99		\$546.63
Total Production Cost			407.66		442.03		457.31		472.04		485.23
Net Income Before Taxes			\$ 85.54		\$ 76.48		\$ 75.51		\$ 66.95		\$ 61.40
Value - Light Refinery Liquid	\$/BBL.	-		5.07		4.54		4.33		4.30	

Notes: (1) Determined by setting the same return of investment for all cases.

FIGURE 4

VALUE OF LIGHT  
REFINERY LIQUID  
VERSUS  
PERCENTAGE OF  
REFINERY FEED



As the net octane required from the processing of crude decreases, the value of incremental barrels of high octane blend stock also decreases. This change continues until the refinery becomes a predominantly coal liquid refinery, when the value of the coal liquid reformat and the coal liquid itself stabilizes. Due to the gasoline pool effect, the additive value of mixing coal liquid with crude can be expected to increase with an increase in the required pool octane value. The clear octane used in the study is 93 RON clear; however, values up to 95 RON clear or higher are being discussed and projected for the 1980 gasoline pool.

### POTENTIAL VARIATIONS IN COAL LIQUID VALUE

The above results illustrate that coal-derived liquid can be a very valuable feedstock to a petroleum refinery even in comparison to a good quality feedstock such as Southwest Louisiana crude. Even though this study indicates that the value of the coal liquid is greatest when it is used to supplement crude oil in a petroleum refinery, it is significant that an all coal liquid refinery would save approximately \$25,000,000 in investment over a conventional refinery. This would have economic advantages if the petroleum refinery were included as part of the COG Refinery.

This study was made for a typical refinery in the Kentucky-Illinois area but even a typical refinery does not adequately illustrate the full extent of benefits available by supplementing crude oil with coal liquid. Several examples are discussed below to indicate how the value of the coal liquid would be greater if different bases were used for the LP comparisons.

One obvious case is that with a refinery making more than 60% gasoline. The LP in all cases indicates that there is incentive to relax the restriction on gasoline yield. According to the LP calculations the total profitability for the refinery would be increased in all cases by increasing the gasoline yield, but the increase in profitability would be greater for the coal liquid cases.

A second example would be to permit the refinery LP model to make some chemicals rather than all fuels. It is known that there are considerable quantities of benzene, toluene and xylenes in the reformates produced from the coal liquid. The presence of significant quantities of aromatics has been confirmed by other investigations. If these materials were recovered as chemicals, the profitability of the refinery would be greater in all cases but would be increased more significantly when coal liquid was used. Thus, production of benzene, toluene and xylene from the refinery should significantly increase the calculated value of the coal liquid.

A third case would be to compare the coal liquid against a different type of crude oil. Much of the value of the coal liquid is due to the high yields of high octane reformates. This characteristic makes the coal liquid very valuable even with a high cyclic content feed material such as Southwest Louisiana crude. With a crude having a lower cyclic content in the naphtha boiling range the coal liquid would become even more valuable.

It is recognized that the calculated value of the coal liquid is somewhat dependent on the assumed value of the crude oil it replaces. For example, if the crude oil were available at no cost the calculated value of the coal liquid would be very low. On the other hand if the assumed value were higher than \$3.50 per barrel the coal liquid would have a greater calculated value. Even though transportation costs were considered, the \$3.50/Bbl for Southwest Louisiana crude may actually be higher for a location in the Kentucky-Illinois area. The assumed value of the crude affects the overall profitability but does not affect the refinery configuration or the schedule of products.

The assumed prices for products also have a significant effect on the calculated value of the coal liquids. Unlike changes in the crude price, however, the product prices can have a significant effect on the refinery configuration and the product slate. Sensitivity evaluation of the effect of product prices would require additional optimization studies which are beyond the intended scope of this project.

In addition to its high cyclic content, one of the most significant features of the coal-derived liquid is its low sulfur content (less than 0.01%). Since there is a shortage of low-sulfur fuels of all types, the alternate use of this material directly as a fuel rather than as a refinery feedstock should also be considered. In the Kentucky-Illinois area residual fuel of less than 1% sulfur sells for \$4.62 per barrel<sup>(3)</sup>. Therefore after a simple distillation to remove light ends, the light refinery liquid could be sold directly as a fuel and should be worth at least \$4.62. It would appear that under the current assumptions a refinery could afford to pay this price for the coal liquid only if it represents less than half of the total refinery feed. Thus, it is likely that the coal liquid would be sold in some cases as a low-sulfur fuel oil. If sold as a fuel oil, however, there would really be no advantage in producing such a low-boiling material. This would allow the investment for the COG Refinery to be decreased and thereby increase its profitability. This means that a complete optimization study would have to include the entire COG Refinery. While it is an interesting possibility, it is well beyond the scope of this work. The important point here is that there would be some competition between a refinery and industrial fuel uses for the liquid produced in a COG Refinery.

#### SUMMARY

The results of this study clearly show that compared to \$3.50 per barrel for Southwest Louisiana crude oil, the value of the light refinery liquid produced from a COG Refinery varied from \$4.30 to \$5.07 per barrel depending upon the relative amounts of crude oil and coal liquid fed to the refinery. Even though the highest value is calculated when the coal-derived liquid is used to supplement the crude oil, it offers significant investment savings when used as the sole feedstock to the refinery. The basis selected for this study are felt to be conservative and it is probable that other equally reasonable cases would have yielded an even higher value for the light refinery liquid.

- (1) PROJECT COED, U.S. Government Contract 14-01-001-498, Hydrotreating Studies - Part II - Appendix IX.
- (2) Project Gasoline Pre Pilot Plant Phase I Research on CSF Process, Vol. II., Part II.
- (3) Oil & Gas Journal, Vol. 69, No. 45, (Nov. 8, 1971).