

CHEMICALS FROM COAL

Interim Report

for

USBM SYNTHOIL

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## ABSTRACT

This document contains the results of an investigation to determine the suitability of the USBM Synthoils Product as a petrochemical feedstock. A sample of the whole crude was distilled into two straight run fractions; 350-650°F mid-distillate and 650°F+ residue. Laboratory studies in metal reactors and computer and mathematical simulations were performed to provide overall material balance data for a conceptual plant. The mid-distillate was hydrocracked to produce naphtha which was further processed by hydrotreating and reforming. The reformate from the mid-distillate was then mathematically hydrodealkylated to convert it to a product slate consisting of methane, LPG's, benzene, and fuel, along with the total hydrogen consumed. The value of the products obtained per 100 pounds of mid-distillate was \$6.89. The high aromatic yield obtained from the hydrocrackate naphtha makes this fraction very attractive as a petrochemical feedstock. Because the gas oil would be extremely difficult to process, it was not investigated.

## SUMMARY

The data presented herein was obtained from processing studies on a sample of USBM Synthoil Product under contract with the United States Energy Research and Development Administration. The experimental work was done in the Hydrocarbons and Energy Research Laboratory of The Dow Chemical Company in Midland, Michigan. Included in this report is the data from laboratory inspections using hydro-processing operations on one fraction distilled from the Synthoil whole crude. A sample of the whole crude was distilled into two straight run fractions, whose boiling range and elemental composition are listed in Table 1.

TABLE 1

### BOILING RANGE AND ELEMENTAL COMPOSITION OF SYNTHOIL STRAIGHT RUN FRACTIONS

	A-2 MID- DISTILLATE 350-650°F	A-4 RESIDUE 650°F +
WT. % OF CRUDE	34.0	66.0
API GRAVITY, 60°F	10.5	--
ELEMENTAL COMPOSITION		
C wt. %	86.3	--
H wt. %	9.3	--
O ppm	33000	--
N ppm	7400	--
S ppm	2800	--

### BOILING RANGE, OF

IBP	359	--
10 wt. %	425	--
20 wt. %	462	--
30 wt. %	489	--
40 wt. %	515	--
50 wt. %	542	--
60 wt. %	569	--
70 wt. %	596	--
80 wt. %	622	--
90 wt. %	653	--

The straight run mid-distillate was hydrocracked over Harshaw HT-400 E cobalt molybdenum catalyst. This catalyst was chosen for its neutral alumina support and its resistance to deactivation by nitrogen, oxygen, and sulfur in the feed. A higher ratio of normal/iso paraffins was also expected from this catalyst. Operating conditions of 1500-2500 psig and 920-950°F with LHSV's of 0.62 to 1.47 were surveyed. The naphtha created from hydrocracking the mid-distillate was distilled off and the unconverted mid-distillate was hydrocracked a second time. Nominal requirements for 60% conversion to C<sub>1</sub>-C<sub>9</sub> were 2500 psig, 941°F, and 0.75 LHSV.

The combined naphthas from two-pass hydrocracking the straight run mid-distillate were hydrotreated over Cyanamid Aeroform® HDS-9A nickel molybdenum catalyst. This catalyst was chosen for its resistance to deactivation by heteroatoms in the feed and for its superior activity for denitrogenation. Sulfur was reduced from 30 to 1 ppm, oxygen from 5100 to 80 ppm, and nitrogen from 50 to 9 ppm in the hydrotreating step.

The hydrotreated hydrocrackate naphtha was reformed over Cyanamid Aeroform® PHF-4 platinum chloride catalyst. This catalyst was chosen as a typical example of a readily available bifunctional reforming catalyst. At 500 psig and 964°F, the hydrocrackate naphtha was reformed with a first day conversion of 95.3%. After 70 hours, the naphthene conversion was still at 92.6%.

In addition to the hydroprocessing studies, the mid-distillate was subjected to mathematical recycle hydrocracking to naphtha, hydrotreating, reforming, and hydrodealkylation (HDA). As a result, this fraction was converted to methane, LPG's, benzene, and liquid fuel and the hydrogen required was also calculated. From this data, presented in Table 2, the value of the fraction was determined.



TABLE 2

PRODUCT PATTERNS AND VALUE FOR  
SYNTHOIL STRAIGHT RUN FRACTIONS

	<u>STRAIGHT RUN MID-DISTILLATE 350-650°F</u>
Processing Sequence	Recycle Hydrocrack
	Hydrotreat
	Reform
	HDA
PRODUCT PATTERN, Wt. %	
HYDROGEN	-7.9
METHANE	19.1
LPG	47.6
BENZENE	33.1
LIQUID FUEL	3.2
VALUE/100 lb DISTILLATE (1980)	\$6.89

Based on the yield data calculated for the mid-distillate fraction and the wt. % of the fraction from distillation, a mass balance for a conceptual plant operating on 100.00 lb/hr Synthoil whole crude was calculated. With the flow rates and compositions of key streams known, the preliminary estimate for capital requirements and operating costs could be made. The 34.0 lb/hr straight run mid-distillate was recycle hydrocracked mathematically, consuming 2.18 lb/hr hydrogen and producing 2.10 lb/hr methane, 10.06 lb/hr LPG's and 22.35 lb/hr naphtha. The hydrocrackate naphtha, 22.35 lb/hr, was hydrotreated mathematically, consuming 0.07 lb/hr hydrogen and producing 1.75 lb/hr gas. The hydrotreated naphtha was then reformed, producing 0.32 lb/hr hydrogen, 0.92 lb/hr gas and 19.39 lb/hr reformate. An in house mathematical model for hydrodealkylation was used to convert the reformate to 4.25 lb/hr methane, 3.54 lb/hr ethane, 11.26 lb/hr benzene, and 1.12 lb/hr liquid fuel, while consuming 0.74 lb/hr hydrogen. With hydrogen needs met by converting part of the methane to hydrogen in an oil fired methane reformer, overall yields from the conceptual plant in pounds per 100 pounds of crude are presented in Table 3.

TABLE 3

OVERALL YIELD FROM CONCEPTUAL PLANT USING  
SYNTHOIL WHOLE CRUDE AS FEEDSTOCK

Yield, lb/100 lb crude

Methane	0.96
LPG's	16.02
42.13 wt. % ethane	
23.47 wt. % propane	
22.72 wt. % butanes	normal/iso = 5.7
11.73 wt. % pentanes	normal/iso = 1.5
Benzene	11.26
Fuel (HDA)	1.12 (no allowance for plant fuel)
Residue	66.00

## PART I - EXPERIMENTAL

### Introduction

An increasing awareness of the energy crisis now facing the United States has prompted many to seriously consider the status of our fossil fuel resources and the factors shaping their future use patterns. The current situation with respect to gas and oil is worsening rapidly. Not only has there been a serious reduction of gas found to that which is used, the amount used is consistently greater than that produced. Similarly, oil production has been much less than the amount consumed. The deficit has been made up through increased imports which have compromised the independence of the country. In contrast, coal is the resource with the distinct advantage of long-term availability. It is also the resource with the highest sulfur and ash content, and the most difficult transportation requirements. Despite the problems associated with coal, it becomes clear that its availability warrants the development of schemes for prompt, optimum usage. It is not a question of development for chemical or energy needs but a necessity that both needs be met. In the "crisis" atmosphere related to energy, the dependence of petrochemical requirements on fossil fuels is commonly overlooked since these feedstocks currently comprise a relatively small percentage of total resource consumption. It is apparent, however, that hydrocarbon feedstock demands will continue to rise, putting increased pressure on already short supplies. Although social, political, and economic factors may alter the timing of a considerable shift in the use pattern of remaining supplies of fossil fuels, some conclusions can still be reached. Domestic oil and gas supplies will not meet future chemicals demands for hydrocarbons, let alone handle the larger energy needs. Coal, the largest single hydrocarbon resource left, must therefore be developed for future chemicals production needs as a supplement to current coal-to-clean-energy development activities. It was with this in mind that The Dow Chemical Company proposed, and was subsequently granted, a contract by the United States Energy Research and Development Administration (ERDA), to evaluate coal derived liquid products as petrochemical feedstocks.

As stated in the ERDA Contract, the purpose of this research effort was to study the feasibility of using coal liquefaction products for the production of chemicals, with the following work objective:

To estimate preliminary capital requirements and operating costs for a commercial plant which would use coal liquefaction products for the production of useful aliphatic and aromatic compounds.

In order to limit the scope of this investigation to a manageable size, certain boundary conditions were established prior to the beginning of experimental work. The large quantities of aromatic and saturated cyclic compounds found in coal derived liquids suggested that, with appropriate choices in hydroprocessing operations, high yields of benzene should be obtained. Furthermore, if the aliphatic by-products from benzene production could be directed toward normal paraffins, useful olefins might also be produced to supplement the benzene value. It was decided that since this was a preliminary study, it would be limited to using "standard" hydroprocessing operations. No attempts were made to recover or further process the tar acids and bases present in these materials. This program was also limited to the use of only readily available commercial catalysts. It was not anticipated that the data generated from this research effort would be capable of being used to scale-up to commercialization in a single step. Rather, the plan was to produce laboratory data that could be reduced to a form where it would be useful in predicting the behavior of the material as it would exist in the commercial process and therefore form the basis for comparing various liquefaction products. As a final step in satisfying the objective of this contract, this data would provide the overall mass, elemental, and componential information needed to make a preliminary estimate of the capital investment and operating costs for a commercial plant.

#### Liquefaction Product

The sample of Synthoil subjected to the hydroprocessing experiments was produced in the Pittsburgh Energy Research Center from West Virginia Coal. The source was Pittsburgh seam from the Ireland Mine. The oil was made using the nominal 1/2-ton/day unit with a 14.5 foot long catalytic reactor. Conditions were 4000 psig, 842°F, feeding 35 percent solid slurry in lined-out, coal-derived oil at 25 lb per hour. The catalyst was 1/8" pellets of cobalt molybdenum on silica alumina, Harshaw No. 0402T. The process product yield, based on dry coal, is estimated at 59.3% by weight. The material had an API Gravity of approximately 0° at 60°F, had a viscosity of 30 SSU at 180°F, contained about 40% asphaltenes, and about 50% had a boiling range between 350 and 850°F.

An attempt was made to hydrogenate the full range Synthoil with a Cobalt-Moly on alumina catalyst. The objective was to reduce molecular weight (boiling range). Little conversion of Synthoil was obtained at 2000 psig and 860°F. No net mid-distillate was produced. Asphaltene conversion was 37%.

#### Processing Approach

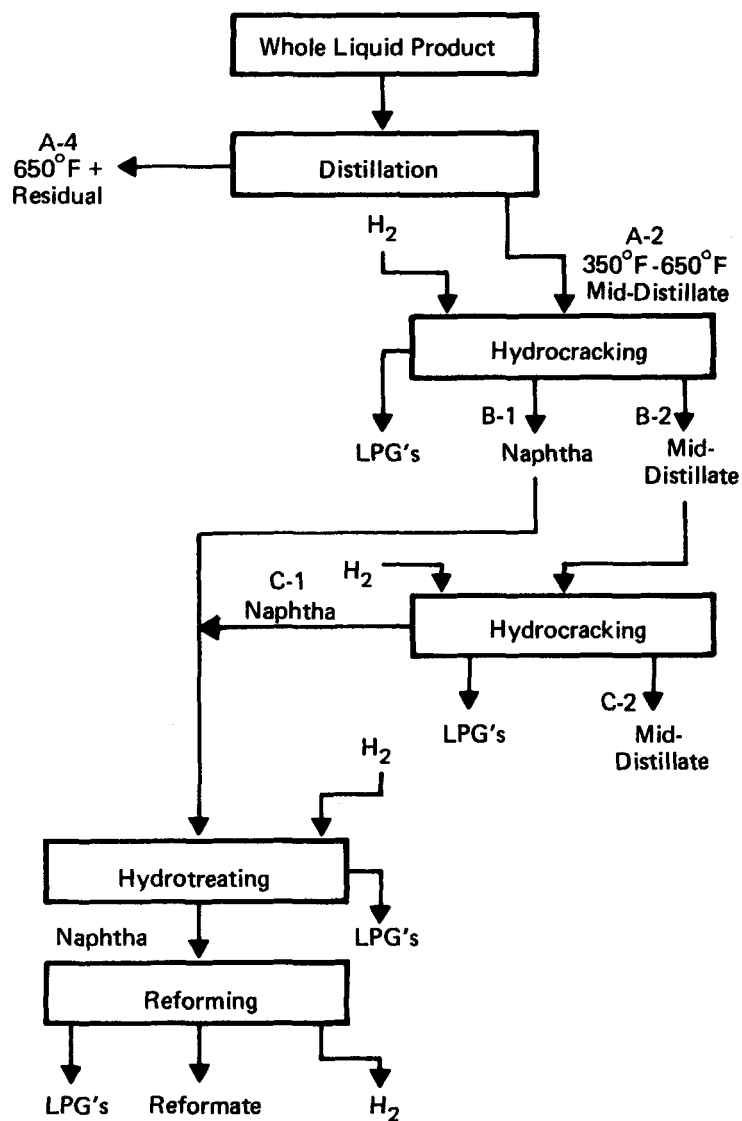
In order to parallel existing processing technology for producing petrochemicals from crude oil, the following processing sequence was followed for the USBM Synthoil:

- 1) Distillation into nominally two cuts --  
A-2 350°F-650°F (straight run mid-distillate)  
A-4 650°F-Plus (residue)
- 2) Hydrocracking of the mid-distillate to produce naphtha with some LPG's.
- 3) Hydrotreating of the hydrocrackate naphtha to remove the heteroatoms.
- 4) Reforming of the hydrotreated naphtha to produce maximum yields of aromatics.

These steps are shown schematically in Figure 1 and discussed sequentially below.

Distillations were carried out in a 72 liter Podbielniak® Fractioneer A batch distillation unit, instrumented to operate unattended. This still is capable of operating at pressures from 10mm Hg to atmospheric and temperatures up to 350°C.

Figure 1  
PROCESSING SEQUENCE



The three hydroprocessing steps were carried out in three similar reactors. The nominal 1 inch diameter tubular stainless steel reactors were operated continuously in<sub>3</sub> downflow with a fixed catalyst bed varying from 50 to 200 cm<sup>3</sup> in volume. Pressures up to 3000 psi, at 1300°F are attainable with these units. Either of two feed reservoir systems, one an unheated 1 gallon plastic bottle set upon scales and the other a heated 5 gallon tank equipped with a bubbler level indicator, provided a constant feed supply to a metering pump. The liquid product collected from the reactors was weighed periodically. Both hydrogen and vent gas flow rates were measured with calibrated integral orifice flowmeters. The vent gas flowmeter was equipped with a square root integrator to provide a time weighted average rate.

On-line analysis of the hydrocarbons in the vent gas was done on a gas chromatograph with a 20 ft Poropak Q® column using an internal standard method. In many cases, the use of the internal standard also allowed calculation of hydrogen in the vent gas by difference. A Beckman 3AM3 Gas Density Balance was used to provide a check on the vent gas density, needed to calculate mass flow rates from orifice pressure drop data. Mass balance closure for these experiments was typically better than  $\pm 2\%$ .

In addition to on-line vent gas analysis, the following analyses were performed on liquid samples as required:

- 1) Carbon-Hydrogen; Initially, a Perkin Elmer Model 240 CHN analyzer was used which required encapsulation of the volatile liquids in quartz vials. This was later replaced with a Model 1200 Chemical Data Systems Elemental Analyzer.
- 2) Sulfur; the Dohrmann Oxidative Microcoulemetric method was used.
- 3) Nitrogen; A Dohrmann Microcoulemetric Reactor first being used in the reductive mode was later replaced with an Antek Model 771 Pyroreactor with a chemiluminescent Nitrogen Detector.
- 4) Oxygen; a Karman Model A711 Neutron Generator was used for neutron activation analysis.
- 5) Water; an Aquatest I analyzer was used to measure dissolved water in a liquid sample with a coulometric Karl-Fisher titration.
- 6) Naphtha Componential; analysis of the C<sub>3</sub>-C<sub>9</sub> hydrocarbons was accomplished on a gas chromatograph with a 200 ft Squalane Capillary Column and a Flame Ionization Detector.

- 7) Simulated Distillations; the boiling range was measured on a gas chromatograph with an 8 ft Bonded Methyl Silicone Column and a Flame Ionization Detector (see ASTM D-2887-73). A simple internal standard variation was employed for non-distillates.
- 8) Mercury and Gallium; a General Electric TRIGA reactor provides slow neutrons for the neutron activation analysis of these metals at the 10 to 50 ppb detection level.
- 9) Common Metals; standard emission spectroscopy was used for this analysis.

All hydroprocessing experiments were conducted in much the same way. The reactor systems were instrumented to allow for 24 hr operation with only 8 hr per day being attended operation. This led to 24 hr minimum runs. Often, the lag between completion of a run and the corresponding analytical data increased the run time to 48 hours or more. Another important procedure to point out is that since the hydroprocessing steps must occur sequentially, both run data and the feed material for the next series of experiments were created simultaneously. As a result, the composite material produced from one hydroprocessing step, which was carried out at various operating conditions, is not likely to accurately represent material created in a production unit operating at optimum conditions. Differences between experimental and production derived materials will become greater as the processing sequence is followed from start to finish. Since 50 cc of catalyst seemed to be a real minimum catalyst loading, operating at nominal space velocities meant that some 2-1/2 to 5 or more liters of material was required for each run. This allowed for only three to five runs where the amount of some materials was limited.

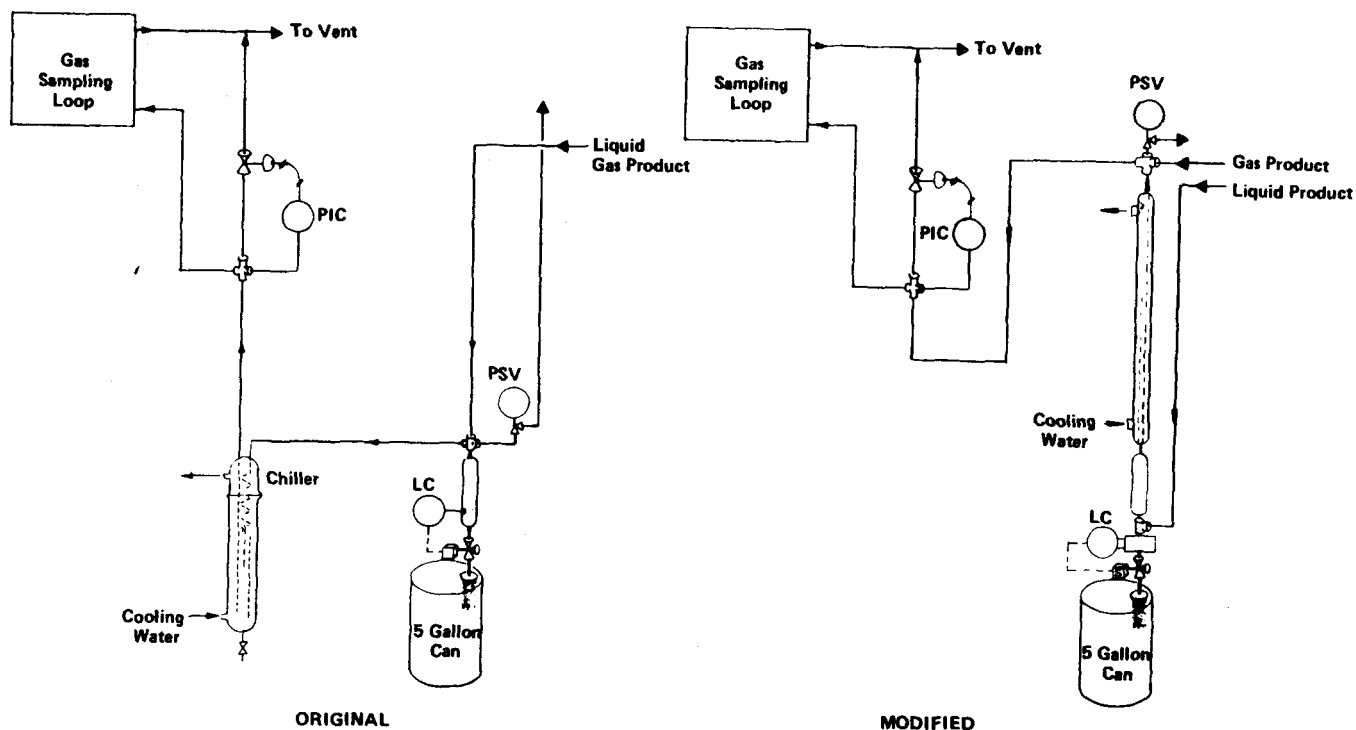
There were some common problems encountered in all of the hydroprocessing experiments. Early results obtained for sulfur and nitrogen levels with the Dohrmann analyzer are suspect. In addition, early oxygen analyses were also suspect. Elemental balances calculated for oxygen on some of the runs resulted in impossible answers, indicating oxygen being produced during hydroprocessing. Another problem, common to all but the last few hydroprocessing runs, was the stripping of C<sub>5</sub>-C<sub>7</sub> hydrocarbons from the liquid product by the vent gas. The mechanical configuration of the product handling system both before and after corrective measures were taken is illustrated in Figure 2. In the original design, the gas and liquid products were recombined after the pressure was reduced. The gas and liquid product was then conveyed via a 1/4 in. tube to the product recovery train. This two-phase flow appears to have been the cause of the large amount of C<sub>5</sub>-C<sub>7</sub> in the vent gas. The product recovery train contained a flash vessel where liquid and gas were separated. The gas was then passed through



a chiller to remove stripped hydrocarbons. The data would indicate that this chiller was inadequate to perform this operation. In order to alleviate this problem, the product recovery train was modified. An additional line between the reactor and product recovery train was installed so that the liquid and gas products could be transferred separately. In addition, only the liquid product was routed through the flash vessel. This was done so that any vapor formed by the flash accompanying liquid transfer would be separated. The gas separated in this manner was routed through a new chiller with larger surface area. The results of this modification are illustrated in Table 4. As a result of this problem, the liquids being processed beyond the first hydroprocessing step have artificially low fractions of C<sub>5</sub>-C<sub>7</sub> components.

Figure 2

PRODUCT RECOVERY TRAIN



The raw data collected in the hydroprocessing experiments was reduced to a usable form with a series of computer programs. Programs were written for vent gas analysis, naphtha componentials, simulated distillations, elemental balances, and overall mass balances including C<sub>1</sub>-C<sub>9</sub> componential yields. Chromatograph data from vent gas and naphtha componential analyses was converted to area percent of each component using a Varian Aerograph Chromatography Data System with a Model No. 220-20D, Class IV computer. The area percent data was in turn used to calculate mole and weight percent of each component using Fortran programs on an IBM 370 computer. In the case of hydrocracking, a sample of the composite material produced was distilled on a spinning band column to a 350°F naphtha, which was analyzed componentially, and a 350°F<sup>+</sup> fraction. Material balance data from the distillation was used to check conversion of mid-distillates or gas oils to naphtha. No distillations were required for hydrotreating and reforming experiments, as these were all conducted using a naphtha feed. Results from the data reduction sequence are presented in the appendices of this report.

TABLE 4

VENT GAS FLOW RATE AND COMPOSITION

	ORIGINAL			MODIFIED		
	Run No. 6-13-3 Flow Rate - 11.86 Composition: G/100G. Feed			Run No. 6-18-2 Flow Rate - 6.18 Composition: G/100G. Feed		
	<u>PARAFFIN</u>	<u>NAPHTHENE</u>	<u>AROMATIC</u>	<u>PARAFFIN</u>	<u>NAPHTHENE</u>	<u>AROMATIC</u>
C <sub>1</sub>	.000			.003		
C <sub>2</sub>	.014			.004		
C <sub>3</sub>	.027			.010		
C <sub>4</sub>	.071			.012		
C <sub>5</sub>	.334	.186		.078	.007	
C <sub>6</sub>	.363	1.611	.991	.238	.870	.461
C <sub>7</sub>	.559	1.112	.962	.327	.829	.634

## PROCESSING RESULTS

### Distillation

The Synthoil whole liquid was distilled, yielding the following fractions:

Straight Run Mid-Distillate -	34.0%
Residual -	66.0%

The residual bottoms had a melting point near 240°F.

Because so little light oil is obtained from the Synthoil process, and because the gas oil would be extremely difficult to process, it was decided to continue investigating only the mid-distillate as a petrochemical feedstock. Results of the analytical scans of the mid-distillate fraction are presented in Table 5. An important result of these inspections which should be noted is the relatively high concentrations of heavy metals, specifically Hg and Ga, not observed in the other coal liquids processed. There is no obvious reason for this, as contamination from an external source was ruled out as a possibility.

### Hydrocracking

The Synthoil straight run mid-distillate fraction was single-pass hydrocracked. The first pass product was distilled to a 350°F naphtha fraction and a 350°F<sup>+</sup> mid distillate. Only the mid-distillate fraction was hydrocracked a second time. The reactions were conducted using excess hydrogen, which was run through the reactor once and vented along with the LPG's produced. Both passes were conducted over a fixed bed of Harshaw HT-400 E 1/8" extrudate cobalt molybdate catalyst which had the following physical characteristics:

Composition - 3% cobalt oxide and 15% molybdenum dioxide  
on alumina.  
Average Bulk Density - 50 lb/cu ft  
Crush Strength - 12 lb  
Surface Area - 220 M<sup>2</sup>/g  
Pore Volume - 0.5 cc/g

This catalyst was chosen because of its high activity for desulfurization and denitrogenation and because of its neutral alumina support. An alumina, or neutral support, was desired for two reasons. First, the unusually high levels of nitrogen and oxygen expected to be in some of the coal derived oil fractions would quickly deactivate Lewis acid sites, such as would be found in a silica supported catalyst. Secondly, Lewis acid site cracking creates C<sub>4</sub>-C<sub>9</sub> paraffins with very low normal/iso ratios, typically around 0.6, as compared to 3 to 5 for

neutral sites. A high yield of normal paraffins was desired because they are the better aliphatic feedstock for ethylene production in an ethylene cracker. A stainless steel wire mesh was placed into the bottom of the reactor to act as a filter, keeping catalyst dust and chips out of the small diameter tubing downstream. One-quarter inch Berl saddles were loaded on top of the screen to the point where the catalyst bed was to be located. The appropriate amount of catalyst, based on the desired liquid hourly space velocity (LHSV), was then loaded into the reactor. Finally, more Berl saddles were placed on top of the catalyst bed.

TABLE 5

ANALYTICAL RESULTS FOR SYNTHOIL MID-DISTILLATE

METALS ANALYSIS

Fe	Ni	Cr	Mn	Cu	Zn	Co	Al	Ti	Sn	Pb	Mg	Ca	Hg	Ga
2	<1	<1	<0.5	<0.2	<3	<1	<1	<1	<1	<3	<1	<1	0.21	0.12

A-2  
MID-DISTILLATE  
350-650°F

API GRAVITY, 60°F 10.5

ELEMENTAL COMPOSITION

C wt. %	86.3
H wt. %	9.3
O ppm	33000
N ppm	7400
S ppm	2800

BOILING RANGE FROM  
SIMULATED DISTILLATION, °F

IBP	359
10 wt. %	425
20 wt. %	462
30 wt. %	489
40 wt. %	515
50 wt. %	542
60 wt. %	569
70 wt. %	596
80 wt. %	622
90 wt. %	653

Presulfiding of the catalyst was necessary to convert cobalt and molybdenum oxides to sulfides, thereby fully developing the catalyst activity. This was accomplished by passing a light naphtha (Stoddard Solvent) containing approximately 1% by weight carbon disulfide over the catalyst in a hydrogen atmosphere at moderate pressure and under carefully controlled temperature conditions. The cold reactor was brought up to 400 psig with hydrogen, the flow being fixed at 2 SCFH per 100 cc catalyst. The carbon disulfide in naphtha feed was started at 1 g. feed/g. catalyst/hour or 1 weight hourly space velocity (WHSV). After establishing flows, the reactor was heated to 200°C in steps of 25°C/half-hour and held at that temperature for four hours. The temperature was then increased to 325°C at 25°C/half-hour and held for 10 to 16 hours. The reactor pressure was then increased to that specified for run conditions and the presulfiding feed was replaced by the experimental feed. Finally, the reactor temperature was increased at 25°C/half-hour to the specified temperature for the run.

A range of processing conditions were surveyed by varying the reactor temperature, pressure, and the LHSV. Nominal reactor temperatures of 920 to 950°F were required for reasonable conversion rates. Pressures of 2500 and 1500 psig and LHSV's of 0.62 to 1.47 were surveyed. The limited amount of time and feedstock available did not allow for variable studies followed by continuous operation at a single set of conditions to create naphtha and unconverted mid-distillate for further processing. The composite product from the process variable studies was used for further studies. As would be expected, increasing pressure, decreasing LHSV, and increasing temperature all contributed to increased conversion. A notable aspect of these hydrocracking experiments is the reduction of heteroatom levels. Composite first pass hydrocracking removal of oxygen, nitrogen, and sulfur was 97, 86, and 96 percent respectively. Second pass removal was 77, 89, and 74 percent respectively. Difficulties arose from the need to handle approximately 4% water produced (due to O<sub>2</sub> in the feed) along with the liquid product. This was not a problem with the COED and H-COAL samples since the water was present in small enough quantities to be carried out with the vent gas. As a result, the computer programs for data reduction had to be modified to handle the water produced. A major difficulty was encountered while trying to hydrocrack the straight run mid-distillate. After approximately 100 hours of operation, a plug of ammonium chloride formed in the reactor downstream from the catalyst at a point where the temperature was 400-600°F. The formation of this "salt" plug necessitated reactor cleaning, reloading, and presulfiding each 100 hours. Because the plug occurred downstream of the reactor while running a distillate, the chloride present was assumed to be organic. No inspections were conducted to verify this.

The mid-distillate recovered from distillation of the first pass hydrocracked straight run mid-distillate was hydrocracked over a fresh load of Harshaw HT-400E 1/8" cobalt molybdenum catalyst

at 2500 psig, 944-984°F, and a LHSV of 1. Formation of ammonium chloride plugs did not occur during the second pass hydrocracking experiments. The feed to the second pass hydrocracking experiments was significantly different from the straight run mid-distillate as indicated from the boiling range and gravity data in Tables 5 and 6.

TABLE 6

BOILING RANGE AND GRAVITY DATA FOR FIRST PASS  
HYDROCRACKED SYNTHOIL MID-DISTILLATE

	<u>B-2</u> <u>MID-DISTILLATE</u>
API GRAVITY, 60°F	32.8
BOILING RANGE FROM SIMULATED DISTILLATION, °F	
IBP	330
10 wt. %	365
20 wt. %	389
30 wt. %	399
40 wt. %	412
50 wt. %	436
60 wt. %	456
70 wt. %	484
80 wt. %	513
90 wt. %	541

Simplified results from the Synthoil mid-distillate hydrocracking experiments are presented in Table 7. Included are the operating conditions, C<sub>1</sub>-C<sub>9</sub> yield expressed as weight %, a componential analysis of the C<sub>1</sub>-C<sub>9</sub> fraction, the amount of hydrogen consumed, and the heteroatom concentrations in both feed and product liquids. Complete run data is included in the appendices.

Hydrotreating

The naphtha produced from the two-pass hydrocracked mid-distillate was hydrotreated twice to create a feedstock with heteroatoms reduced to levels low enough for successful reforming with a conventional bifunctional reforming catalyst. The single pass reactions were conducted with an excess of hydrogen, at a ratio of 2000 and 3000 SCF/BBL of feed for

TABLE 7

HYDROCRACKING SYNTHOIL MID-DISTILLATE FRACTIONS  
SIMPLIFIED DATA

	Liquid														
	Run	Temp.	Press.	LHSV	PPM	PPM	PPM	C <sub>1</sub> -C <sub>9</sub>	H <sub>2</sub>	H <sub>2</sub> O	Componential Analysis Wt. %				
					O	N	S	Yield	G/100G	G/100G	C <sub>2</sub> -C <sub>4</sub>		C <sub>5</sub> -C <sub>9</sub>		
					C <sub>5</sub> +	C <sub>5</sub> +	C <sub>5</sub> +	Wt. %	Feed	Feed	Methane	LPG's	Paraf.	Naph.	Arom.
No.	°f	PSIG	HR <sup>-1</sup>												
-18-	STRAIGHT RUN														
	MID-DISTILLATE				33000	7400	2800								
	7-2-3	932	2460	0.62	240	10	30	54.5	-4.4	3.4	4.3	19.7	13.7	36.0	26.3
	7-5-2	917	2400	0.91	450	30	90	45.4	-4.3	3.7	5.1	24.7	9.7	32.1	26.3
	7-6-4	926	2500	1.04	1020	340	110	56.3	-4.9	3.6	4.8	32.6	13.3	26.0	22.9
	7-8-2	932	2540	1.31	1050	40	100	44.5	-3.7	3.7	6.2	20.7	8.6	30.8	32.4
	7-10-2	924	2430	1.47	1290	570	140	47.6	-3.9	2.6	5.7	28.2	11.2	27.5	26.9
	7-11-2	924	1550	1.11	1380	560	60	38.7	-2.5	1.7	5.4	22.6	9.9	23.9	31.9
	7-12-2	946	1520	0.95	970	590	150	49.2	-2.9	3.2	7.8	29.4	11.3	19.6	31.8
	7-14-2	946	2510	0.88	2080	1050	220	62.2	-4.4	2.7	6.7	30.4	11.7	23.9	25.8
	7-14-3	950	2540	0.97	1360	550	160	63.7	-4.6	3.4	6.8	32.7	11.8	22.4	25.0
	7-14-4	950	2690	1.04	1320	620	150	64.7	-4.4	3.1	6.7	30.6	11.0	24.8	26.8
HYDROCRACKED															
MID-DISTILLATE				1200	400	120									
7-17-2	950	2525	0.98	3040	10	100	66.1	-3.4	--	5.8	27.9	15.5	22.3	28.5	
7-17-3	944	2525	0.97	1080	<10	10	56.8	-3.0	--	5.9	29.8	14.2	21.0	29.0	
7-17-4	946	2525	1.00	1680	<10	<10	51.8	-2.7	--	5.8	30.0	13.2	20.4	30.4	
7-17-5	949	2525	1.00	0	<10	10	54.0	-2.7	--	5.7	28.2	13.9	19.7	30.0	
7-21-2	984	2510	1.00	2960	<10	10	74.3	-3.6	--	7.0	33.7	13.7	17.6	27.8	
7-21-3	983	2520	1.00	4010	<10	10	72.4	-3.3	--	7.1	32.9	14.7	16.1	28.8	

the first pass and 2000 SCF/BBL for the second pass, which passed through once and was vented with the LPG's produced. Runs were carried out over a fixed bed of American Cyanamid Aeroform HDS-9A 1/16" extrudate hydrotreating catalyst. This catalyst consisted of nickel and molybdenum on an alumina support and had the following physical characteristics:

Composition -	3% nickel oxide and 18% molybdenum trioxide on alumina
Average Bulk Density -	45-50 lb/cu ft
Crush Strength -	12 lb

The HDS-9A catalyst was used because of its demonstrated superior activity for removal of nitrogen compounds without the loss in sulfur removal effectiveness apparent in other Ni-Mo catalysts. It was expected that the use of this catalyst would result in a favorable trade off between nitrogen removal and aromatic saturation, the latter being considered detrimental to the goal of producing aromatic feedstocks. The catalyst was loaded in the reactor, in the same manner as for the hydrocracking catalyst, with two volumes of 16-20 mesh silicon carbide diluent and presulfided with  $H_2S$  at atmospheric pressure according to the following procedure:

After the catalyst was loaded in the cold reactor, hydrogen flow was established at 2.89 SCFH. Hydrogen sulfide flow was then established at 0.24 SCFH. The reactor temperature was increased at  $25^{\circ}C/15$  min. to  $400^{\circ}C$  and held for two hours. The temperature was then reduced to  $360^{\circ}C$  and the  $H_2S$  flow was stopped. While maintaining the hydrogen flow, the reactor pressure was increased to 1000 psig.

The hydrotreating runs for this feedstock were conducted over the same catalyst load as the H-COAL hydrocrackate naphtha. This catalyst load had previously been run for 50 hours on the H-COAL naphtha. Reactor conditions of  $680^{\circ}F$ , 1000 psig, and a LHSV of 2 were used for the first pass, while the temperature was increased to  $690^{\circ}F$  for the second pass with the other two variables remaining the same.

Results from the hydrotreating runs conducted after gaseous presulfiding indicate that sulfur contamination from this source occurs to a lesser degree but is still significant. This contributed in part, along with insufficient removal of nitrogen to the need for a second pass in order to produce suitable reformer feedstock. Because of the limited amount of material available, more processing conditions for hydrotreating were not surveyed. Consequently, the need for a second pass was not absolutely established. Data from the hydrotreating runs performed on the Synthoil hydrocrackate naphtha is presented in Table 8.



TABLE 8

HYDROTREATING SYNTHOIL HYDROCRACKATE NAPHTHA  
SIMPLIFIED DATA

RUN NO.	1st Pass Feed	6-13-2	6-13-3	6-15-2	2nd Pass Feed	6-18-2	6-18-3	6-18-4	6-21-2
TEMPERATURE °F		682	680	682		689	689	689	689
PRESSURE, PSIG		1025	1020	1004		1000	1000	1000	1005
LHSV HR <sup>-1</sup>		2.09	2.05	2.08		1.95	1.96	1.95	1.95
<u>YIELD, G/100G FEED</u>									
HYDROGEN		-0.27	-0.62	-0.72		-1.13	-1.24	-0.83	-0.91
C <sub>1</sub> -C <sub>4</sub> GAS		0.22	0.09	0.08		0.03	0.02	0.02	0.02
C <sub>5</sub> -C <sub>10</sub> + LIQUID		100.05	100.53	100.64		101.10	101.22	100.81	100.89
AROMATIC SATURATION %/100G FEED		6.49	6.99	5.88		7.64	7.19	7.14	6.21
OXYGEN, PPM	5100	1900	1700	233	240	140	140	100	100
NITROGEN, PPM	51	21	25	20	20	3	8	11	3
SULFUR, PPM	30	11	8	5	15	1	1	1	1

## Reforming

The Synthoil hydrotreated naphtha was reformed over a conventional bifunctional platinum reforming catalyst to maximize aromatics. A hydrogen ratio of 4000 SCF/BBL of feed was used and the excess was vented with the LPG's produced. The single pass reactions were carried out over a fixed bed of Cyanamid Aeroform® PHF-4 1/16" extrudate reforming catalyst consisting of platinum and chloride on alumina with the following physical characteristics:

Composition - 0.3% platinum and 0.6% chloride on alumina  
Crush Strength - 10 lb  
Average Bulk Density - 35-40 lb/cu ft

The platinum catalyst was chosen over the newer bimetallics for several reasons. Bimetallics are much more susceptible to poisons, which were presumed to be in coal derived oils. Further, by operating at "severe" conditions, the expected hydrocracking activity of the platinum catalyst would purify the aromatics produced by selectively cracking away the paraffins. The result would be a reformat with a high enough aromatic content to be fed to a hydrodealkylator with the non-aromatics being converted to methane and ethane. Another alternative, which was not pursued, would have been to operate at less severe conditions while maintaining high naphthene conversions but reducing the likelihood of hydrocracking and isomerization. In this case the reformat would be extracted with raffinate going to a naphtha cracker and the extract to hydrodealkylation. Calculating the economic balance between these two alternatives requires more data than the scope of this investigation allows. The intent was to operate the reformer at constant conditions in order to better compare naphthas.

The catalyst was loaded into the reactor in the same manner as the hydrotreating catalyst, with the screen in the bottom of the reactor and Berl saddles to position the bed in the thermocouple zone. The catalyst was diluted with two volumes of 16-20 mesh silicon carbide to prevent backmixing and channeling in the catalyst bed, as well as to permit better monitoring of the endotherm. The catalyst was calcined as follows:

Hydrogen flow was established at ~ 1.25 SCFH with the reactor pressure at 50 psig. The temperature was increased at 25°C/half hour to 530°C and held at these conditions for 2 hours. The temperature was then reduced to 455°C and again held for 2 hours. Pressure was then increased to that specified for the run and the hydrocarbon feed introduced. Finally, the hydrogen flow rate was established at that specified for the run and the reactor temperature was increased at 25°C/half hour to the temperature specified for the run.

The hydrocrackate hydrotreated naphtha was reformed at 964°F and 500 psig with a LHSV of 2. The initial activity was very encouraging, but catalyst activity declined as the naphthene conversion data in Table 9 indicates. The limited amount of this material allowed for only a 100 hour run at these conditions, making it difficult to determine if the deactivation would continue.

TABLE 9

REFORMING SYNTHOIL HYDROTREATED HYDROCRACKATE NAPHTHA  
SIMPLIFIED DATA

RUN NO.	<u>Feed</u>	<u>6-23-2</u>	<u>6-23-3</u>	<u>6-23-4</u>
TEMPERATURE, °F		963	964	964
PRESSURE, <sup>1</sup> PSIG		500	500	500
LHSV, HR		2.08	2.06	2.06
CHEM. OXYGEN, PPM	82			
WATER, PPM	58			
NITROGEN, PPM	9			
SULFUR, PPM	1			
<u>YIELD, G/100G FEED</u>				
HYDROGEN		2.77	2.46	2.29
C <sub>1</sub> -C <sub>5</sub> GAS		12.74	12.60	12.40
C <sub>6</sub> -C <sub>9</sub>				
PARAFFIN	3.31	8.06	8.92	9.34
NAPHTHENE	49.04	2.31	2.86	3.61
AROMATIC	25.56	66.56	65.45	60.61
C <sub>10</sub> <sup>+</sup>	22.09	7.57	7.70	11.70
% NAPHTHENE CONVERSION		95.3	94.2	92.6
% AROMATIC C <sub>6</sub> -C <sub>9</sub>	32.8	86.5	84.7	82.4

Steam Coil Cracking

Because prior experience with coal liquefaction products showed the mid-distillate fraction to be unattractive as an ethylene cracker feedstock, no steam coil cracking experiments were performed on the Synthoil product.

## PART II - CONCEPTUAL PROCESS

### Introduction

A conceptual process is to be used as the basis for comparison of the various coal liquefaction products surveyed under this contract. The data included in the conceptual process will be used to calculate preliminary capital and operating costs, which will in turn serve as the data for economic evaluations of the proposed process. The laboratory data presented in Part I of this report was reduced to kinetic equations which describe the conversions and selectivities observed. Where necessary, engineering judgement has been used to "smooth" inconsistencies in the laboratory data. The kinetic expressions derived from the laboratory data were utilized to determine mass, componential, and elemental balances for a conceptual process. The mid-distillate fraction from the distillation step was analyzed as a feedstock to the conceptual plant. The product patterns presented in the tables following are therefore based on 100.00 weight percent of each fraction. From this data, the relative value of the fraction can be readily assessed based on the respective yields of aliphatic and aromatic products along with the hydrogen consumed.

Also included in this section of the report is a schematic diagram of the conceptual process. Mass-per-unit-time, elemental, and componential data for selected streams is also presented. The basis for this data is a flow rate of 100.00 lb/hr of whole crude to the distillation column. Componential data for the selected streams presented is given in weight percent of each component in the stream.

### REDUCTION OF LABORATORY DATA

#### Hydrocracking Mid-Distillate

The data obtained from the laboratory inspections on the two-pass hydrocracked Synthoil mid-distillate was reduced to obtain average first order rate constants for each pass. Rate constants were calculated from conversion and process variable data for each run according to the following equation:

$$\ln (1-C) = -k e^{\frac{-E}{RT}} P_{H_2}^{-0.5} \text{ LHSV}$$

where - C = C<sub>1</sub>-C<sub>9</sub> yield, wt. fraction

k = rate constant

E = 38000 cal/g mole

R = 1.987 cal/g mole °K

T = reactor temperature, °K

P<sub>H<sub>2</sub></sub> = pressure, psig

LHSV = liquid space velocity, vol/vol-hr

The average rate constants determined by this method were used as a basis for estimating the rate constants for consecutive passes so that recycle hydrocracking calculations might be made. In order to complete the recycle hydrocracking calculations, selectivity data for each pass was also needed. This data was obtained from laboratory inspections for first and second pass and was estimated for consecutive passes. Several assumptions were used in making recycle hydrocracking calculations. First, it was assumed that the reaction rate for virgin material is unaffected by the presence of recycle material. Second, after having been recycled three times, there is no further change in reaction rate for that material. Finally, it was assumed that selectivities would remain constant after the second pass. Laboratory data obtained for Synthoil hydrocracking runs were used to obtain selectivities for the first and second pass. A plot of experimental versus the calculated conversions computed from the first and second pass average rate constants is presented in Figure 3. The straight line 45° plot confirms the assumed first order kinetics for mid-distillate hydrocracking conversions. Table 10, contains the reactor conditions, rate constants, and selectivities used to make recycle hydrocracking calculations.

TABLE 10

MID-DISTILLATE RECYCLE HYDROCRACKING DATA

Reactor Conditions

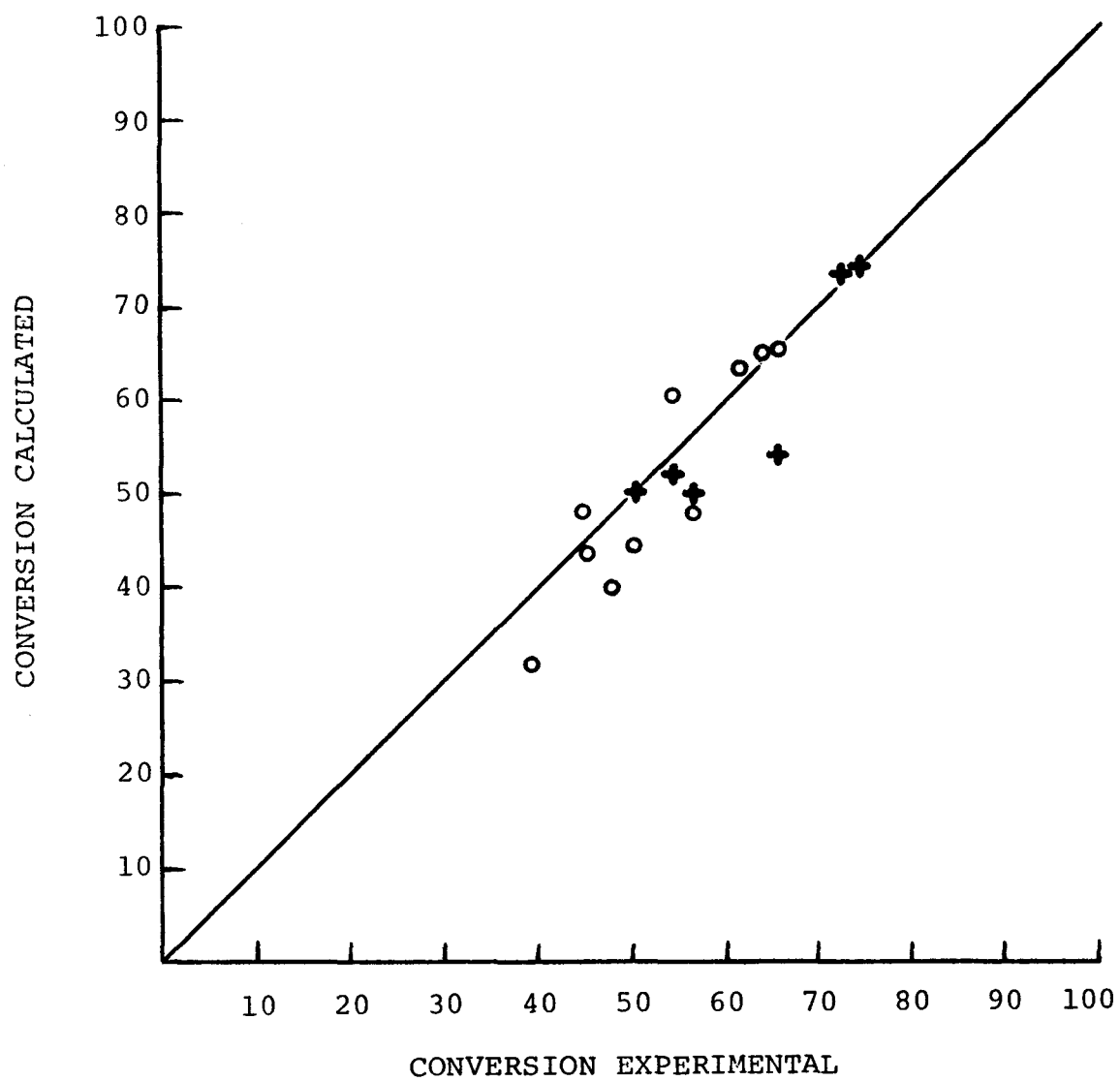
941°F  
 2500 psig  
 LHSV 0.75 volumes/volume - hr  
 Recycle = 0.65/1 virgin

Rate Constants

1st Pass	$1.63 \times 10^7 \text{ hr}^{-1}$	
2nd Pass	$1.22 \times 10^7 \text{ hr}^{-1}$	
3rd+ Pass	$1.00 \times 10^7 \text{ hr}^{-1}$	- assumed -

Figure 3

PLOT OF EXPERIMENTAL VERSUS  
CALCULATED CONVERSIONS



- FIRST PASS
- + SECOND PASS

TABLE 10 Cont'd

1ST PASS SELECTIVITIES  
lb/100 lb Feed

	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	<u>CYCLO HEXANE</u>	<u>AROMATIC</u>
Methane	6.8				
Ethane	10.3				
Propane	11.2				
C <sub>4</sub>	8.7	1.4			
C <sub>5</sub>	2.2	1.3	1.4		
C <sub>6</sub>	1.7	1.0	5.3	4.8	6.3
C <sub>7</sub>	1.2	2.4	1.6	6.2	10.5
C <sub>8</sub>	0.6	0.4	1.7	2.1	5.3
C <sub>9</sub>	0.4	0.3	0.3	0.6	4.1

2ND PASS SELECTIVITIES  
lb/100 lb Feed

	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	<u>CYCLO HEXANE</u>	<u>AROMATIC</u>
Methane	5.8				
Ethane	7.5				
Propane	10.4				
C <sub>4</sub>	9.9	1.7			
C <sub>5</sub>	2.7	1.6	1.8		
C <sub>6</sub>	1.9	0.9	6.0	2.0	8.2
C <sub>7</sub>	1.3	2.9	2.5	3.1	11.5
C <sub>8</sub>	0.8	0.6	1.9	1.4	6.0
C <sub>9</sub>	0.5	0.6	0.6	1.1	4.9

OVERALL HETEROATOM PRODUCTION  
lb/100 lb Feed

Water	3.71
Ammonia	0.90
Hydrogen Sulfide	0.30

### Hydrotreating Naphthas

Laboratory data from single pass hydrotreating the Synthoil hydrocrackate naphtha was reduced to provide selectivity data. Because of the relatively low heteroatom levels in this material, all of the hydrogen consumed was assumed to go to saturating aromatics to naphthenes. Conversion levels of aromatics to naphthenes were calculated for all carbon numbers. Therefore, the appropriate level of aromatic saturation was calculated to yield the hydrogen consumption calculated from analytical carbon-hydrogen data. The selectivity data for hydrotreating Synthoil hydrocrackate naphtha is presented in Table 11 below.

TABLE 11

#### HYDROTREATING SYNTHOIL HYDROCRACKATE NAPHTHA SELECTIVITY DATA

##### Reactor Conditions

680°F  
1000 psig  
LHSV 2 vol/vol - hr

##### Selectivity, lb/100 lb Feed

C <sub>1</sub>	--
C <sub>2</sub>	0.01
C <sub>3</sub>	0.01
C <sub>4</sub>	0.06

##### Conversion of Aromatics in Feed, wt. %

C <sub>6</sub>	--
C <sub>7</sub>	14.0
C <sub>8</sub>	21.0
C <sub>9</sub>	16.0

The C<sub>4</sub>-C<sub>9</sub> paraffins and C<sub>5</sub> naphthenes were assumed to be unchanged during the hydrotreating step.

### Reforming Naphthas

The laboratory data for reforming the hydrotreated hydrocrackate naphtha was reduced to give conversion and selectivity data for the conceptual process. Conversions of both paraffins and C<sub>5</sub> and C<sub>6</sub> naphthenes were calculated and are presented in Table 12.



It should be noted that C<sub>6</sub>-C<sub>9</sub> paraffins were not converted in these runs as they were for other liquids processed. Some of the aromatics produced resulted from conversion of C<sub>10</sub><sup>+</sup> material and all of the paraffins produced were calculated to come from C<sub>8</sub> and C<sub>9</sub> naphthenes and C<sub>10</sub><sup>+</sup> material. The paraffin product normal/iso ratios for C<sub>4</sub>-C<sub>9</sub> hydrocarbons are also presented in Table 12. Hydrogen production was then calculated from analytical carbon-hydrogen data collected from analyses of the feed and product streams.

TABLE 12

HYDROCRACKATE NAPHTHA REFORMING DATA  
CONVERSIONS, WT. % OF COMPONENT IN FEED

	PARAFFIN	NAPHTHENE	
		CYCLO PENT	CYCLO HEXANE
C <sub>6</sub>	--	-0-	98.0
C <sub>7</sub>	--	90.2	98.4
C <sub>8</sub>	-0-	95.1	99.5
C <sub>9</sub>	-0-	96.5	100
C <sub>10</sub> <sup>+</sup>	64.7		

Selectivity

C<sub>8</sub> Naphthenes converted to 62 wt. % Aromatic, 38 wt. % Paraffin  
 C<sub>9</sub> Naphthenes converted to 81 wt. % Aromatic, 19 wt. % Paraffin  
 C<sub>10</sub><sup>+</sup> Converted to 21 wt. % Benzene, 17 wt. % Toluene,  
 62 wt. % Paraffin

Paraffin Selectivity as Wt. % of Paraffin  
Produced From  
C<sub>8</sub> Naphthene, C<sub>9</sub> Naphthene, And C<sub>10</sub><sup>+</sup>

	PARAFFIN	CYCLO PENT
C <sub>1</sub>	10	
C <sub>2</sub>	15	
C <sub>3</sub>	17	
C <sub>4</sub>	16	
C <sub>5</sub>	13	2
C <sub>6</sub>	15	
C <sub>7</sub>	11	

TABLE 12 Cont'd

Paraffin Normal/Iso Ratio (Total Product)

C <sub>4</sub>	1.85
C <sub>5</sub>	0.84
C <sub>6</sub>	0.79
C <sub>7</sub>	0.45
C <sub>8</sub>	0.31
C <sub>9</sub>	0.35

Hydrodealkylating Reformates

The hydrocrackate reformat was mathematically hydrodealkylated. Selectivity data for converting paraffins, naphthenes, and aromatics to methane, ethane, benzene, and liquid fuel as well as the hydrogen required was calculated from an internally developed model. The selectivity data is reported as weight percent of each product for each hydrocarbon classification by carbon number. This data is presented in Table 13.

TABLE 13

REFORMATE HYDRODEALKYLATION SELECTIVITY DATA

	<u>C<sub>6</sub></u>	<u>C<sub>7</sub></u>	<u>C<sub>8</sub></u>	<u>C<sub>9</sub></u>
PARAFFIN				
HYDROGEN	-0.074	-0.077	-0.080	-0.081
METHANE	0.434	0.426	0.421	0.417
ETHANE	0.640	0.651	0.659	0.664
NAPHTHENE				
HYDROGEN	-0.088	-0.089	-0.090	-0.090
METHANE	0.440	0.431	0.425	0.421
ETHANE	0.648	0.658	0.665	0.669
AROMATIC				
HYDROGEN	-0-	-0.024	-0.041	-0.057
METHANE	-0-	0.146	0.261	0.347
ETHANE	-0-	0.004	0.047	0.069
BENZENE	1.00	0.843	0.689	0.581
LIQ. FUEL	-0-	0.031	0.044	0.060

## CONCEPTUAL PROCESS YIELDS AND PLANT BALANCE

The Synthoil straight run mid-distillate was subjected to mathematical recycle hydrocracking, hydrotreating, reforming, and hydrodealkylation. Componential data for the products from each hydroprocessing step were determined. Mass balance data for each stream in a conceptual plant, including flow rates and elemental data where known, were determined. A schematic diagram of the conceptual plant, with selected streams identified by number is included in Figure 4. The basis for the mass balance data is a flow of 100.00 lb/hr of the whole crude to the distillation step. The componential data for each stream identified is presented as weight percent of each component by carbon number. Tables 14 through 17 contain the componential data for conceptual recycle hydrocracking, hydrotreating, reforming, and hydrodealkylation. Table 18 contains the total conceptual product pattern from the mid-distillate along with the value. The values of the products were derived from those published by Spitz and Ross<sup>1</sup>. Hydrogen was estimated at \$2.10/MCF from a methane reformer operating on \$3.25/MM BTU gas. Tables 19 through 24 contain the mass balance data for a conceptual plant operating on Synthoil whole crude.

<sup>1</sup>Spitz, P. H. and Ross, G. N., "What is Feedstock Worth?" Hydrocarbon Processing, April, 1976.

Figure 4  
CONCEPTUAL PLANT

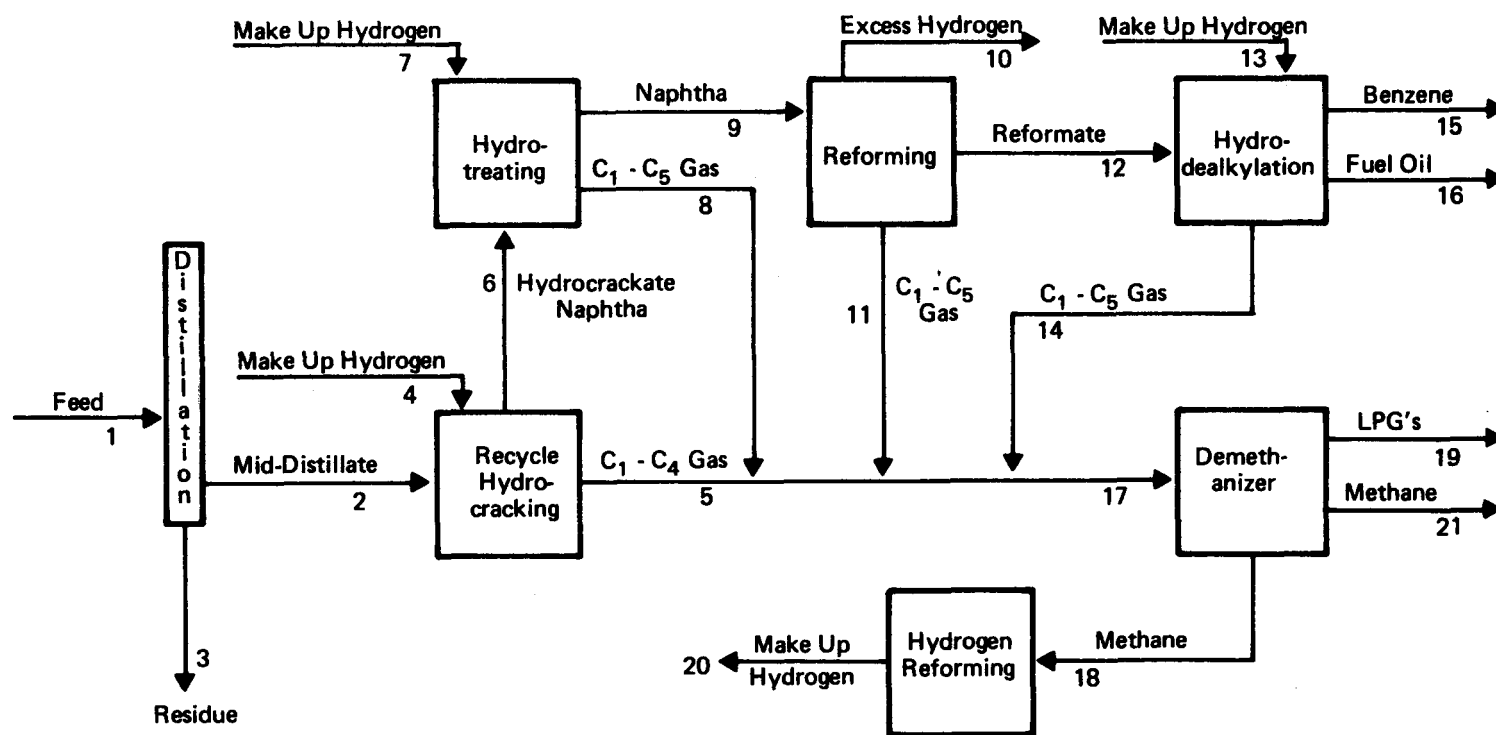


TABLE 14

CONCEPTUAL RECYCLE HYDROCRACKING SYNTHOIL  
MID-DISTILLATE COMPONENTIAL DATA

	WT. %				
	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	<u>CYCLO HEXANE</u>	<u>AROMATIC</u>
Hydrogen	-6.41				
Methane	6.17				
Ethane	8.99				
Propane	10.46				
C <sub>4</sub>	8.73	1.40			
C <sub>5</sub>	2.28	1.36	1.48		
C <sub>6</sub>	1.73	0.94	5.32	3.69	6.65
C <sub>7</sub>	1.18	2.45	1.81	4.90	10.38
C <sub>8</sub>	0.60	0.47	1.67	1.78	5.27
C <sub>9</sub>	0.37	0.41	0.38	0.71	4.16
C <sub>10</sub> <sup>+</sup>	5.74				
Water	3.71				
Ammonia	0.90				
Hydrogen Sulfide	0.30				

TABLE 15

CONCEPTUAL HYDROTREATING SYNTHOIL MID-DISTILLATE  
HYDROCRACKATE NAPHTHA COMPONENTIAL DATA

	WT. %				
	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	<u>CYCLO HEXANE</u>	<u>AROMATIC</u>
Hydrogen	-0.30				
Methane	0.00				
Ethane	0.01				
Propane	0.01				
C <sub>4</sub>	0.06	0.00			
C <sub>5</sub>	3.45	2.06	2.24		
C <sub>6</sub>	2.61	1.42	8.12	5.62	10.15
C <sub>7</sub>	1.79	3.71	2.73	9.85	13.61
C <sub>8</sub>	0.09	0.72	2.52	4.49	6.35
C <sub>9</sub>	0.56	0.62	0.58	2.14	5.33
C <sub>10</sub> <sup>+</sup>	8.75				

TABLE 16

CONCEPTUAL REFORMING SYNTHOIL MID-DISTILLATE  
HYDROCRACKATE HAPHTHA COMPONENTIAL DATA

	WT. %				
	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	<u>CYCLO HEXANE</u>	<u>AROMATIC</u>
Hydrogen	1.53				
Methane	0.63				
Ethane	0.95				
Propane	1.07				
C <sub>4</sub>	0.66	0.35			
C <sub>5</sub>	0.37	0.45	0.13		
C <sub>6</sub>	2.34	2.96	8.77	0.12	17.77
C <sub>7</sub>	2.06	4.58	0.29	0.17	28.06
C <sub>8</sub>	0.41	1.34	0.13	0.02	12.55
C <sub>9</sub>	0.33	0.94	0.02	0.00	7.50
C <sub>10</sub> <sup>+</sup>	3.34				

TABLE 17

CONCEPTUAL HYDRODEALKYLATION SYNTHOIL MID-DISTILLATE  
HYDROCRACKATE NAPHTHA COMPONENTIAL DATA

WT. %	
Hydrogen	-3.84
Methane	21.93
Ethane	18.25
Benzene	58.08
Liquid Fuel	5.56

TABLE 18

CONCEPTUAL PROCESS PRODUCTS  
SYNTHOIL MID-DISTILLATE

Basis - 100 lb From Distillation	
Hydrogen	-7.87
Methane	19.06
Ethane	19.98
Propane	11.12
Butanes	10.78
Pentanes	5.67
Benzene	33.11
Liquid Fuel	3.17
Value/100 lb	
Distillate (1980)	\$6.89

TABLE 19  
DISTILLATION

Whole Crude

Stream Identification No. 1  
Flow Rate 100.0 lb/hr

Mid-Distillate

Stream Identification No. 2  
Flow Rate 34.0 lb/hr

API Gravity, 60°F - 10.5

	<u>Wt. %</u>
Carbon	86.3
Hydrogen	9.3
Oxygen	3.3
Nitrogen	0.74
Sulfur	0.28

Residue

Stream Identification No. 3  
Flow Rate 64.0 lb/hr

TABLE 20

CONCEPTUAL PLANT HYDROPROCESSING LIQUID STEAM

Hydrocrackate Naphtha

Stream Identification No. 6  
Flow Rate 22.35 lb/hr

	<u>Wt. %</u>
Carbon	86.9
Hydrogen	12.6
Nitrogen	.005
Oxygen	.510
Sulfur	.003

	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	<u>CYCLO HEXANE</u>	<u>AROMATIC</u>
C <sub>5</sub>	3.45	2.06	2.24		
C <sub>6</sub>	2.61	1.42	8.12	5.62	10.15
C <sub>7</sub>	1.79	3.71	2.73	7.47	15.84
C <sub>8</sub>	.90	.72	2.52	2.69	8.05
C <sub>9</sub>	.56	.62	.58	1.07	6.35
C <sub>10</sub> <sup>+</sup>	8.75				



TABLE 20 Cont'd

Hydrotreated Naphtha

Stream Identification No. 9  
Flow Rate 20.69 lb/hr

					<u>Wt. %</u>
			Carbon	87.62	
			Hydrogen	12.38	
	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	<u>CYCLO HEXANE</u>	<u>AROMATIC</u>
C <sub>6</sub>	2.82	1.53	8.77	6.07	10.96
C <sub>7</sub>	1.93	4.01	2.95	10.64	14.70
C <sub>8</sub>	.97	.78	2.72	4.85	6.86
C <sub>9</sub>	.60	.67	.63	2.31	5.76
C <sub>10</sub> <sup>+</sup>	9.45				

Reformate C<sub>6</sub><sup>+</sup>

Stream Identification No. 12  
Flow Rate 19.39 lb/hr

					<u>Wt. %</u>
			Carbon	89.17	
			Hydrogen	10.83	
	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	<u>CYCLO HEXANE</u>	<u>AROMATIC</u>
C <sub>6</sub>	2.50	3.16	9.36	.12	18.96
C <sub>7</sub>	2.20	4.89	.31	.18	29.95
C <sub>8</sub>	.44	1.43	.14	.02	13.39
C <sub>9</sub>	.35	1.00	.02	.00	8.00
C <sub>10</sub> <sup>+</sup>	3.56				

TABLE 21

CONCEPTUAL PLANT HYDROPROCESSING GAS STREAMSHydrocracking Gas Make

Stream Identification No. 5  
Flow Rate 12.16 lb/hr

			<u>Wt. %</u>
		Carbon	80.26
		Hydrogen	19.74
	<u>NORM PARAF</u>	<u>ISO PARAF</u>	
Methane	17.26		
Ethane	25.15		
Propane	29.26		
C <sub>4</sub>	24.42	3.92	

Hydrotreating Gas Make

Stream Identification No. 8  
Flow Rate 1.62 lb/hr

				<u>Wt. %</u>
			Carbon	83.85
			Hydrogen	16.15
	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	
Methane	--			
Ethane	0.13			
Propane	0.13			
C <sub>4</sub>	0.77	--		
C <sub>5</sub>	44.06	26.31	28.61	

Reformer Gas Make

Stream Identification No. 11  
Flow Rate 0.89 lb/hr

				<u>Wt. %</u>
			Carbon	80.91
			Hydrogen	19.09
	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	
Methane	13.67			
Ethane	20.61			
Propane	23.21			
C <sub>4</sub>	14.32	7.59		
C <sub>5</sub>	8.03	9.76	2.82	

TABLE 22

CONCEPTUAL PLANT HYDRODEALKYLATOR STREAMSHydrodealkylator Gas Make

Stream Identification No. 14  
Flow Rate 7.79 lb/hr

			<u>Wt. %</u>
Methane	59.95	Carbon	76.80
Ethane	40.05	Hydrogen	23.20

Benzene Product

Stream Identification No. 15  
Flow Rate 11.26 lb/hr

			<u>Wt. %</u>
Benzene	100.0	Carbon	92.2
		Hydrogen	7.8

Hydrodealkylator Bottoms

Stream Identification No. 16  
Flow Rate 1.12 lb/hr

			<u>Wt. %</u>
C <sub>10</sub> <sup>+</sup>		Carbon	84.4
		Hydrogen	15.6

TABLE 23

CONCEPTUAL PLANT DEMETHANIZER STREAMSFeed to Demethanizer

Stream Identification No. 17

Flow Rate 22.46 lb/hr

				<u>Wt. %</u>
			Carbon	79.34
			Hydrogen	20.66
	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYLCO PENT</u>	
Methane	28.67			
Ethane	30.06			
Propane	16.73			
C <sub>4</sub>	13.80	2.42		
C <sub>5</sub>	3.54	2.45	2.34	

Methane to Hydrogen Production (Reformer)

Stream Identification No. 18

Flow Rate 5.48 lb/hr

			<u>Wt. %</u>
Methane	100.0	Carbon	74.8
		Hydrogen	25.2

LPG's

Stream Identification No. 19

Flow Rate 16.02 lb/hr

				<u>Wt. %</u>
			Carbon	81.35
			Hydrogen	18.65
	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	
Ethane	42.13			
Propane	23.47			
C <sub>4</sub>	19.35	3.37		
C <sub>5</sub>	4.99	3.43	3.31	

TABLE 23 Cont'd

Methane to Export

		Stream Identification No. 21	
		Flow Rate 0.96 lb/hr	
		<u>Wt. %</u>	
Methane	100.0	Carbon	74.8
		Hydrogen	25.2

TABLE 24

HYDROGENFlow Rate

To Hydrocracking	-2.18 lb/hr	Stream I.D. 4
To Hydrotreating	-0.07 lb/hr	Stream I.D. 7
From Reforming	+0.32 lb/hr	Stream I.D. 10
To Hydrodealkylation	-0.74 lb/hr	Stream I.D. 13
From Methane Reforming	+2.67 lb/hr	Stream I.D. 20

APPENDICES

TO

PART I

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## PROCESS EQUIPMENT DESCRIPTION

### HYDROPROCESSING EQUIPMENT

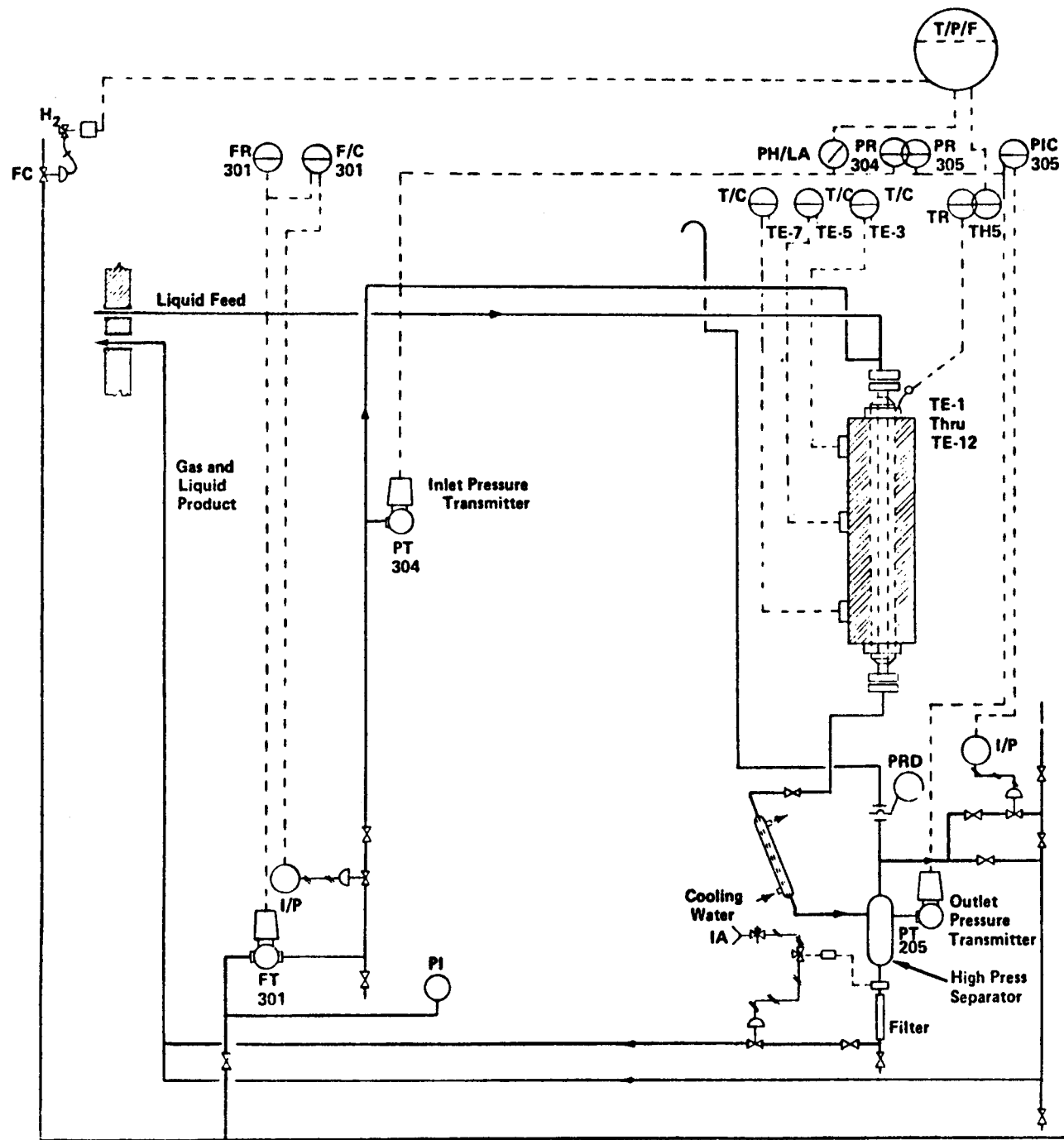
The equipment used for the hydroprocessing experiments is shown in Figures I, II, III, and IV. Figures I and II are engineering sketches of the original reactor and product recovery train. Figures III and IV are sketches of the same equipment after modifications were made to reduce stripping of light hydrocarbons from the liquid by the gaseous product. All descriptions of the experimental equipment reported in this text refer to these figures.

Gaseous Feed - Hydrogen is supplied to the laboratory as a utility at two different pressures, nominally 1200 and 3200 psig. The hydrogen is routed to each reactor via a header system and through a flow transmitter. The Foxboro integral orifice differential pressure cell flow transmitters used for hydrogen flow control were equipped with orifices ranging from 0.003 to 0.007 inches in diameter. Pressure differentials of 0 to 20 or 0 to 40 inches of water were used. In order to obtain maximum accuracy for a given hydrogen flow rate, orifice size and differential pressure drop were chosen so that control settings of greater than 30% of maximum flow were utilized. Also, flow transmitters were zeroed before the start of each experiment using a Foxboro current calibrator. From the flow transmitter, the hydrogen is routed to the top of the reactor and the pressure at that point is recorded.

Liquid Feed - Each reactor has provision for liquid feed from either a one-gallon jug on scales, or a five-gallon feed tank equipped with a bubbler level indicator. A multiple head Milton Roy metering pump delivers the liquid feed to the reactor at operating pressure at a controlled rate, nominally 25 to 400 ml/hr.

The Reactor - Three similar reactors were used for the hydroprocessing studies. All of the reactors consisted of a heavy wall nickel-free stainless steel tube suspended in a furnace. The furnace is divided into three heating zones on two of the reactors and eight zones on the third. The temperature of each zone is controlled through the use of thermocouples located on the outside wall of each reactor. During normal operations a thermowell is placed in the center of the reactor. The thermowell consists of a closed end piece of 430 stainless 1/4 inch tubing with a 0.035 inch wall. It is silver soldered into special



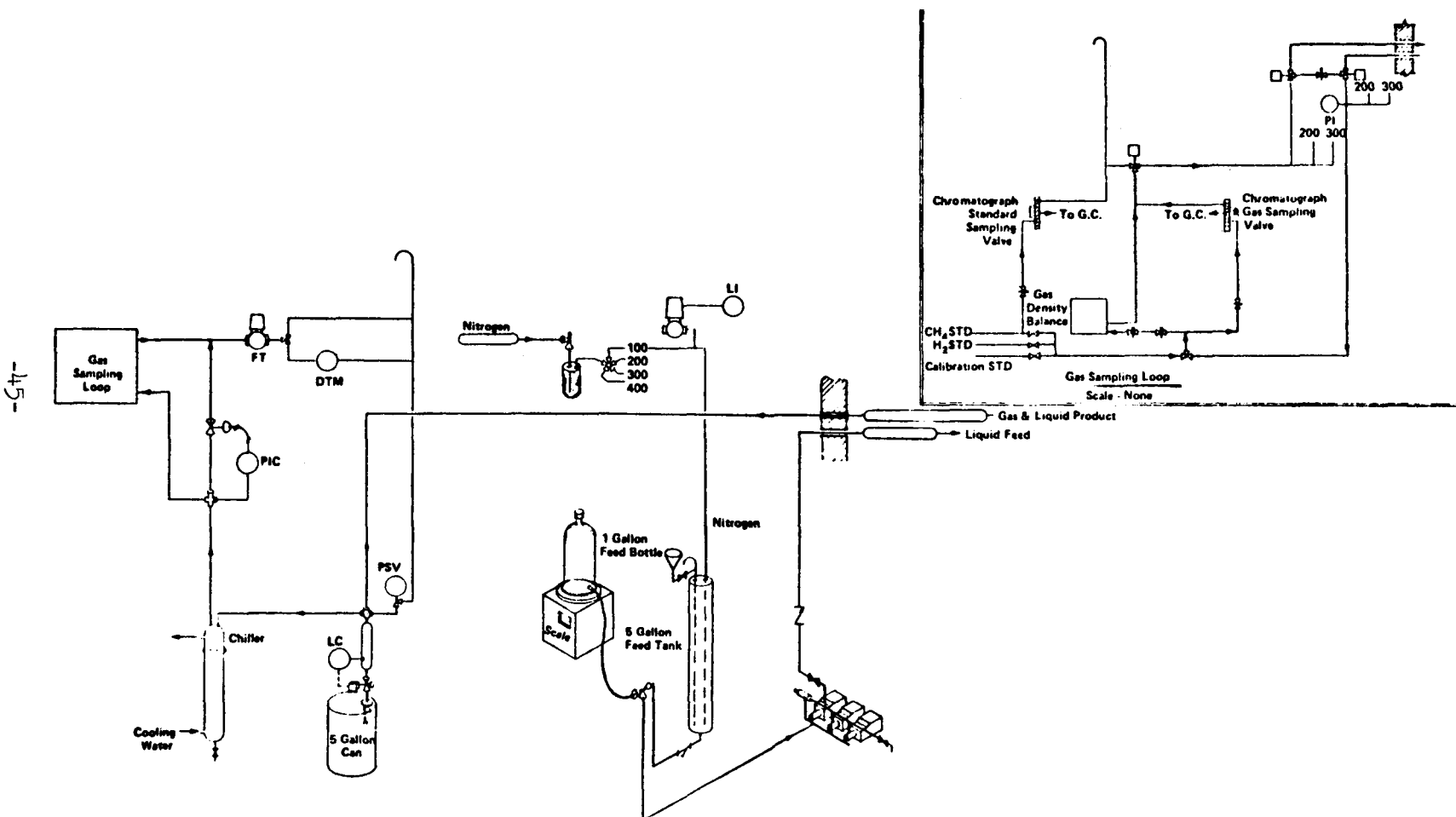


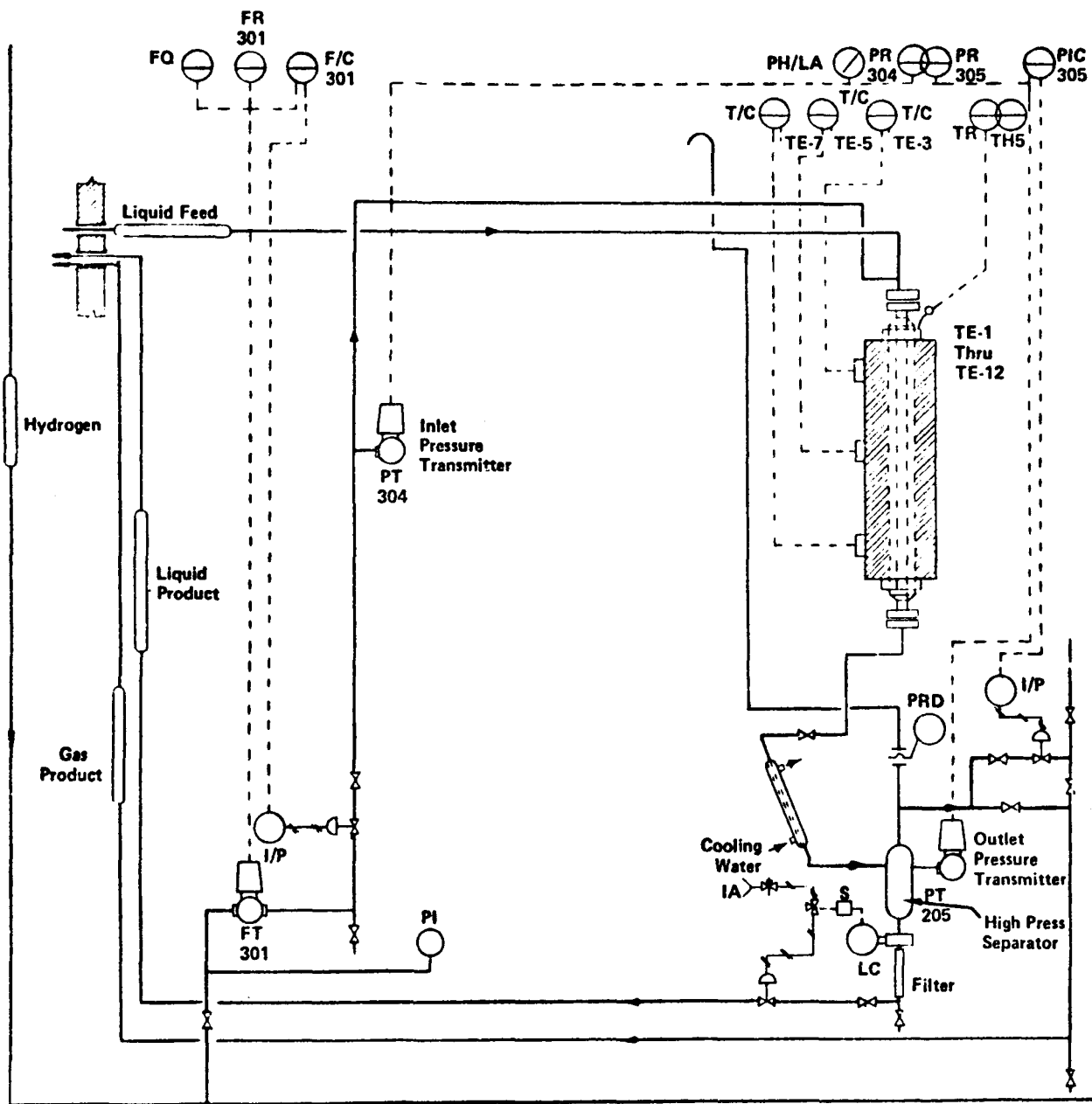
ORIGINAL REACTOR

Figure 1

Figure II

ORIGINAL FEED AND PRODUCT  
RECOVERY EQUIPMENT



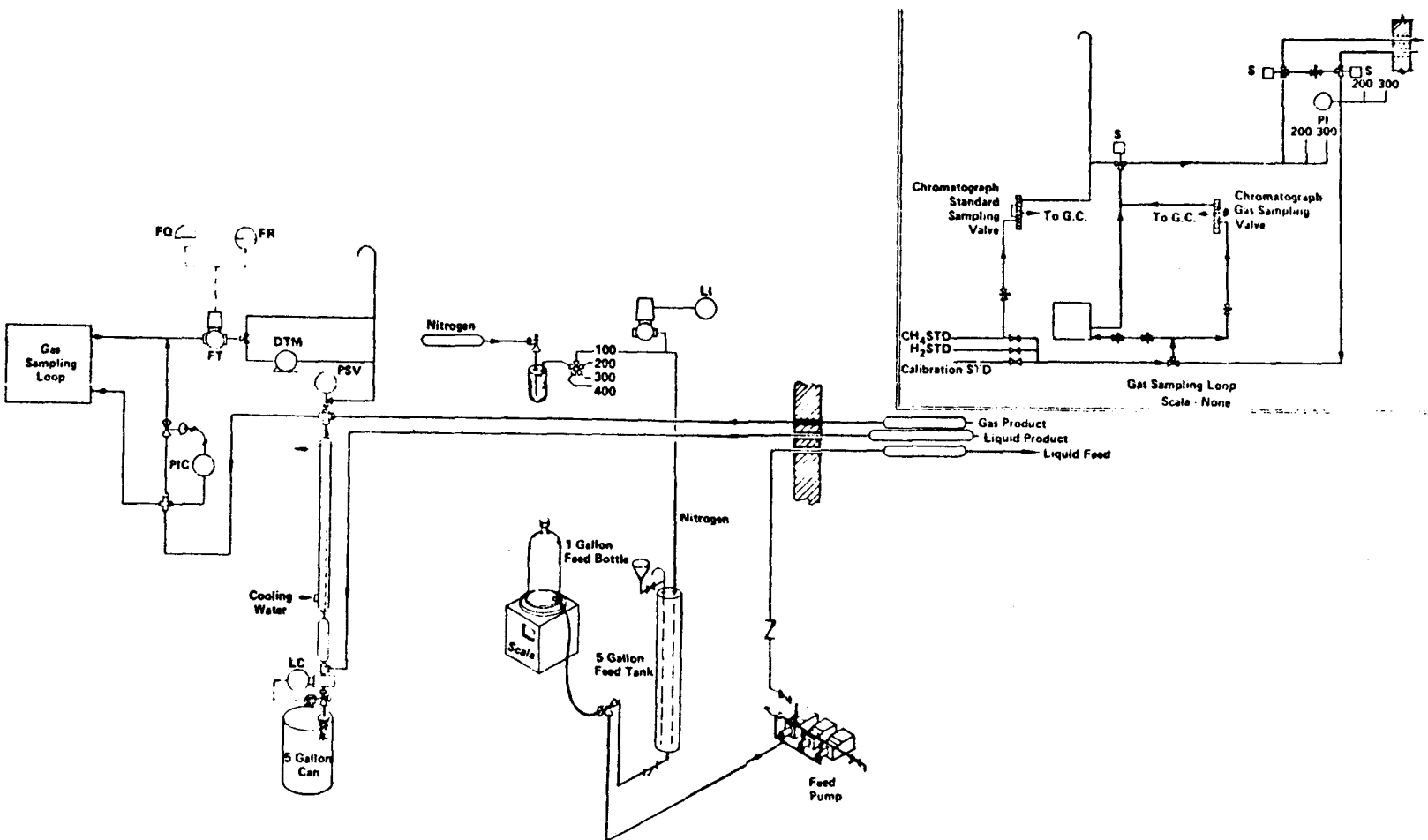


MODIFIED REACTOR

Figure III

Figure IV

MODIFIED FEED AND PRODUCT RECOVERY EQUIPMENT



Conax® fittings and drilled with some dozen very small holes. Four 0.062 inch Megapak® type thermocouples are led through the Conax® fitting and sealed leak tight against the reactor pressure. The four internal thermocouples are positioned to measure temperature variations across the catalyst bed. One reactor has a one inch schedule 40 Type 446 stainless steel pipe inside a machined pressure shell of Type 316 stainless steel. The maximum operating pressure at temperatures below 1350°F is 1000 psig for this reactor. Because of the low pressure rating, this reactor was used for reforming runs. The other two reactors have a one inch schedule 80 Type 430 stainless steel pipe inside a machined pressure shell of "MO-RE" 1®. The maximum operating pressure at temperatures below 1250°F is 3000 psig for these reactors. Hydrocracking and hydro-treating experiments were conducted in these reactors.

High Pressure Separator - The reactor effluent is cooled in a tubular heat exchanger and the gas products are separated from the liquid in the high pressure separator. A pressure transmitter on the separator provides a signal for the recording of reactor outlet pressure, and through a controller and control valve, the back pressure control on the reactor. The gases are let down through the reactor pressure control valve, while the liquid level in the high pressure separator is controlled by a sonic level switch, which periodically energizes a solenoid valve which in turn opens the liquid level control valve. The liquid and gaseous products are recombined in the transfer line to the low pressure receiver in the original design. This was modified later when separate lines for each were provided.

Low Pressure Separator - In the original design the recombined gas and liquid products entered the low pressure separator at about 3 psig. Here the final liquid-gas separation took place. In the modified design only the liquid product entered the separator where the gas produced from the flash associated with the pressure drop from the high pressure to low pressure separators was disengaged from the liquid. Both gas streams were then recombined. The liquid level is controlled by a sonic level switch which operates a solenoid valve, dropping the liquid into an appropriate receiver. The gaseous products are further cooled in a tubular heat exchanger. A Taylor Fulscope® controller and control valve provide the 3 psig back pressure control. The back pressure control provides a continuous flow gas sample through paired solenoid valves located in the control room near the gas sampling loop and hence back to a flow transmitter. When energized, the paired solenoid valves provide a gas sample for

analysis while maintaining the total gas flow through the flow transmitter. The flow rate is displayed at the control panel and is integrated, the square root integral is displayed as well. If desired, the total vent gas flow can be routed through a test meter for verification of the vent rate integral. The Foxboro integral orifice differential pressure cell flow transmitter used to measure the gaseous product flow rate was equipped with orifices ranging from 0.015 to 0.050 inches in diameter and operated at differential pressures from 0 to 20 inches of water. This flow transmitter was also calibrated before the start of each run with a Foxboro current calibrator.

#### DISTILLATION EQUIPMENT

The 20 gallon Podbielniak distillation column used to separate the various oils is designed to run unattended. It is capable of handling either light or heavy oils. The distillation kettle, column, and receivers are steam traced and the overhead condenser is cooled by a tempered water cooling system. A cold trap is also provided for very low boiling materials.

Distillations may be conducted at atmospheric pressure or under vacuum. The vacuum is provided by two vacuum pumps and is controlled by setting the vacuum rate metering valve and setting the set point using a mercury switch.

The boil-up rate is controlled by a pressure drop controller which controls the kettle heaters. The kettle is equipped with a hot oil temperature limit switch to prevent boiling the kettle dry.

The vapors going overhead are condensed in a reflux condenser at the top of the column. Condensed vapors are removed from the column just below the condenser. The overheads are split between reflux back to the column and overheads product by the overheads splitter which is controlled by two timers, one of which opens the valve in the overheads product line, and the other closes the valve. The overheads valve is maintained in the closed or total reflux position by the condenser temperature recorder controller when the cut point is reached.

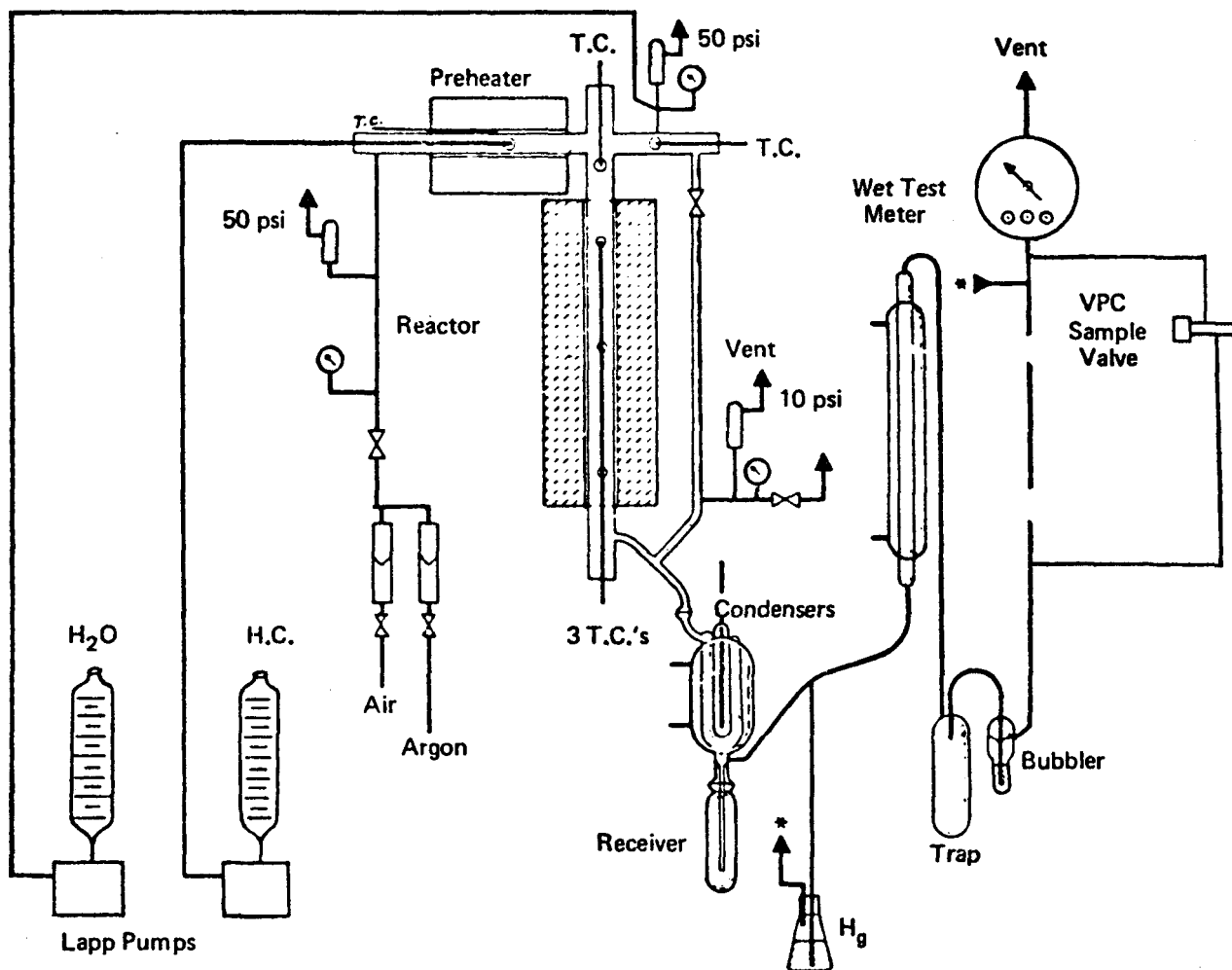
The cold trap provided for condensing very light materials can only be used for atmospheric distillations.

#### STEAM COIL CRACKING EQUIPMENT

The equipment used for the steam coil cracking experiments is shown in Figure V. Lapp metering pumps of 2000 ml/hr capacity are used to pump hydrocarbon and water from

Figure V

STEAM COIL CRACKING EQUIPMENT



graduated funnels into the reactor. After the water and liquid hydrocarbon are vaporized and preheated to about 500°C, the vapors enter the reactor where they are rapidly heated to cracking temperature. The hot effluent stream is cooled to below room temperature in a glass condenser using refrigerated glycol-water as coolant. The liquid products are collected in the receiver and the gases pass through a vapor phase chromatograph (V.P.C.) sampling valve and then through a wet test meter. The reactor and preheater are constructed of one inch Incoloy pipe and are electrically heated. The feed samples and both the liquid and gas phases of the cooled effluent stream were analyzed by V.P.C. methods. Gas samples were injected via two 7-Port Microtek sampling valves into the chromatographs for hydrogen and hydrocarbon analyses. An Aerograph Isothermal V.P.C. equipped with an activated charcoal column was used for hydrogen analysis with Argon as carrier gas. Using a standard set of operating conditions, the hydrogen concentration can be read from a standard curve of mole percent hydrogen versus peak area. The curve was prepared from analyses of known mixtures. An F&M temperature programmed Model 300 Chromatograph with a 10 ft flourosilicone on a activated alumina column was used for the analysis of the hydrocarbons in the gas phase. The liquid phase samples were first separated in a spinning band distillation column into an IBP-210°C cut, a 210-280°C, and a 280°C plus.

The IBP-210°C was analyzed using a squalane capillary column, 0.01 inch I.D. by 200 ft long. The 210-280°C was analyzed on a carbowax capillary column, 0.01 inch I.D. by 300 ft long. The 280°C plus material was not analyzed. Using the measured liquid sample weight and gas volume, the analyses of the two effluent streams were combined in the appropriate ratio to give the composition of the hot effluent stream from the reactor.

#### DATA REDUCTION TECHNIQUES

The data reduction techniques, methodology and assumptions described below were used to convert the hydroprocessing data to a useful form. With aid of the computer programs developed, fast accurate data reduction was possible.

Reactor Vent Gas Analysis - The objective of the vent gas analysis is to obtain material balance and hydrogen uptake information. To achieve this, the componential makeup of the vent gas and the mass flowrate must be determined. Vent gas hydrocarbons are quantitatively identified via gas chromatography. The sample injection



is followed by a constant volume injection of methane. By injecting a sample gas of known composition, a methane response factor ( $RF_{CH_4}$ ) may be defined as:

$$RF_{CH_4} = \frac{\text{Area \% of Pure } CH_4 \text{ Injection}}{\text{Area \% of Calibration Gas } CH_4} \times \text{mole \% } CH_4 \text{ in calibration gas}$$

Non-methane response factors are then related to the methane response factor in a computer program which uses area percent of each identified component in the gas as input data. Mole percent of each component and the corresponding weight percents are calculated. The unanalyzed portion of the gas is assumed to have a molecular weight of 2.016. The specific gravity is back calculated from these results and can be checked against the specific gravity measured on-line by a Beckman 3AM3 Gas Density balance. Weight percent carbon and hydrogen are also calculated. This program does not take into account the  $H_2O$ ,  $H_2S$ , and  $NH_4$  present in the vent gas.

SIMULATED DISTILLATION - The purpose of this analysis is to obtain a true boiling point distribution of a hydrocarbon. The assumption behind this test is that any hydrocarbon in the sample boiling at "x"°F will elute from the particular G.C. column used with the same retention time. A calibration mixture containing normal  $C_5$  to  $C_{44}$  paraffins with known boiling points are used to obtain a boiling point versus time correlation. The sample chromatogram is divided by the Varian® computer into constant area percents, the end of each segment correlating with a boiling point. The result is a set of data points relating weight percent off versus boiling point.

SPINNING BAND DISTILLATION - The purpose of this procedure is to separate a sample of the composite material produced from hydrocracking experiments into a 350°F minus naphtha and a 350°F plus bottoms. In this manner, the simulated distillation results can be checked against the weight percent off at 350°F. More important, however, is that the naphtha distilled can be further analyzed to obtain componential data. This number is also used to identify the weight percent of  $C_{10}^+$  material in a sample. The approximately 40 theoretical plates in this column allow for very accurate distillation cuts.

NAPHTHA COMPONENTIALS - The purpose of this analysis is to quantitatively identify the C<sub>4</sub> to C<sub>12</sub> hydrocarbons in a 375°F endpoint naphtha. The chromatogram of the sample is compared to a chromatogram with previously identified peaks. Peaks are assigned identification numbers. These identification numbers and their corresponding area percents are then fed into a program which calculates individual compound weight percent, mole percent, and liquid volume percent as well as the sample's average molecular weight, liquid specific gravity, API gravity, atomic H/C ratio and weight percent hydrogen. The compounds are then classified by carbon number and structural type. Weight percents and volume percents in each category are reported.

DATA REDUCTION PROGRAM - The purpose of this program is to combine the elemental and componential data from the vent gas, naphtha componential, and in the case of hydrocracking a weight percent off at 350°F (all C<sub>10</sub><sup>+</sup> material) in the appropriate ratio to give the composition of the total effluent leaving the reactor. Mass flow rate data obtained from the experiments conducted was also input data to the computer program. Hydrogen consumed or produced, as well as a C<sub>1</sub>-C<sub>9</sub> compounds classified by carbon number and structural type and the weight percent C<sub>10</sub><sup>+</sup> material for the total hydroprocessing product.

ELEMENTAL BALANCE PROGRAM - The purpose of this program is to provide a carbon, hydrogen, oxygen, nitrogen, and sulfur elemental balance check on the data obtained from hydroprocessing experiments. Analytical results for weight percent C, H, O, N, S in the feedstock and liquid product are combined with the vent gas analysis for weight percent carbon and hydrogen in the appropriate ratio, based on mass flow rate data from the experiments, to give the product/feed balance for the elements present. The difference between the weight percent hydrogen calculated for the feed and for the products yields the hydrogen consumption or production since elements are also calculated in mass flow units.

#### ANALYTICAL EQUIPMENT AND TECHNIQUES

The laboratory is equipped with a number of gas chromatograph (G.C.) instruments for performing various analyses of the samples from the coal liquefaction processes and from our laboratory processing experiments. Process vent gas and liquid streams are both analyzed by this procedure. A varian Aerograph Chromatography Data System with a model No. 220-20D, Class IV computer completes this analytical capability.

### NAPHTHA COMPONENTIAL

Analyses of C<sub>3</sub>-C<sub>9</sub> hydrocarbon components, up to a 350°F endpoint, in the liquid product are performed using a Hewlett Packard 5710A G.C. equipped as follows:

Detector: Flame Ionization Detector (F.I.D.)

Column: 200 ft, 0.01 in. I.D. Squalane Capillary Column

Temperature Program: Time 1 : 0  
Temp 1 : 0°C  
Rate : 2°C/min  
Temp 2 : 100°C  
Time 2 : Hold

A 0.5 micro liter sample is used.

### VENT GAS COMPONENTIAL

Analysis of vent gas, generated by laboratory processing experiments, for hydrocarbon components is performed by using a Hewlett Packard 5700A G.C. with a methane internal standard method. The G.C. is equipped as follows:

Detector: Thermal Conductivity Detector (T.C.)

Column: 20 ft Porapak Q 80/100 mesh

Temperature Program: Time 1 : 4 min  
Temp 1 : 70°C  
Rate : 16°C/min  
Temp 2 : 230°C  
Time 2 : 16 min

### SIMULATED DISTILLATION

An analysis to obtain a true boiling point distribution for a liquid hydrocarbon sample which boils below 1000°F is performed using a Hewlett Packard 5710A G.C. A Varian Aerograph Simulated Distillation package included with the Varian Chromatography Data System implements programs that acquire and accept information through a teletype and store the data in the computer. The computer calibrates the chromatograph, calculates the boiling point temperature, and lists these versus the percent samples eluted. A 0.2 micro liter sample is used. For hydrocarbon containing fractions that boil above 1000°F, an internal standard variation may be used. The method instituted on the Varian

apparatus is D 2887-73, adopted by the American Society for Testing and Materials (ASTM). The G.C. is equipped as follows:

Detector: F.I.D.

Column: 2 mm I.D. x 8 ft Bonded Methyl Silicone  
on 100-110 Anakrom AW

Effluent Splitter: 1:10

Temperature Program: Temp 1 : -20°C  
Time 1 : 0  
Rate : 16°C/min  
Temp 2 : 350°C  
Temp 2 : 4 min

#### CARBON AND HYDROGEN

Liquid samples are analyzed for the relative amounts of carbon and hydrogen present using a Model 1200 Chemical Data System Elemental Analyzer Peak Identifier. A 0.2 micro liter sample is passed over a copper oxide catalyst at 800°C where the carbon and hydrogen are converted to CO<sub>2</sub> and H<sub>2</sub>O respectively. The amounts of carbon dioxide and water are determined with a vapor phase chromatograph equipped with a Porapak column and a T.C. detector.

#### NITROGEN

Determination of the amount of nitrogen present in a liquid sample is made using an Antek Model 771 Pyroreactor. Nitrogen in the sample is converted to NO<sub>x</sub> at 1000°C. The level of nitrogen oxides produced is measured with a model 720 Chemiluminescent Nitrogen Detector and compared with a known standard.

#### SULFUR

The apparatus used for performing sulfur analyses on liquid samples is a Dohrmann Microcoulometric Reactor. Sulfur present in the samples is converted to SO<sub>2</sub>. Sulfur dioxide levels are determined by titrating with iodine and comparing results with known standards.

#### WATER

The concentration of water present in liquid samples is measured using a Photovolt Aquatest I analyzer. The Aquatest I is a coulometer, designed specifically for Karl Fischer titrations of water. Titration indicates the addition of a reagent. Electrical current adds the reagent in the case of the Aquatest I. Faraday's Law applies (1 equivalent = 96,500 coulombs), and the instrument reads out directly in micrograms of water.

### TOTAL OXYGEN

Total oxygen content of liquid hydrocarbon samples is determined using neutron activation analysis. A Karman Model A711 Neutron Generator ( $14.3 \times 10^6$  electron volts) produces the necessary activation energy. Samples are conveyed to and from source and detector via a pneumatic transfer system. A scintillation detector equipped with a sodium iodide crystal detects the induced radioactive isotope (Nitrogen 16) at energies of 6.1 and  $7.3 \times 10^6$  electron volts. The isotope has a 7.1 sec half-life, and decays back to oxygen, making the analysis a non-destructive method.

### MERCURY AND GALLIUM

Analyses of various liquid samples for Mercury and Gallium at a 100 ppb detection level are carried out using a General Electronics TRIGA Reactor. Samples are irradiated in the nuclear reactor for approximately two hours causing them to become radioactive. Radiation count rates characteristic for the elements being detected are measured with an ORTEC (Ge)(Li) detector and compared to known standards.

### COMMON METALS

Analyses of the liquid fractions for common metals are performed at detection levels from 0.1 to 3 ppm, depending on the particular element measured, by Atomic Emission. The samples are digested using sulfuric and nitric acids. The residue is taken up in a 20%  $\text{NaNO}_3$  buffer. An aliquot of the buffer solution is dried on the ends of graphite electrodes and excited in a 9 amp A.C. arc discharge. The energy emitted from the discharge is dispersed by a grating spectrograph and collected on a photographic plate. The intensity of the spectral lines produced from the atoms in the discharge are converted to concentrations.

### API GRAVITY

The API Gravity reported for the various fractions was determined using a hydrometer and was corrected to 60°F.

### HYDROPROCESSING AND STEAM COIL CRACKING RUN DATA

Tables of the run data obtained from the hydroprocessing and steam coil cracking experiments are presented. The reactor conditions listed are the averages for the data set. Conversions were calculated from simulated distillation results for the hydrocracking runs. The

componential data, including hydrogen consumption or production, was calculated from analyses performed on the gas and liquid products and combined in the computer programs. The elemental material balance data was derived from analytical results for elemental analyses and the flow rates from the run data and was calculated from a computer program.

## HYDROPROCESSING DATA

DATE 2-9-76  
 RUN, SAMPLE NO. 103-7-2-3  
 PROCESS: HYDROCRACKING MID-DISTILLATE  
 CATALYST: HARSHAW HT-400-1/8-E  
 FEED: SYNTHOIL ST. RUN MID-DISTILLATE

DATA BOOK NO. 103-7-2

REACTOR CONDITIONS

PRESSURE - PSIG	2460	TEMPERATURE °F	932
LHSV - VOL/VOL-HR	0.62	CATALYST VOLUME CC	150
MATERIAL BALANCE %	97.06	FORCE BALANCED ON	OIL PRODUCT
HYDROGEN RATIO SCF/BBL	19850	OIL PRODUCT RATE G/HR	69.5
OIL FEED RATE G/HR	92.9	TAIL GAS RATE G/HR	49.9
HYDROGEN FEED RATE G/HR	29.7	WATER PRODUCT G/HR	3.2

CONVERSIONS WEIGHT PERCENT

450°F + 79.6

550°F + 91.6

YIELD: G/100G OIL FEED

HYDROGEN	-3.14 <sup>A</sup>	-4.42 <sup>B</sup>	WATER	3.44
METHANE	2.25			
ETHANE	3.32			
PROPANE	3.42			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	3.11	.39				3.50
C <sub>5</sub>	1.05	.56	.42			2.04
C <sub>6</sub>	.85	.98	2.24	3.86	2.41	10.35
C <sub>7</sub>	.62	1.41	1.33	5.60	4.70	13.65
C <sub>8</sub>	.72	.30	2.05	2.68	3.62	9.37
C <sub>9</sub>	.23	.42	.25	.36	2.97	4.23
TOTAL	6.59	4.05	6.31	12.50	13.70	43.14
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	0.0		C <sub>10</sub> <sup>+</sup>	47.52		
HYDROGEN YIELD SCF/BBL	-1950 <sup>A</sup>		-2745 <sup>B</sup>			

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.3	9.3	.28	3.3	.74	100.0
HYDROGEN		31.97				31.97
TOTAL	86.3	41.27	.28	3.3	.30	132.01

PRODUCTS

LIQUID	65.76	9.05	.001	.024	.003	74.84
HC GAS	20.70	4.15				24.84
HYDROGEN		28.83				28.83
NH <sub>3</sub>		.06	.28			.34
H <sub>2</sub> O		.41		3.2		3.69
H <sub>2</sub> S		.05			.74	.79
TOTAL	86.46	42.55	.28	3.3	.74	133.33

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 2-16-76  
 RUN, SAMPLE NO. 103-7-5-2  
 PROCESS: HYDROCRACKING MID-DISTILLATE  
 CATALYST: HARSHAW HT-400-1/8-E  
 FEED: SYNTHOIL ST. RUN MID-DISTILLATE

DATA BOOK NO. 103-7-5

REACTOR CONDITIONS

PRESSURE - PSIG	2400	TEMPERATURE °F	917
LHSV - VOL/VOL-HR	0.91	CATALYST VOLUME CC	150
MATERIAL BALANCE %	98.95	FORCE BALANCED ON	OIL PRODUCT
HYDROGEN RATIO SCF/BBL	19100	OIL PRODUCT RATE G/HR	99.87
OIL FEED RATE G/HR	135.8	TAIL GAS RATE G/HR	72.70
HYDROGEN FEED RATE G/HR	41.77	WATER PRODUCT G/HR	5.00

CONVERSIONS WEIGHT PERCENT

450°F + 72.4

550°F + 86.6

YIELD: G/100G OIL FEED

HYDROGEN	-3.32 <sup>A</sup>	-4.26 <sup>B</sup>	WATER	3.68
METHANE	2.20			
ETHANE	3.37			
PROPANE	3.62			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	3.34	.45				3.79
C <sub>5</sub>	.88	.56	.32			1.76
C <sub>6</sub>	.61	.71	1.70	3.27	2.08	8.35
C <sub>7</sub>	.50	.84	.58	4.15	4.07	10.13
C <sub>8</sub>	.44	.21	1.52	1.80	3.14	7.11
C <sub>9</sub>	.15	.16	.25	.39	2.16	3.11
TOTAL	5.91	2.93	4.37	9.61	11.44	34.25
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	0.04		C <sub>10</sub> <sup>+</sup>	56.08		
HYDROGEN YIELD SCF/BBL	-2062 <sup>A</sup>		-2645 <sup>B</sup>			

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.3	9.3	.34	3.8	.30	100.00
HYDROGEN		30.76				30.76
TOTAL	86.3	40.06	.34	3.8	.30	130.76

PRODUCTS

LIQUID	64.67	8.75	.003	.045	.009	73.47
HC GAS	21.77	4.29				26.06
HYDROGEN		27.46				27.46
NH <sub>3</sub>		.06	.28			.34
H <sub>2</sub> O		.41		3.26		3.67
H <sub>2</sub> S		.05			.74	.79
TOTAL	86.44	41.02	.28	3.3	.74	131.79

A From Hydrogen Mass Balance

B From Elemental Balance



## HYDROPROCESSING DATA

DATE 2-27-76

DATA BOOK NO. 103-7-6

RUN, SAMPLE NO. 103-7-6-4

PROCESS: HYDROCRACKING MID-DISTILLATE

CATALYST: HARSHAW HT-400-1/8-E

FEED: SYNTHOIL ST. RUN MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	926
LHSV - VOL/VOL-HR	1.04	CATALYST VOLUME CC	100
MATERIAL BALANCE %	106.01	FORCE BALANCED ON	OIL PRODUCT
HYDROGEN RATIO SCF/BBL	17500	OIL PRODUCT RATE G/HR	70.21
OIL FEED RATE G/HR	103.00	TAIL GAS RATE G/HR	58.11
HYDROGEN FEED RATE G/HR	29.03	WATER PRODUCT G/HR	3.71

CONVERSIONS WEIGHT PERCENT

450°F + 77.4

550°F + 86.5

YIELD: G/100G OIL FEED

HYDROGEN	-4.93 <sup>A</sup>	-4.87 <sup>B</sup>	WATER	3.60
METHANE	2.59			
ETHANE	4.02			
PROPANE	5.73			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	6.99	.89				7.89
C <sub>5</sub>	1.98	1.17	.89			4.04
C <sub>6</sub>	1.13	.55	2.25	3.25	2.58	9.76
C <sub>7</sub>	.43	1.08	1.21	3.40	3.84	9.95
C <sub>8</sub>	.26	.19	1.09	1.68	3.03	6.25
C <sub>9</sub>	.17	.22	.10	.18	2.95	3.62
TOTAL	10.96	4.10	5.54	8.15	12.39	41.50
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>		0.17	C <sub>10</sub> <sup>+</sup>	47.28		
HYDROGEN YIELD SCF/BBL	-3060 <sup>A</sup>	-3025 <sup>B</sup>				

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.3	9.3	.28	3.3	.74	100.00
HYDROGEN		28.18				28.18
TOTAL	86.3	37.48	.28	3.3	.74	128.18
PRODUCTS						
LIQUID	60.05	7.98	.034	.102	.011	68.18
HC GAS	27.45	5.69				33.13
HYDROGEN		23.25				23.25
NH <sub>3</sub>		.05	.25			.30
H <sub>2</sub> O		.40		3.20		3.60
H <sub>2</sub> S		.05			.73	.78
TOTAL	87.50	37.42	.28	3.3	.74	129.24

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 3-4-76

DATA BOOK NO. 103-7-8

RUN, SAMPLE NO. 103-7-8-2

PROCESS: HYDROCRACKING MID-DISTILLATE

CATALYST: HARSHAW HT-400-1/8-E

FEED: SYNTHOIL ST. RUN MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2540	TEMPERATURE °F	932
LHSV - VOL/VOL-HR	1.31	CATALYST VOLUME CC	100
MATERIAL BALANCE %	100	FORCE BALANCED ON	--
HYDROGEN RATIO SCF/BBL	19550	OIL PRODUCT RATE G/HR	104.85
OIL FEED RATE G/HR	130.26	TAIL GAS RATE G/HR	61.63
HYDROGEN FEED RATE G/HR	41.02	WATER PRODUCT G/HR	4.80

CONVERSIONS WEIGHT PERCENT

450°F + 71.2

550°F + 83.2

YIELD: G/100G OIL FEED

HYDROGEN	-2.88 <sup>A</sup>	-3.65 <sup>B</sup>	WATER	3.68
METHANE	2.66			
ETHANE	3.61			
PROPANE	3.08			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	1.94	.29				2.23
C <sub>5</sub>	.65	.34	.40			1.39
C <sub>6</sub>	.57	.26	1.45	2.63	2.09	7.00
C <sub>7</sub>	.43	.71	1.05	3.66	5.24	11.09
C <sub>8</sub>	.05	.25	1.37	2.11	4.20	7.98
C <sub>9</sub>	.20	.26	.26	.37	2.45	3.54
TOTAL	3.84	2.11	4.52	8.77	13.99	33.22
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>		0.23	C <sub>10</sub> <sup>+</sup>	56.00		
HYDROGEN YIELD SCF/BBL	-1784 <sup>A</sup>	-2265 <sup>B</sup>				

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.3	9.3	.28	3.3	.74	100.00
HYDROGEN		31.49				31.49
TOTAL	86.3	40.79	.28	3.3	.74	131.49
PRODUCTS						
LIQUID	71.24	9.18	.004	.105	.010	80.53
HC GAS	15.33	3.27				18.60
HYDROGEN		28.61				28.61
NH <sub>3</sub>		.06	.28			.34
H <sub>2</sub> O		.40		3.20		3.60
H <sub>2</sub> S		.05			.73	.78
TOTAL	86.57	41.56	.28	3.3	.74	132.46

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 3-11-76  
 RUN, SAMPLE NO. 103-7-10-2  
 PROCESS: HYDROCRACKING MID-DISTILLATE  
 CATALYST: HARSHAW HT-400-1/8-E  
 FEED: SYNTHOIL ST. RUN MID-DISTILLATE

DATA BOOK NO. 103-7-10

REACTOR CONDITIONS

PRESSURE - PSIG	2430	TEMPERATURE °F	924
LHSV - VOL/VOL-HR	1.47	CATALYST VOLUME CC	100
MATERIAL BALANCE %	99.33	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	17370	OIL PRODUCT RATE G/HR	105.12
OIL FEED RATE G/HR	146.5	TAIL GAS RATE G/HR	78.59
HYDROGEN FEED RATE G/HR	40.99	WATER PRODUCT G/HR	3.78

CONVERSIONS WEIGHT PERCENT

450°F + 70.0

550°F + 80.6

YIELD: G/100G OIL FEED

HYDROGEN	-2.43 <sup>A</sup>	-3.88 <sup>B</sup>	WATER	2.58
METHANE	2.60			
ETHANE	4.57			
PROPANE	4.36			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	3.44	.52				3.96
C <sub>5</sub>	.97	.55	.56			2.08
C <sub>6</sub>	.88	.38	1.79	2.68	2.39	8.13
C <sub>7</sub>	.53	.96	.77	3.63	5.21	11.10
C <sub>8</sub>	.23	.20	1.17	1.60	2.64	5.84
C <sub>9</sub>	.17	.28	.17	.21	2.03	2.86
TOTAL	6.22	2.88	4.46	8.13	12.28	33.96
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>		.19	C <sub>10</sub> <sup>+</sup>	54.12		
HYDROGEN YIELD SCF/BBL	-1510 <sup>A</sup>	-2410 <sup>B</sup>				

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.3	9.3	.28	3.3	.74	100.00
HYDROGEN		27.98				27.98
TOTAL	86.3	37.28	.28	3.3	.74	127.98
PRODUCTS						
LIQUID	63.57	7.96	.057	.129	.014	71.74
HC GAS	23.33	4.72				28.05
HYDROGEN		25.55				25.55
NH <sub>3</sub>		.05	.22			.27
H <sub>2</sub> O		.40		.17		3.57
H <sub>2</sub> S		.05			.73	.78
TOTAL	86.91	38.73	.28	3.3	.74	129.96

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 3-16-76  
 RUN, SAMPLE NO. 103-7-11-2  
 PROCESS: HYDROCRACKING MID-DISTILLATE  
 CATALYST: HARSHAW HT-400-1/8-E  
 FEED: SYNTHOIL ST. RUN MID-DISTILLATE

DATA BOOK NO. 103-7-11

REACTOR CONDITIONS

PRESSURE - PSIG	1550	TEMPERATURE °F	924
LHSV - VOL/VOL-HR	1.11	CATALYST VOLUME CC	100
MATERIAL BALANCE %	98.30	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	16095	OIL PRODUCT RATE G/HR	84.00
OIL FEED RATE G/HR	110.60	TAIL GAS RATE G/HR	53.37
HYDROGEN FEED RATE G/HR	28.67	WATER PRODUCT G/HR	1.90

CONVERSIONS WEIGHT PERCENT

450°F + 5.80

550°F + 68.7

YIELD: G/100G OIL FEED

HYDROGEN	+1.12 <sup>A</sup>	-2.54 <sup>B</sup>	WATER	1.72
METHANE	2.18			
ETHANE	3.59			
PROPANE	3.03			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	2.15	.34				2.49
C <sub>5</sub>	.83	.45	.48			1.75
C <sub>6</sub>	.73	.31	1.38	2.15	1.92	6.50
C <sub>7</sub>	.38	.71	.51	2.57	4.58	8.74
C <sub>8</sub>	.12	.13	.78	1.02	3.90	5.95
C <sub>9</sub>	.14	.13	.12	.39	2.02	2.79
TOTAL	4.35	2.07	3.27	6.13	12.42	28.24
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>		0.14	C <sub>10</sub> <sup>+</sup>	60.84		
HYDROGEN YIELD SCF/BBL	+72 <sup>A</sup>		-1580 <sup>B</sup>			

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.3	9.3	.28	3.3	.74	100.00
HYDROGEN		25.92				25.92
TOTAL	86.3	35.22	.28	3.3	.74	125.92

PRODUCTS

LIQUID	68.13	7.67	.056	.138	.006	76.00
HC GAS	18.38	3.67				22.05
HYDROGEN		26.04				26.04
NH <sub>3</sub>		.05	.22			.27
H <sub>2</sub> O		.40		3.16		3.56
H <sub>2</sub> S		.05			.73	.78
TOTAL	86.51	37.88	.28	3.3	.74	128.70

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 3-23-76

DATA BOOK NO. 103-7-12

RUN, SAMPLE NO. 103-7-12-2

PROCESS: HYDROCRACKING MID-DISTILLATE

CATALYST: HARSHAW HT-400-1/8-E

FEED: SYNTHOIL ST. RUN MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	1520	TEMPERATURE °F	946
LHSV - VOL/VOL-HR	0.95	CATALYST VOLUME CC	100
MATERIAL BALANCE %	98.99	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	18660	OIL PRODUCT RATE G/HR	61.04
OIL FEED RATE G/HR	94.85	TAIL GAS RATE G/HR	59.31
HYDROGEN FEED RATE G/HR	28.50	WATER PRODUCT G/HR	3.00

CONVERSIONS WEIGHT PERCENT

450°F + 71.1

550°F + 80.0

YIELD: G/100G OIL FEED

HYDROGEN	-.72 <sup>A</sup>	-2.88 <sup>B</sup>	WATER	3.16
METHANE	3.67			
ETHANE	4.67			
PROPANE	5.15			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	3.40	.61				4.01
C <sub>5</sub>	1.03	.61	.78			2.42
C <sub>6</sub>	.98	.45	2.64	1.74	3.08	8.89
C <sub>7</sub>	.55	1.05	.49	2.03	6.23	10.35
C <sub>8</sub>	.20	.13	.59	.56	3.81	5.29
C <sub>9</sub>	.18	.13	.11	.29	1.83	2.54
TOTAL	6.34	2.97	4.61	4.62	14.95	33.50
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	0.0		C <sub>10</sub> <sup>+</sup>	50.53		
HYDROGEN YIELD SCF/BBL	-450 <sup>A</sup>		-1790 <sup>B</sup>			

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.3	9.3	.28	3.3	.74	100.00
HYDROGEN		30.05				30.05
TOTAL	86.3	39.35	.28	3.3	.74	130.05

PRODUCTS

LIQUID	58.05	6.18	.059	.097	.015	64.40
HC GAS	27.65	5.50				33.16
HYDROGEN		29.32				29.33
NH <sub>3</sub>		.05	.22			.27
H <sub>2</sub> O		.40		3.20		3.60
H <sub>2</sub> S		.05			.72	.77
TOTAL	85.70	41.50	.28	3.3	.74	131.53

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 3-26-76  
 RUN, SAMPLE NO. 103-7-14-2  
 PROCESS: HYDROCRACKING MID-DISTILLATE  
 CATALYST: HARSHAW HT-400-1/8-E  
 FEED: SYNTHOIL ST. RUN MID-DISTILLATE

DATA BOOK NO. 103-7-14

REACTOR CONDITIONS

PRESSURE - PSIG	2510	TEMPERATURE °F	947
LHSV - VOL/VOL-HR	0.88	CATALYST VOLUME CC	100
MATERIAL BALANCE %	99.45	FORCE BALANCED ON	--
HYDROGEN RATIO SCF/BBL	20460	OIL PRODUCT RATE G/HR	50.2
OIL FEED RATE G/HR	87.43	TAIL GAS RATE G/HR	63.03
HYDROGEN FEED RATE G/HR	28.81	WATER PRODUCT G/HR	2.37

CONVERSIONS WEIGHT PERCENT

450°F + 80.5

550°F + 85.8

YIELD: G/100G OIL FEED

HYDROGEN	-3.54 <sup>A</sup>	-4.39 <sup>B</sup>	WATER	2.71
METHANE	4.04			
ETHANE	5.82			
PROPANE	6.65			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	5.19	.81				5.99
C <sub>5</sub>	1.37	.78	1.00			3.15
C <sub>6</sub>	1.15	.46	3.38	2.91	3.80	11.70
C <sub>7</sub>	.74	1.54	.81	3.74	6.37	13.20
C <sub>8</sub>	.44	.19	.84	1.36	3.31	6.14
C <sub>9</sub>	.19	.20	.08	.25	2.09	2.82
TOTAL	9.08	3.97	6.11	8.27	15.57	43.00
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	0.0		C <sub>10</sub> <sup>+</sup>	40.55		

HYDROGEN YIELD SCF/BBL -2190<sup>A</sup> -2725<sup>B</sup>

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.3	9.3	.28	3.3	.74	100.00
HYDROGEN		32.95				32.95
TOTAL	86.3	42.25	.28	3.3	.74	132.95

PRODUCTS

LIQUID	50.93	6.14	.105	.208	.022	57.41
HC GAS	35.57	7.07				42.65
HYDROGEN		29.42				29.42
NH <sub>3</sub>		.04	.18			.22
H <sub>2</sub> O		.39		3.09		3.48
H <sub>2</sub> S		.05			.72	.77
TOTAL	86.50	43.11	.28	3.3	.74	133.95

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 3-29-76  
 RUN, SAMPLE NO. 103-7-14-3  
 PROCESS: HYDROCRACKING MID-DISTILLATE  
 CATALYST: HARSHAW HT-400-1/8-E  
 FEED: SYNTHOIL ST. RUN MID-DISTILLATE

DATA BOOK NO. 103-7-14

REACTOR CONDITIONS

PRESSURE - PSIG	2540	TEMPERATURE °F	950
LHSV - VOL/VOL-HR	0.97	CATALYST VOLUME CC	100
MATERIAL BALANCE %	97.14	FORCE BALANCED ON	HYDROGEN
HYDROGEN RATIO SCF/BBL	15970	OIL PRODUCT RATE G/HR	55.90
OIL FEED RATE G/HR	96.8	TAIL GAS RATE G/HR	62.50
HYDROGEN FEED RATE G/HR	24.9	WATER PRODUCT G/HR	3.30

CONVERSIONS WEIGHT PERCENT

450°F + 83.5

550°F + 89.0

YIELD: G/100G OIL FEED

HYDROGEN	-3.24 <sup>A</sup>	-4.62 <sup>B</sup>	WATER	3.41
METHANE	4.17			
ETHANE	6.57			
PROPANE	7.07			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	5.65	.88				6.52
C <sub>5</sub>	1.39	.84	.61			2.84
C <sub>6</sub>	.94	.89	3.15	2.82	3.86	11.67
C <sub>7</sub>	.72	1.44	1.01	3.59	6.40	13.16
C <sub>8</sub>	.32	.33	.90	1.23	2.38	5.15
C <sub>9</sub>	.22	.20	.15	.39	2.80	3.75
TOTAL	9.23	4.59	5.82	8.02	15.43	43.10
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>		.01	C <sub>10</sub> <sup>+</sup>	38.10		
HYDROGEN YIELD SCF/BBL	-2010 <sup>A</sup>	-2870 <sup>B</sup>				

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.3	9.3	.28	3.3	.74	100.00
HYDROGEN		25.72				25.72
TOTAL	86.3	35.02	.28	3.3	.74	125.72

PRODUCTS

LIQUID	51.28	6.29	.055	.136	.016	57.78
HC GAS	34.92	7.13				42.05
HYDROGEN		22.48				22.48
NH <sub>3</sub>		.05	.23			.28
H <sub>2</sub> O		.40		3.16		3.56
H <sub>2</sub> S		.05			.72	.77
TOTAL	86.20	36.40	.28	3.3	.74	126.92

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 3-31-76  
 RUN, SAMPLE NO. 103-7-14-4  
 PROCESS: HYDROCRACKING MID-DISTILLATE  
 CATALYST: HARSHAW HT-400-1/8-E  
 FEED: SYNTHOIL ST. RUN MID-DISTILLATE

DATA BOOK NO. 103-7-14

REACTOR CONDITIONS

PRESSURE - PSIG	2690	TEMPERATURE °F	950
LHSV - VOL/VOL-HR	1.04	CATALYST VOLUME CC	100
MATERIAL BALANCE %	97.77	FORCE BALANCED ON	HYDROGEN
HYDROGEN RATIO SCF/BBL	15350	OIL PRODUCT RATE G/HR	60.0
OIL FEED RATE G/HR	103.30	TAIL GAS RATE G/HR	65.61
HYDROGEN FEED RATE G/HR	25.54	WATER PRODUCT G/HR	3.23

CONVERSIONS WEIGHT PERCENT

450°F + 83.5

550°F + 89.1

YIELD: G/100G OIL FEED

HYDROGEN	-1.93 <sup>A</sup>	-4.42 <sup>B</sup>	WATER	3.13
METHANE	4.15			
ETHANE	6.44			
PROPANE	6.64			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	5.08	.80				5.88
C <sub>5</sub>	1.27	.76	.95			2.98
C <sub>6</sub>	1.08	.47	3.15	3.07	3.83	11.59
C <sub>7</sub>	.73	1.50	1.08	3.91	6.36	13.58
C <sub>8</sub>	.26	.29	1.33	1.22	3.89	6.99
C <sub>9</sub>	.22	.21	.28	.36	2.49	3.55
TOTAL	8.64	4.03	6.79	8.55	16.57	44.58
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	0.0		C <sub>10</sub> <sup>+</sup>	36.96		
HYDROGEN YIELD SCF/BBL	-1195 <sup>A</sup>		-2745 <sup>B</sup>			

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.3	9.3	.28	3.3	.74	100.00
HYDROGEN		24.72				24.72
TOTAL	86.3	34.02	.28	3.3	.74	124.72

PRODUCTS

LIQUID	51.58	6.33	.062	.132	.015	58.12
HC GAS	33.80	6.89				40.68
HYDROGEN		22.80				22.80
NH <sub>3</sub>		.05	.22			.27
H <sub>2</sub> O		.40		.16		3.56
H <sub>2</sub> S		.05			.73	.78
TOTAL	85.38	36.52	.28	3.3	.74	126.21

A From Hydrogen Mass Balance

B From Elemental Balance



## HYDROPROCESSING DATA

DATE 4-9-76  
 RUN, SAMPLE NO. 103-7-17-2  
 PROCESS: HYDROCRACKING MID-DISTILLATE  
 CATALYST: HARSHAW HT-400-1/8-E  
 FEED: SYNTHOIL 2ND PASS MID-DISTILLATE

DATA BOOK NO. 103-7-17

REACTOR CONDITIONS

PRESSURE - PSIG	2525	TEMPERATURE °F	950
LHSV - VOL/VOL-HR	0.98	CATALYST VOLUME CC	100
MATERIAL BALANCE %	97.62	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	12080	OIL PRODUCT RATE G/HR	50.2
OIL FEED RATE G/HR	84.3	TAIL GAS RATE G/HR	53.06
HYDROGEN FEED RATE G/HR	18.96	WATER PRODUCT G/HR	--

CONVERSIONS WEIGHT PERCENT

450°F + 87.8

550°F + 85.3

YIELD: G/100G OIL FEED

HYDROGEN	-1.92 <sup>A</sup>	-3.44 <sup>B</sup>	WATER	---
METHANE	3.84			
ETHANE	4.77			
PROPANE	6.27			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	6.28	1.12				7.40
C <sub>5</sub>	1.84	1.18	1.42			4.44
C <sub>6</sub>	1.39	.68	5.08	1.04	4.78	12.96
C <sub>7</sub>	.87	2.55	1.67	2.60	7.71	15.39
C <sub>8</sub>	.40	.47	1.15	.74	2.85	5.61
C <sub>9</sub>	.34	.50	.33	.69	3.53	5.39
TOTAL	11.12	6.50	9.65	5.07	18.87	51.20
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	0.0		C <sub>10</sub> <sup>+</sup>	35.82		
HYDROGEN YIELD SCF/BBL	-1030 <sup>A</sup>		-1850 <sup>B</sup>			

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	89.2	10.6	.046	.12	.012	99.98
HYDROGEN		22.49				22.49
TOTAL	89.2	33.09	.046	.12	.012	122.47
PRODUCTS						
LIQUID	52.17	7.03	.001	.304	.010	59.51
HC GAS	35.32	7.02				42.34
HYDROGEN		20.72				20.72
NH <sub>3</sub>		.01	.045			.055
H <sub>2</sub> O		-.023		-.184		-.207
H <sub>2</sub> S		.000			.002	.002
TOTAL	87.48	34.76	.046	.12	.012	122.42

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 4-21-76

DATA BOOK NO. 103-7-17

RUN, SAMPLE NO. 103-7-17-4

PROCESS: HYDROCRACKING MID-DISTILLATE

CATALYST: HARSHAW HT-400-1/8-E

FEED: SYNTHOIL 2ND PASS MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2525	TEMPERATURE °F	946
LHSV - VOL/VOL-HR	1.00	CATALYST VOLUME CC	100
MATERIAL BALANCE %	92.72	FORCE BALANCED ON	HYDROGEN
HYDROGEN RATIO SCF/BBL	6900	OIL PRODUCT RATE G/HR	63.25
OIL FEED RATE G/HR	85.88	TAIL GAS RATE G/HR	33.67
HYDROGEN FEED RATE G/HR	11.04	WATER PRODUCT G/HR	--

CONVERSIONS WEIGHT PERCENT

450°F + 74.8

550°F + 61.8

YIELD: G/100G OIL FEED

HYDROGEN	-3.00 <sup>A</sup>	-2.69 <sup>B</sup>	WATER ---
METHANE	2.99		
ETHANE	3.94		
PROPANE	5.63		

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	5.13	.89				6.02
C <sub>5</sub>	1.37	.84	.96			3.17
C <sub>6</sub>	.93	.46	3.18	1.06	4.47	10.10
C <sub>7</sub>	.66	1.40	1.41	1.48	5.83	10.78
C <sub>8</sub>	.37	.28	.97	.69	2.98	5.29
C <sub>9</sub>	.23	.31	.35	.49	2.47	3.86
TOTAL	8.70	4.18	6.87	3.72	15.75	39.21
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	0.0		C <sub>10</sub> <sup>+</sup>	51.19		
HYDROGEN YIELD SCF/BBL	-1610 <sup>A</sup>		-1440 <sup>B</sup>			

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	89.2	10.6	.046	.12	.012	99.98
HYDROGEN		12.86				12.86
TOTAL	89.2	23.46	.046	.12	.012	112.84
PRODUCTS						
LIQUID	65.33	8.25	.000	.168	.000	73.74
HC GAS	24.29	5.04				29.33
HYDROGEN		9.84				9.84
NH <sub>3</sub>		.010	.046			.056
H <sub>2</sub> O		-.006		-.048		-.054
H <sub>2</sub> S		.001			.012	.013
TOTAL	89.62	23.13	.046	.12	.012	112.92

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 4-21-76

DATA BOOK NO. 103-7-17

RUN, SAMPLE NO. 103-7-17-4

PROCESS: HYDROCRACKING MID-DISTILLATE

CATALYST: HARSHAW HT-400-1/8-E

FEED: SYNTHOIL 2ND PASS MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2525	TEMPERATURE °F	946
LHSV - VOL/VOL-HR	1.00	CATALYST VOLUME CC	100
MATERIAL BALANCE %	92.72	FORCE BALANCED ON	HYDROGEN
HYDROGEN RATIO SCF/BBL	6900	OIL PRODUCT RATE G/HR	63.25
OIL FEED RATE G/HR	85.88	TAIL GAS RATE G/HR	33.67
HYDROGEN FEED RATE G/HR	11.04	WATER PRODUCT G/HR	--

CONVERSIONS WEIGHT PERCENT

450°F + 74.8

550°F + 61.8

YIELD: G/100G OIL FEED

HYDROGEN	-3.00 <sup>A</sup>	-2.69 <sup>B</sup>	WATER	---
METHANE	2.99			
ETHANE	3.94			
PROPANE	5.63			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	5.13	.89				6.02
C <sub>5</sub>	1.37	.84	.96			3.17
C <sub>6</sub>	.93	.46	3.18	1.06	4.47	10.10
C <sub>7</sub>	.66	1.40	1.41	1.48	5.83	10.78
C <sub>8</sub>	.37	.28	.97	.69	2.98	5.29
C <sub>9</sub>	.23	.31	.35	.49	2.47	3.86
TOTAL	8.70	4.18	6.87	3.72	15.75	39.21
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	0.0		C <sub>10</sub> <sup>+</sup>	51.19		

HYDROGEN YIELD SCF/BBL	-1610 <sup>A</sup>	-1440 <sup>B</sup>
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ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	89.2	10.6	.046	.12	.012	99.98
HYDROGEN		12.86				12.86
TOTAL	89.2	23.46	.046	.12	.012	112.84

PRODUCTS

LIQUID	65.33	8.25	.000	.168	.000	73.74
HC GAS	24.29	5.04				29.33
HYDROGEN		9.84				9.84
NH <sub>3</sub>		.010	.046			.056
H <sub>2</sub> O		-.006		-.048		-.054
H <sub>2</sub> S		.001			.012	.013
TOTAL	89.62	23.13	.046	.12	.012	112.92

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 4-23-76  
 RUN, SAMPLE NO. 103-7-17-5  
 PROCESS: HYDROCRACKING MID-DISTILLATE  
 CATALYST: HARSHAW HT-400-1/8-E  
 FEED: SYNTHOIL 2ND PASS MID-DISTILLATE

DATA BOOK NO. 103-7-17

REACTOR CONDITIONS

PRESSURE - PSIG	2525	TEMPERATURE °F	949
LHSV - VOL/VOL-HR	1.00	CATALYST VOLUME CC	100
MATERIAL BALANCE %	100.61	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	12000	OIL PRODUCT RATE G/HR	59.56
OIL FEED RATE G/HR	85.82	TAIL GAS RATE G/HR	46.08
HYDROGEN FEED RATE G/HR	19.18	WATER PRODUCT G/HR	--

CONVERSIONS WEIGHT PERCENT

450°F + 81.9

550°F + 70.9

YIELD: G/100G OIL FEED

HYDROGEN	-1.34 <sup>A</sup>	-2.69 <sup>B</sup>	WATER ---
METHANE	3.07		
ETHANE	3.94		
PROPANE	5.28		

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	5.16	.83				5.99
C <sub>5</sub>	1.45	.86	.94			3.25
C <sub>6</sub>	1.09	.52	3.10	.97	4.06	9.74
C <sub>7</sub>	.68	1.59	1.18	1.71	6.19	11.34
C <sub>8</sub>	.41	.33	.97	.79	3.28	5.78
C <sub>9</sub>	.24	.34	.31	.69	2.66	4.25
TOTAL	9.04	4.46	6.50	4.16	16.19	40.35
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	0.0		C <sub>10</sub> <sup>+</sup>	47.35		
HYDROGEN YIELD SCF/BBL	-720 <sup>A</sup>		-1440 <sup>B</sup>			

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	89.2	10.6	.046	.12	.012	99.98
HYDROGEN		22.35				22.35
TOTAL	89.2	32.95	.046	.12	.012	122.33

PRODUCTS

LIQUID	61.49	7.91	.000	.00	.001	69.40
HC GAS	26.56	5.35				31.91
HYDROGEN		20.81				20.81
NH <sub>3</sub>		.010	.046			.056
H <sub>2</sub> O		.015		.12		.135
H <sub>2</sub> S		.001			.011	.012
TOTAL	88.05	34.10	.046	.12	.012	122.32

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 4-29-76

DATA BOOK NO. 103-7-21

RUN, SAMPLE NO. 103-7-21-3

PROCESS: HYDROCRACKING MID-DISTILLATE

CATALYST: HARSHAW HT-400-1/8-E

FEED: SYNTHOIL 2ND PASS MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2520	TEMPERATURE °F	983
LHSV - VOL/VOL-HR	1.00	CATALYST VOLUME CC	100
MATERIAL BALANCE %	98.66	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	12300	OIL PRODUCT RATE G/HR	43.08
OIL FEED RATE G/HR	85.88	TAIL GAS RATE G/HR	62.47
HYDROGEN FEED RATE G/HR	19.67	WATER PRODUCT G/HR	--

CONVERSIONS WEIGHT PERCENT

450°F + 91.3

550°F + 76.3

YIELD: G/100G OIL FEED

HYDROGEN	-1.13 <sup>A</sup>	-3.27 <sup>B</sup>	WATER	---
METHANE	5.15			
ETHANE	6.55			
PROPANE	8.93			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	7.05	1.38				8.42
C <sub>5</sub>	1.67	1.14	1.65			4.46
C <sub>6</sub>	1.22	1.20	4.60	1.05	6.77	14.83
C <sub>7</sub>	.88	2.22	.56	1.71	8.31	13.70
C <sub>8</sub>	.33	1.52	.61	.60	3.65	6.71
C <sub>9</sub>	.20	.30	.31	.55	2.13	3.49
TOTAL	11.33	7.76	7.73	3.91	20.86	51.61
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	---		C <sub>10</sub> <sup>+</sup>	---		
HYDROGEN YIELD SCF/BBL	-604 <sup>A</sup>		-1760 <sup>B</sup>			

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	89.2	10.6	.046	.12	.012	99.98
HYDROGEN		22.9				22.90
TOTAL	89.2	33.5	.046	.12	.012	122.88
PRODUCTS						
LIQUID	44.75	5.42	.000	.401	.001	50.56
HC GAS	42.35	8.48				50.83
HYDROGEN		22.03				22.03
NH <sub>3</sub>		.010	.046			.056
H <sub>2</sub> O		-.035		-.281		-.317
H <sub>2</sub> S		.001			.011	.01
TOTAL	87.10	35.90	.046	.12	.012	123.17

A From Hydrogen Mass Balance

B From Elemental Balance

SYNTHOIL HYDROCRACKATE NAPHTHA  
FEED TO HYDROTREATING

	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	<u>CYCLO HEXANE</u>	<u>AROMATIC</u>
C <sub>6</sub>	0.41	0.27	1.76	2.88	2.50
C <sub>7</sub>	0.77	0.43	4.31	6.71	12.77
C <sub>8</sub>	0.16	0.76	2.58	7.52	13.04
C <sub>9</sub>	0.17	----	2.17	9.50	17.42
C <sub>10</sub> <sup>+</sup>	13.87				

## HYDROPROCESSING DATA

DATE 6-24-76

DATA BOOK NO. 103-6-13

RUN, SAMPLE NO. 103-6-13-3

PROCESS: HYDROTREATING

CATALYST: CYANAMID HDS-9A 1/16"

FEED: SYNTHOIL B-1 &amp; C-1 HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	1020	TEMPERATURE °F	680
LHSV - VOL/VOL-HR	2.05	CATALYST VOLUME CC	50
MATERIAL BALANCE %	98.1	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	3154	OIL PRODUCT RATE G/HR	78.88
OIL FEED RATE G/HR	83.58	TAIL GAS RATE G/HR	9.91
HYDROGEN FEED RATE G/HR	5.21	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	-0.62 <sup>A</sup>	-0.78 <sup>B</sup>	-0.37 <sup>C</sup>
GAS	11.86		
	NORMPARAF		
METHANE	---		
ETHANE	0.01		
PROPANE	0.01	ISOPARAF	
C <sub>4</sub>	0.07	---	
LIQUID	100.53		

AROMATIC SATURATION: G/100G OIL FEED      % OF FEED

C <sub>6</sub>	---	---
C <sub>7</sub>	1.66	13.3
C <sub>8</sub>	3.06	24.1
C <sub>9</sub>	2.27	13.3
TOTAL	6.99	15.0

HYDROGEN YIELD SCF/BBL	-315 <sup>A</sup>	-396 <sup>B</sup>	-188 <sup>C</sup>
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ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.8	11.7	.0051	.5100	.0030	100.00
HYDROGEN		6.23				6.23
TOTAL	87.8	17.93	.0051	.5100	.0030	106.23

PRODUCTS

LIQUID	82.51	11.68	.0025	.1700	.0008	94.36
HC GAS	5.41	0.80				6.21
HYDROGEN		5.61				5.61
NH <sub>3</sub>		.000	.0026			.003
H <sub>2</sub> O		.038		.3400		.378
H <sub>2</sub> S		.000			.0020	.002
TOTAL	87.92	18.13	.0051	.5100	.0030	106.56

A From Hydrogen Mass Balance

B From Elemental Balance

C From Aromatic Saturation

## HYDROPROCESSING DATA

DATE 6-22-76

DATA BOOK NO. 103-6-13

RUN, SAMPLE NO. 103-6-13-2

PROCESS: HYDROTREATING

CATALYST: CYANAMID HDS-9A 1/16"

FEED: SYNTHOIL B-1 &amp; C-1 HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	1025	TEMPERATURE °F	682
LHSV - VOL/VOL-HR	2.09	CATALYST VOLUME CC	50
MATERIAL BALANCE %	97.6	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	3125	OIL PRODUCT RATE G/HR	78.54
OIL FEED RATE G/HR	83.75	TAIL GAS RATE G/HR	10.44
HYDROGEN FEED RATE G/HR	5.23	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	-0.27 <sup>A</sup>	-0.95 <sup>B</sup>	-0.35 <sup>C</sup>
GAS	12.45		
	NORMPARAF		
METHANE	0.02		
ETHANE	0.01		
PROPANE	0.01	ISOPARAF	
C <sub>4</sub>	0.07	0.11	
LIQUID	100.05		

AROMATIC SATURATION: G/100G OIL FEED      % OF FEED

C <sub>6</sub>	--	--
C <sub>7</sub>	1.82	14.6
C <sub>8</sub>	2.80	22.0
C <sub>9</sub>	1.87	11.0
TOTAL	6.49	14.2

HYDROGEN YIELD SCF/BBL	-137 <sup>A</sup>	-483 <sup>B</sup>	-178 <sup>C</sup>
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ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.8	11.7	.0051	.5100	.0030	100.00
HYDROGEN		6.24				6.24
TOTAL	87.8	17.94	.0051	.5100	.0030	106.24
PRODUCTS						
LIQUID	81.8	11.8	.0021	.1900	.0011	93.79
HC GAS	5.65	0.85				6.50
HYDROGEN		.97				5.97
NH <sub>3</sub>		.001	.0030			.004
H <sub>2</sub> O		.036		.3200		.356
H <sub>2</sub> S		.000			.0019	.002
TOTAL	87.45	18.66	.0051	.5100	.0030	106.62

A From Hydrogen Mass Balance

B From Elemental Balance

C From Aromatic Saturation



## HYDROPROCESSING DATA

DATE 6-25-76

DATA BOOK NO. 103-6-15

RUN, SAMPLE NO. 103-6-15-2

PROCESS: HYDROTREATING

CATALYST: CYANAMID HDS-9A 1/16"

FEED: SYNTHOIL B-1 &amp; C-1 HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	1004	TEMPERATURE °F	682
LHSV - VOL/VOL-HR	2.08	CATALYST VOLUME CC	50
MATERIAL BALANCE %	97.4	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	1870	OIL PRODUCT RATE G/HR	80.79
OIL FEED RATE G/HR	83.32	TAIL GAS RATE G/HR	5.64
HYDROGEN FEED RATE G/HR	3.11	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	-0.72 <sup>A</sup>	-0.69 <sup>B</sup>	-0.32 <sup>C</sup>
GAS	6.77		
	NORMPARAF		
METHANE	---		
ETHANE	0.01		
PROPANE	0.01	ISOPARAF	
C <sub>4</sub>	0.06	---	
LIQUID	100.64		

AROMATIC SATURATION: G/100G OIL FEED

	<u>G/100G OIL FEED</u>	<u>% OF FEED</u>
C <sub>6</sub>	---	---
C <sub>7</sub>	1.79	14.4
C <sub>8</sub>	2.16	17.0
C <sub>9</sub>	1.93	19.8
TOTAL	5.88	16.4

HYDROGEN YIELD SCF/BBL	-360 <sup>A</sup>	-346 <sup>B</sup>	-160 <sup>C</sup>
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ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.8	11.7	.0051	.5100	.0030	100.00
HYDROGEN		3.73				3.73
TOTAL	87.8	15.43	.0051	.5100	.0030	103.73

PRODUCTS

LIQUID	84.95	11.91	.0020	.0233	.0005	96.89
HC GAS	3.24	0.48				3.72
HYDROGEN		3.01				3.01
NH <sub>3</sub>		.001	.0031			.004
H <sub>2</sub> O		.054		.4867		.541
H <sub>2</sub> S		.002			.0025	.005
TOTAL	88.19	15.46	.0051	.5100	.0030	104.17

A From Hydrogen Mass Balance

B From Elemental Balance

C From Aromatic Saturation

## HYDROPROCESSING DATA

DATE 8-4-76

DATA BOOK NO. 103-6-18

RUN, SAMPLE NO. 103-6-18-2

PROCESS: HYDROTREATING

CATALYST: CYANAMID HDS-9A 1/16"

FEED: SYNTHOIL 1 PASS HYDROTREATED B-1 &amp; C-1 HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	1000	TEMPERATURE °F	689
LHSV - VOL/VOL-HR	1.95	CATALYST VOLUME CC	50
MATERIAL BALANCE %	99.3	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	2058	OIL PRODUCT RATE G/HR	76.42
OIL FEED RATE G/HR	78.67	TAIL GAS RATE G/HR	5.45
HYDROGEN FEED RATE G/HR	3.20	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	-1.13 <sup>A</sup>	-1.02 <sup>B</sup>	-0.42 <sup>C</sup>
GAS	6.93		
	NORMPARAF		
METHANE	---		
ETHANE	0.01		
PROPANE	0.01	ISOPARAF	
C <sub>4</sub>	0.01	---	
LIQUID	101.10		

AROMATIC SATURATION: G/100G OIL FEED      % OF FEED

C <sub>6</sub>	0.24	13.1
C <sub>7</sub>	2.37	22.7
C <sub>8</sub>	2.65	25.1
C <sub>9</sub>	2.38	15.4
TOTAL	7.64	20.0

HYDROGEN YIELD SCF/BBL	-727 <sup>A</sup>	-656 <sup>B</sup>	-270 <sup>C</sup>
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ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.3	12.7	.0020	.0240	.0015	100.03
HYDROGEN		4.07				4.07
TOTAL	87.3	16.77	.0020		.0015	105.10
PRODUCTS						
LIQUID	83.93	13.21	.0003	.0140	.0001	97.15
HC GAS	3.46	0.51				3.97
HYDROGEN		2.94				2.94
NH <sub>3</sub>		.000	.0017			.002
H <sub>2</sub> O		.001		.0100		.011
H <sub>2</sub> S		.000			.0014	.001
TOTAL	87.39	16.66	.0020	.0240	.0015	104.07

A From Hydrogen Mass Balance

B From Elemental Balance

C From Aromatic Saturation

## HYDROPROCESSING DATA

DATE 8-5-76

DATA BOOK NO. 103-6-18

RUN, SAMPLE NO. 103-6-18-3

PROCESS: HYDROTREATING

CATALYST: CYANAMID HDS-9A 1/16"

FEED: SYNTHOIL 1 PASS HYDROTREATED B-1 &amp; C-1 HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	1000	TEMPERATURE °F	689
LHSV - VOL/VOL-HR	1.96	CATALYST VOLUME CC	50
MATERIAL BALANCE %	97.0	FORCE BALANCED ON	OIL PROD
HYDROGEN RATIO SCF/BBL	2039	OIL PRODUCT RATE G/HR	77.68
OIL FEED RATE G/HR	79.38	TAIL GAS RATE G/HR	4.90
HYDROGEN FEED RATE G/HR	3.20	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	-1.24 <sup>A</sup>	-0.65 <sup>B</sup>	-0.40 <sup>C</sup>
GAS	6.17		
	NORMPARAF		
METHANE	---		
ETHANE	---		
PROPANE	0.01	ISOPARAF	
C <sub>4</sub>	0.01	---	
LIQUID	101.22		

AROMATIC SATURATION: G/100G OIL FEED      % OF FEED

C <sub>6</sub>	0.34	18.6
C <sub>7</sub>	2.24	21.5
C <sub>8</sub>	2.79	26.5
C <sub>9</sub>	1.82	11.8
TOTAL	7.19	18.8

HYDROGEN YIELD SCF/BBL	-797 <sup>A</sup>	-418 <sup>B</sup>	-257 <sup>C</sup>
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ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.3	12.7	.0020	.0240	.0015	100.03
HYDROGEN		4.03				4.03
TOTAL	87.3	16.73	.0020	.0240	.0015	104.06
PRODUCTS						
LIQUID	84.94	12.92	.0008	.0140	.0001	97.88
HC GAS	2.93	0.43				3.36
HYDROGEN		2.79				2.79
NH <sub>3</sub>		.000	.0012			.001
H <sub>2</sub> O		.001		.0100		.011
H <sub>2</sub> S		.000			.0014	.001
TOTAL	87.87	16.14	.0020	.0240	.0015	104.04

A From Hydrogen Mass Balance

B From Elemental Balance

C From Aromatic Saturation

## HYDROPROCESSING DATA

DATE 8-9-76 DATA BOOK NO. 103-6-18  
 RUN, SAMPLE NO. 103-6-18-4  
 PROCESS: HYDROTREATING  
 CATALYST: CYANAMID HDS-9A 1/16"  
 FEED: SYNTHOIL 1 PASS HYDROTREATED B-1 & C-1 HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	1000	TEMPERATURE °F	689
LHSV - VOL/VOL-HR	1.95	CATALYST VOLUME CC	50
MATERIAL BALANCE %	96.5	FORCE BALANCED ON	OIL PROD
HYDROGEN RATIO SCF/BBL	2047	OIL PRODUCT RATE G/HR	76.36
OIL FEED RATE G/HR	78.76	TAIL GAS RATE G/HR	5.60
HYDROGEN FEED RATE G/HR	3.20	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	-0.83 <sup>A</sup>	-0.78 <sup>B</sup>	-0.42 <sup>C</sup>
GAS	7.11		
	NORMPARAF		
METHANE	---		
ETHANE	---		
PROPANE	0.01	ISOPARAF	
C <sub>4</sub>	0.01	--	
LIQUID	100.81		

AROMATIC SATURATION: G/100G OIL FEED      % OF FEED

C <sub>6</sub>	0.27	14.9
C <sub>7</sub>	2.59	24.9
C <sub>8</sub>	2.22	21.1
C <sub>9</sub>	2.06	13.3
TOTAL	7.14	18.2

HYDROGEN YIELD SCF/BBL	-531 <sup>A</sup>	-499 <sup>B</sup>	-269 <sup>C</sup>
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ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.3	12.7	.0020	.0240	.0015	100.03
HYDROGEN		4.06				4.06
TOTAL	87.3	16.76	.0020	.0240	.0015	104.09
PRODUCTS						
LIQUID	83.94	12.99	.0011	.0140	.0001	96.95
HC GAS	3.36	.49				3.85
HYDROGEN		3.23				3.23
NH <sub>3</sub>		.000	.0009			.001
H <sub>2</sub> O		.001		.0100		.011
H <sub>2</sub> S		.000			.0014	.001
TOTAL	87.30	16.71	.0020	.0240	.0015	104.04

A From Hydrogen Mass Balance

B From Elemental Balance

C From Aromatic Saturation

## HYDROPROCESSING DATA

DATE 8-10-76 DATA BOOK NO. 103-6-21  
 RUN, SAMPLE NO. 103-6-21-2  
 PROCESS: HYDROTREATING  
 CATALYST: CYANAMID HDS-9A 1/16"  
 FEED: SYNTHOIL 1 PASS HYDROTREATED B-1 & C-1 HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	1005	TEMPERATURE °F	689
LHSV - VOL/VOL-HR	1.95	CATALYST VOLUME CC	50
MATERIAL BALANCE %	97.1	FORCE BALANCED ON	OIL PROD
HYDROGEN RATIO SCF/BBL	2052	OIL PRODUCT RATE G/HR	76.38
OIL FEED RATE G/HR	78.88	TAIL GAS RATE G/HR	5.70
HYDROGEN FEED RATE G/HR	3.20	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	-0.91 <sup>A</sup>	-0.39 <sup>B</sup>	0.34 <sup>C</sup>
GAS	7.10		
	NORMPARAF		
METHANE	---		
ETHANE	---		
PROPANE	0.01	ISOPARAF	
C <sub>4</sub>	0.01	---	
LIQUID	100.89		

AROMATIC SATURATION: G/100G OIL FEED      % OF FEED

C <sub>6</sub>	0.35	19.1
C <sub>7</sub>	1.87	17.9
C <sub>8</sub>	1.78	16.9
C <sub>9</sub>	2.21	14.3
TOTAL	6.21	16.2

HYDROGEN YIELD SCF/BBL	-584 <sup>A</sup>	-250 <sup>B</sup>	-218 <sup>C</sup>
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ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.3	12.7	.0020	.0240	.0015	100.03
HYDROGEN		4.06				4.06
TOTAL	87.3	16.76	.0020	.0240	.0015	104.09
PRODUCTS						
LIQUID	84.23	12.59	.0003	.0100	.0001	96.83
HC GAS	3.43	.50				3.93
HYDROGEN		3.15				3.15
NH <sub>3</sub>		.000	.0017			.002
H <sub>2</sub> O		.002		.0140		.016
H <sub>2</sub> S		.000			.0014	.001
TOTAL	87.66	16.24	.0020	.0240	.0015	103.93

A From Hydrogen Mass Balance

B From Elemental Balance

C From Aromatic Saturation

## HYDROPROCESSING DATA

DATE 8-25-76

DATA BOOK NO. 103-6-23

RUN, SAMPLE NO. 103-6-23-2

PROCESS: REFORMING HYDROTREATED NAPHTHA

CATALYST: CYANAMID AERO PHF-4

FEED: SYNTHOIL HYDROTREATED HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	500	TEMPERATURE °F	963
LHSV - VOL/VOL-HR	2.08	CATALYST VOLUME CC	50
MATERIAL BALANCE %	101.16	FORCE BALANCED ON	OIL FEED
HYDROGEN RATIO SCF/BBL	3780	OIL PRODUCT RATE G/HR	58.88
OIL FEED RATE G/HR	83.57	TAIL GAS RATE G/HR	30.99
HYDROGEN FEED RATE G/HR	6.30	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	2.77 <sup>A</sup>	2.31 <sup>B</sup>	WATER	---
METHANE	1.72			
ETHANE	2.54			
PROPANE	3.03			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	1.83	.99				2.81
C <sub>5</sub>	1.05	1.25	.34			2.64
C <sub>6</sub>	1.36	1.73	1.35	.06	7.10	11.60
C <sub>7</sub>	.97	2.16	.43	.16	23.00	26.72
C <sub>8</sub>	.32	1.03	.14	.06	18.80	20.35
C <sub>9</sub>	.13	.37	.10	.00	17.66	18.26
TOTAL	5.65	7.52	2.36	.29	66.56	82.38
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	0.0		C <sub>10</sub> <sup>+</sup>	7.57		
HYDROGEN YIELD SCF/BBL	1390 <sup>A</sup>		1160 <sup>B</sup>			

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.8	13.2				100
HYDROGEN		7.54				7.54
TOTAL	86.8	20.74				107.54
PRODUCTS						
LIQUID	63.48	6.98				70.46
HC GAS	22.86	3.92				26.77
HYDROGEN		10.31				10.31
NH <sub>3</sub>						
H <sub>2</sub> O						
H <sub>2</sub> S						
TOTAL	86.34	21.20				107.54

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 8-26-76

DATA BOOK NO. 103-6-23

RUN, SAMPLE NO. 103-6-23-3

PROCESS: REFORMING HYDROTREATED NAPHTHA

CATALYST: CYANAMID AERO PHF-4

FEED: SYNTHOIL HYDROTREATED HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	500	TEMPERATURE °F	964
LHSV - VOL/VOL-HR	2.06	CATALYST VOLUME CC	50
MATERIAL BALANCE %	100.98	FORCE BALANCED ON	OIL FEED
HYDROGEN RATIO SCF/BBL	3800	OIL PRODUCT RATE G/HR	58.29
OIL FEED RATE G/HR	83.70	TAIL GAS RATE G/HR	31.76
HYDROGEN FEED RATE G/HR	6.35	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	2.46 <sup>A</sup>	2.18 <sup>B</sup>	WATER
METHANE	1.59		
ETHANE	2.51		
PROPANE	2.98		

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	1.80	.98				2.78
C <sub>5</sub>	1.10	1.27	.37			2.74
C <sub>6</sub>	1.65	1.78	1.73	.07	6.87	12.10
C <sub>7</sub>	1.09	2.35	.47	.19	22.50	26.60
C <sub>8</sub>	.35	1.11	.17	.08	18.45	20.17
C <sub>9</sub>	.15	.44	.14	.01	17.63	18.37
TOTAL	6.15	7.92	2.87	.36	65.45	82.76
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	0.0		C <sub>10</sub> <sup>+</sup>	7.70		
HYDROGEN YIELD SCF/BBL	1230 <sup>A</sup>		1090 <sup>B</sup>			

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.8	13.2				100
HYDROGEN		7.59				7.59
TOTAL	86.8	20.79				107.59
PRODUCTS						
LIQUID	62.68	6.96				69.64
HC GAS	23.84	4.06				27.89
HYDROGEN		10.05				10.05
NH <sub>3</sub>						
H <sub>2</sub> O						
H <sub>2</sub> S						
TOTAL	86.51	21.07				107.58

A From Hydrogen Mass Balance

B From Elemental Balance

## HYDROPROCESSING DATA

DATE 8-27-76

DATA BOOK NO. 103-6-23

RUN, SAMPLE NO. 103-6-23-4

PROCESS: REFORMING HYDROTREATED NAPHTHA

CATALYST: CYANAMID AERO PHF-4

FEED: SYNTHOIL HYDROTREATED HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	500	TEMPERATURE °F	964
LHSV - VOL/VOL-HR	2.06	CATALYST VOLUME CC	50
MATERIAL BALANCE %	100.93	FORCE BALANCED ON	OIL FEED
HYDROGEN RATIO SCF/BBL	3810	OIL PRODUCT RATE G/HR	58.36
OIL FEED RATE G/HR	83.39	TAIL GAS RATE G/HR	31.37
HYDROGEN FEED RATE G/HR	6.34	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	2.29 <sup>A</sup>	2.18 <sup>B</sup>	WATER	---
METHANE	1.56			
ETHANE	2.48			
PROPANE	2.91			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C <sub>5</sub>	CYCLO C <sub>6</sub>		
C <sub>4</sub>	1.76	.97				2.73
C <sub>5</sub>	1.07	1.23	.38			2.67
C <sub>6</sub>	1.68	1.89	1.92	.11	6.99	12.64
C <sub>7</sub>	1.13	2.42	.57	.29	22.15	26.55
C <sub>8</sub>	.40	1.17	.23	.15	18.04	19.99
C <sub>9</sub>	.18	.47	.20	.14	13.43	14.42
TOTAL	6.21	8.15	3.30	.69	60.61	79.01
UNIDENTIFIED C <sub>4</sub> -C <sub>9</sub>	0.0		C <sub>10</sub> <sup>+</sup>	11.70		
HYDROGEN YIELD SCF/BBL	1150 <sup>A</sup>		1090 <sup>B</sup>			

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.8	13.2				100
HYDROGEN		7.60				7.6
TOTAL	86.8	20.80				107.60

PRODUCTS

LIQUID	62.99	7.00				69.98
HC GAS	23.69	4.03				27.72
HYDROGEN		9.89				9.89
NH <sub>3</sub>						
H <sub>2</sub> O						
H <sub>2</sub> S						
TOTAL	86.68	20.92				107.60

A From Hydrogen Mass Balance

B From Elemental Balance



SYNTHOIL HYDROTREATED  
HYDROCRACKATE NAPHTHA  
FEED TO REFORMING

	<u>NORM PARAF</u>	<u>ISO PARAF</u>	<u>CYCLO PENT</u>	<u>CYCLO HEXANE</u>	<u>AROMATIC</u>
C <sub>6</sub>	0.29	0.17	1.36	2.96	1.55
C <sub>7</sub>	0.73	0.41	4.39	9.72	7.95
C <sub>8</sub>	0.15	1.31	2.86	11.72	7.82
C <sub>9</sub>	0.24	---	2.87	13.14	8.25
C <sub>10</sub> <sup>+</sup>	22.09				