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CHEMICALS FROM COAL

Interim Report

for

HRI H-COAL

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ABSTRACT

This document contains the results of an investigation to determine the suitability of the HRI H-Coal Syncrude as a petrochemical feedstock. A sample of the whole crude was distilled into four straight run fractions; IBP-350°F naphtha, 350-550°F mid-distillate, 450-800°F vacuum gas oil, and 850-FBP°F resid. Laboratory studies in metal reactors and computer and mathematical simulations were performed to provide overall material balance data for a conceptual plant. The naphtha was subjected to hydrotreating and reforming studies. The mid-distillate was hydrocracked to produce more naphtha which was further processed by hydrotreating and reforming. The vacuum gas oil was hydrocracked to produce more hydrocrackate naphtha which was mathematically hydrotreated and reformed. Steam coil cracking of the various naphtha and mid-distillate fractions was also performed to evaluate their potential as feedstocks for direct olefin production. None of the fractions surveyed was very attractive as an ethylene cracker feed. The reformate from each of the three distillates was then mathematically hydrodealkylated so that each fraction was converted 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 each distillate was \$10.06, \$8.12, and \$6.91 for the naphtha, mid-distillate, and vacuum gas oil respectively. Based on these values, and the difficulties encountered in recovering the gas oil, it was concluded to be economically unattractive as a petrochemical feedstock. The high aromatic yield obtained from the straight run and hydrocrackate naphthas, however, make these fractions very attractive as petrochemical feedstocks.

SUMMARY

The data presented herein was obtained from processing studies on a sample of HRI H-Coal Syncrude 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 hydroprocessing operations on three of the fractions distilled from the H-Coal whole crude. A sample of the whole crude was distilled into three straight run fractions, whose boiling range and elemental composition are listed in Table 1.

TABLE 1

BOILING RANGE AND ELEMENTAL COMPOSITION OF H-COAL STRAIGHT RUN FRACTIONS

	A-1 NAPHTHA IBP-350°F	A-2 MID-DISTILLATE 350-550°F	A-4 VACUUM GAS OIL 450-800°F	A-3, A-5, A-6 RESIDUAL 800°F PLUS
Wt. % of Crude	19.8	12.1	11.5	56.6
API Gravity, 60°F	44.9	25.9	7.9	--
Elemental Composition				
C wt. %	86.4	88.0	89.6	--
H wt. %	12.9	11.2	10.4	--
O ppm	390	5800	800	--
N ppm	470	440	83	--
S ppm	2600	1700	1700	--
Boiling Range, of				
IBP	-50	217	434	--
10 wt. %	170	366	552	--
20 wt. %	188	378	597	--
30 wt. %	217	395	627	--
40 wt. %	229	408	655	--
50 wt. %	256	417	675	--
60 wt. %	282	432	695	--
70 wt. %	306	449	716	--
80 wt. %	330	471	740	--
90 wt. %	353	500	767	--

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 2500 psig and 870-1010°F with LHSV's of 0.35 to 1.45 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_1-C_9 were 2500 psig, 962°F, and 0.75 LHSV.

The straight run gas oil was hydrocracked over the same catalyst. Operating difficulties were encountered due to solids in the oil which plugged the check valves on the pump. Only a small amount of material was available. Operating conditions of 2500 psig, with temperatures of 840-996°F and LHSV's from 0.69 to 1.68 were surveyed. Conversions of 55.4 to 83.3% 650°F minus were achieved.

Both the straight run naphtha and the combined naphthas from two-pass hydrocracking the straight run mid-distillate were hydrotreated over Harshaw HT-100 E nickel molybdenum catalyst, Harshaw HT-400 E cobalt molybdenum catalyst, or Cyanamid HDS-9A nickel molybdenum catalyst. These catalysts were chosen for their resistance to deactivation by heteroatoms in the feed and for their superior activity for denitrogenation and desulfurization. The straight run data is sketchy, due to a large extent to analytical and presulfiding technique difficulties. Sulfur, nitrogen, and oxygen were reduced to 4, 5, and 420 ppm respectively in two passes. The hydrocrackate naphtha was also hydrotreated in two passes. Nitrogen in the feed to the hydrotreater was less than 1 ppm due to removal during hydrocracking. Sulfur was reduced from 100 to 5 ppm and oxygen was reduced to the 50 ppm level.

The hydrotreated straight run and hydrocrackate naphthas were 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 250 psig and 930-980°F, the catalyst life was very short, as the straight run naphtha rapidly coked the catalyst. Naphthene conversion dropped from 92% to 67%. At 500 psig and 968°F, the hydrocrackate naphtha was reformed with a substantial increase in catalyst life. With a first day conversion of 95%, after 50 hours, the naphthene conversion was still at 93.5%.

Steam coil cracking experiments were conducted on the straight run mid-distillate and naphtha fractions to evaluate their potential as ethylene feedstocks. Due to the high aromatic content of these feedstocks, coke lay down in the reactor was a significant problem. None of the fractions surveyed was particularly attractive as feedstock for direct olefin production.

In addition to the hydroprocessing studies, each fraction was subjected to mathematical recycle hydrocracking to naphtha, hydrotreating, reforming, and hydroalkylation (HDA). As a result, each 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 relative value of each fraction was determined.

TABLE 2

PRODUCT PATTERNS AND VALUE FOR H-COAL STRAIGHT RUN FRACTIONS

	STRAIGHT RUN NAPHTHA IBP-350°F	STRAIGHT RUN MID-DISTILLATE 350-550°F	STRAIGHT RUN VACUUM GAS OIL 450-800°F
Processing Sequence	Hydrotreat Reform HDA	Recycle Hydrocrack Hydrotreat Reform HDA	Recycle Hydrocrack Gas Oil Recycle Hydrocrack Mid-Distillate Hydrotreat Reform HDA
PRODUCT PATTERN, Wt. %			
HYDROGEN	-1.6	-5.4	-8.9
METHANE	19.1	18.6	19.1
LPG	22.6	48.5	55.8
BENZENE	51.3	36.3	32.6
LIQUID FUEL	8.3	1.4	1.2
VALUE/100 lb DISTILLATE (1980)	$10.06	$8.12	$6.91

Based on the yield data calculated for each fraction and the wt. % of each fraction from distillation, a mass balance for a conceptual plant operating on 100.00 lb/hr H-Coal 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. Only the naphtha and mid-distillate fractions were included in this balance, since the gas oil fraction was concluded to be economically unattractive as a petrochemical feedstock. The 12.1 lb/hr straight run mid-distillate from distillation was recycle hydrocracked mathematically, consuming 0.53 lb/hr hydrogen and producing 0.90 lb/hr methane, 3.70 lb/hr LPG's and 8.1 lb/hr naphtha. The straight run and hydrocrackate naphthas, 19.1 and 7.5 lb/hr respectively, were hydrotreated mathematically, consuming 0.20 lb/hr hydrogen and producing 1.52 lb/hr gas. The hydrotreated naphtha was then reformed, producing 0.58 lb/hr hydrogen, 2.66 lb/hr gas and 23.28 lb/hr reformate. An in house mathematical model for hydrodealkylation was used to convert the reformate to 4.86 lb/hr methane, 2.71 lb/hr ethane, 14.52 lb/hr benzene, and 1.80 lb/hr liquid fuel, while consuming 0.82 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 H-COAL WHOLE CRUDE AS FEEDSTOCK

Yield, lb/100 lb crude

Methane	4.02
LPG's	10.33
41.98 wt. % ethane	
20.76 wt. % propane	
19.04 wt. % butanes	normal/iso = 3.6
18.40 wt. % pentanes	normal/iso = 1.4
Benzene	14.52
Fuel (HDA)	1.80
Fuel (Gas Oil)	11.50 (no allowance for plant fuel)
Residue	56.6

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 H-Coal syncrude subjected to the hydroprocessing experiments was produced by Hydrocarbon Research, Inc. in Trenton, New Jersey from Illinois No. 6 bituminous coal. The oil was made in the H-Coal Process Development Unit, operation number 130-62-9. The material consisted of three separate products; 30.4% atmospheric still overhead, 1.8% atmospheric still bottoms, and 67.8% vacuum still bottoms slurry by weight. The product yield, based on dry coal, was calculated to be 80.3% on a weight basis. The API Gravity at 60°F for the three products was 40.5° for atmospheric still overhead, 20.2° for the atmospheric still bottoms, and -9° for the vacuum still bottoms slurry. The vacuum still bottoms slurry contained 11.2% unreacted coal and 21.1% ash by weight.

Processing Approach

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

1) Distillation into nominally three cuts --
Atmospheric Still Bottoms and Overheads

A-1	IBP -350°F	(straight run naphtha)
A-2	350°F-550°F	(straight run mid-distillate)
A-3	550°F-FBP°F	(straight run gas oil - not recovered)

Vacuum Still Bottoms Slurry
- A-4 450°F plus (straight run vacuum gas oil)
- A-5 (Unreacted coal, ash, and residual oil - not used)
- A-6 (Thermal cracking and coking oil - not used)

2) Hydrocracking of the mid-distillate and vacuum gas oil to produce more naphtha with some LPG's.

3) Hydrotreating of the straight run and hydrocrackate naphthas to remove the heteroatoms.

4) Reforming of the hydrotreated naphthas to produce maximum yields of aromatics.

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

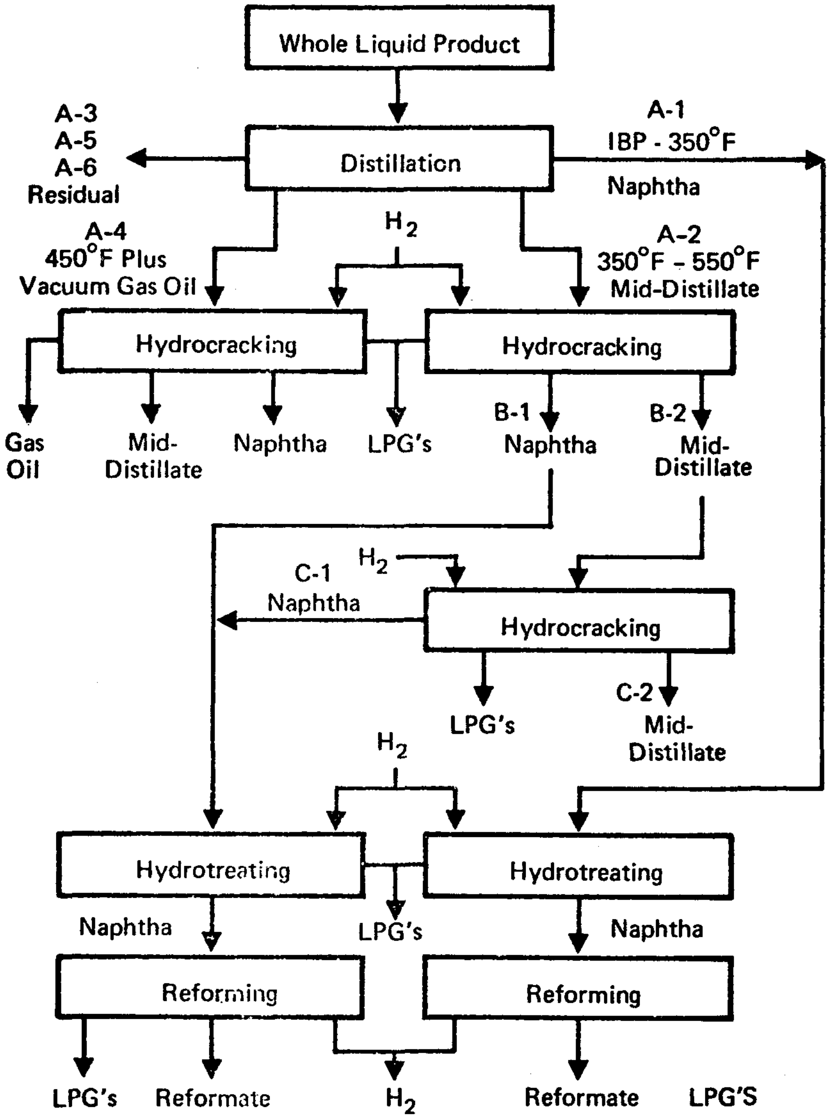
The H-Coal syncrude was received as 32.2% Atmospheric Still Overhead and Bottoms, which was distilled in a 72 liter Podbielniak® Fractioneer A batch distillation unit; and 67.8% Vacuum Still Bottoms Slurry, which was crushed and distilled using an expendable pot designed for this particular distillation.

The remaining three hydroprocessing steps were carried out in three similar reactors. The nominal 1 inch diameter tubular steel reactors were operated continuously in downflow with a fixed catalyst bed varying from 50 to 200 cm^3 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 ±2%.

Figure 1

PROCESSING SEQUENCE



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 coulemetric Karl-Fisher titration.

6) Naphtha Componential; analysis of the C_3-C_9 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 neution activation analysis of these metals at the 10 to 50 ppb detection level.

9) Common Metals; standard emission spectroscopy was used for this analysis.

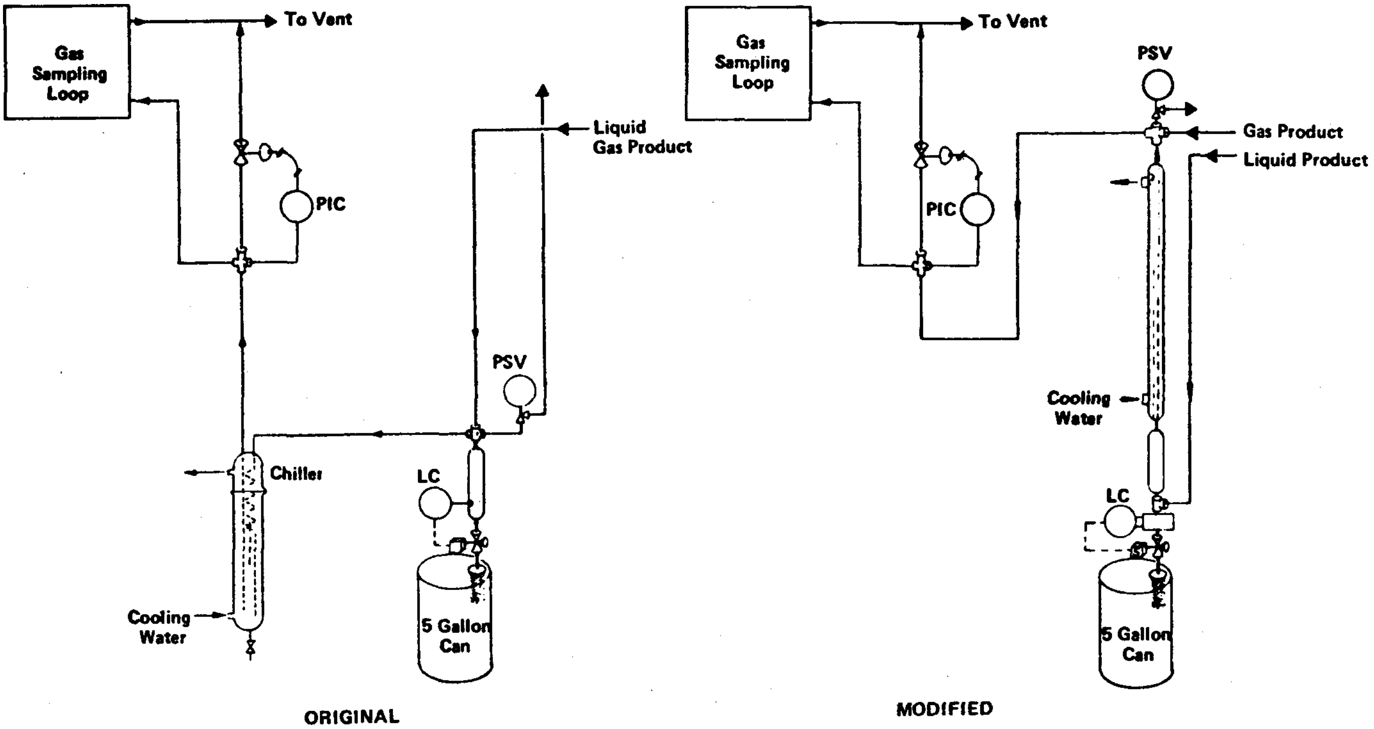
All hydroprocessing experiments were conducted in much the same way. The reactor systems were instrumented to allow for 24 hr operation with only 8 hr per day being attended operation. This led to 24 hr minimum runs. Often, the lag between completion of a run and the corresponding analytical data increased 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_5-C_7 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_5-C_7 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_5-C_7 components.

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_1-C_9 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^{+} 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.

Figure 2

PRODUCT RECOVERY TRAIN



ORIGINAL

MODIFIED

TABLE 4

VENT GAS FLOW RATE AND COMPOSITION

ORIGINAL
Run No. 6-13-3
Flow Rate - 11.86
Composition: G/100G. Feed

MODIFIED
Run No. 6-18-2
Flow Rate - 6.18
Composition: G/100G. Feed

	ORIGINAL			MODIFIED		
	PARAFFIN	NAPHTHENE	AROMATIC	PARAFFIN	NAPHTHENE	AROMATIC
C_1	.000			.003		
C_2	.014			.004		
C_3	.027			.010		
C_4	.071			.012		
C_5	.334	.186		.078	.007	
C_6	.363	1.611	.991	.238	.870	.461
C_7	.559	1.112	.962	.327	.829	.634

PROCESSING RESULTS

Distillation

The H-Coal whole liquid was distilled, yielding the following fractions:

Straight Run Naphtha - 19.8%
Straight Run Mid-distillate - 12.1%
Straight Run Vacuum Gas Oil - 11.5%
Residual - 56.6%

The physical state of the H-Coal syncrude caused considerable difficulties in the distillation step. The Atmospheric Still Overheads and Bottoms were distilled in the batch still used for the separation of the other syncrudes evaluated in this study. This fraction of the H-Coal product, 32.2% by weight, was liquid at room temperature, but the boiling range for this material was much lower than for the liquid fractions of other syncrudes. As a result, the mid-distillate processed had an endpoint of only 550°F instead of 650°F. The balance of the H-Coal product, Vacuum Still Bottoms Slurry (VSBS), was received as a solid at room temperature. A considerable amount of time was spent attempting to recover the oil fraction from this material, which contained unreacted coal and ash as well. The VSBS was first crushed before atmospheric steam distillation and vacuum steam stripping to remove the gas oil were tried unsuccessfully. Solvent extraction using tetrahydrofuran and dioxane with a Soxhlet extractor were also tried. Dioxane was the better of the two solvents, however the resid left after distillation of the extract was not readily redissolved in dioxane. This would cause major problems in removal of the bottoms from the distillation pot. Consequently, a still with an expendable pot was designed to recover the gas oil from the VSBS. The distillation of crushed VSBS proceeded smoothly until temperatures near 800°F were reached. At this point thermal cracking and coking occurred which generated gas and smoke. The volume of gas and smoke generated became so great that the vacuum on the still could not be maintained and the distillation was terminated. The recovered gas oil had a boiling range from 450-850°F. The ideal procedure would have been to separate the 450-650°F portion of the VSBS oil and combine it with the mid-distillate from the Atmospheric Still Overheads and Bottoms. The delay in arriving at a suitable means of removing the oil portion of the VSBS and the time limits for completing experimental work did not allow this. Results of analytical scans of the various straight run fractions are presented in Table 5.

Hydrocracking

The H-Coal 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$^+$ mid distillate. Only the

TABLE 5

ANALYTICAL RESULTS FOR H-COAL FRACTIONS

	A-1 NAPHTHA IBP-350°F	A-2 MID-DISTILLATE 350-550°F	A-4 VACUUM GAS OIL 450°F PLUS
API GRAVITY, 60°F	49.9	25.9	7.9
ELEMENTAL COMPOSITION			
C wt. %	86.4	88.0	89.6
H wt. %	12.9	11.2	10.4
O ppm	0.39	0.58	0.08
N ppm	0.047	0.044	0.083
S ppm	0.26	0.17	0.17
Hg PPB	<5	60	NA
Ga PPB	<1	<1	NA
BOILING RANGE FROM SIMULATED DISTILLATION, °F			
IBP	-50	217	434
10 wt. %	170	366	552
20 wt. %	188	378	597
30 wt. %	217	395	627
40 wt. %	229	408	655
50 wt. %	256	417	675
60 wt. %	282	432	695
70 wt. %	306	449	716
80 wt. %	330	471	740
90 wt. %	353	500	767

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
Surface Area - 220 M^2/g
Crush Strength - 12 lb
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_4-C_9 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.

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.

The H-Coal straight run mid-distillate was hydrocracked after the last two second pass hydrocracking runs for the COED mid-distillate over the same catalyst load. Based upon results obtained for COED mid-distillate hydrocracking experiments, nominal reactor temperatures of 870 to 1010°F and LHSV's of 0.35 to 1.45 with a reactor pressure of 2500 psig 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 experiments. As would be expected, decreasing the LHSV and increasing the temperature contributed to increased conversions. A notable aspect of these hydrocracking experiments is the reduction of nitrogen levels. Virtually all of the nitrogen was converted in the hydrocracking step. The oxygen data reported for these runs is suspect, as in many instances the data indicates that oxygen is being produced in the hydrocracking step.

The straight run vacuum gas oil was also subjected to hydrocracking to evaluate this feedstock for naphtha production. A fresh load of Harshaw HT-400-E-1/8" extrudate hydrocracking catalyst, presulfided with 0.6 weight percent CS_2 in Stoddard Solvent according to the procedure outlined in the previous section, was used. Because the gas oil was very viscous at room temperature, it was fed from the 5 gallon heated feed tank with bubbler level indicator. Some difficulty was encountered in processing this fraction. Even though it was a distillate, the material contained very fine particles which tended to plug the feed pump. A reactor pressure of 2500 psi with temperature from 840 to 996°F and LHSV's from 0.69 to 1.68 were surveyed. Data collected for the conversion of C_{10} plus material in the feed to C_{10} minus material in the product indicate that decreasing LHSV and increasing temperature produces higher conversion rates.

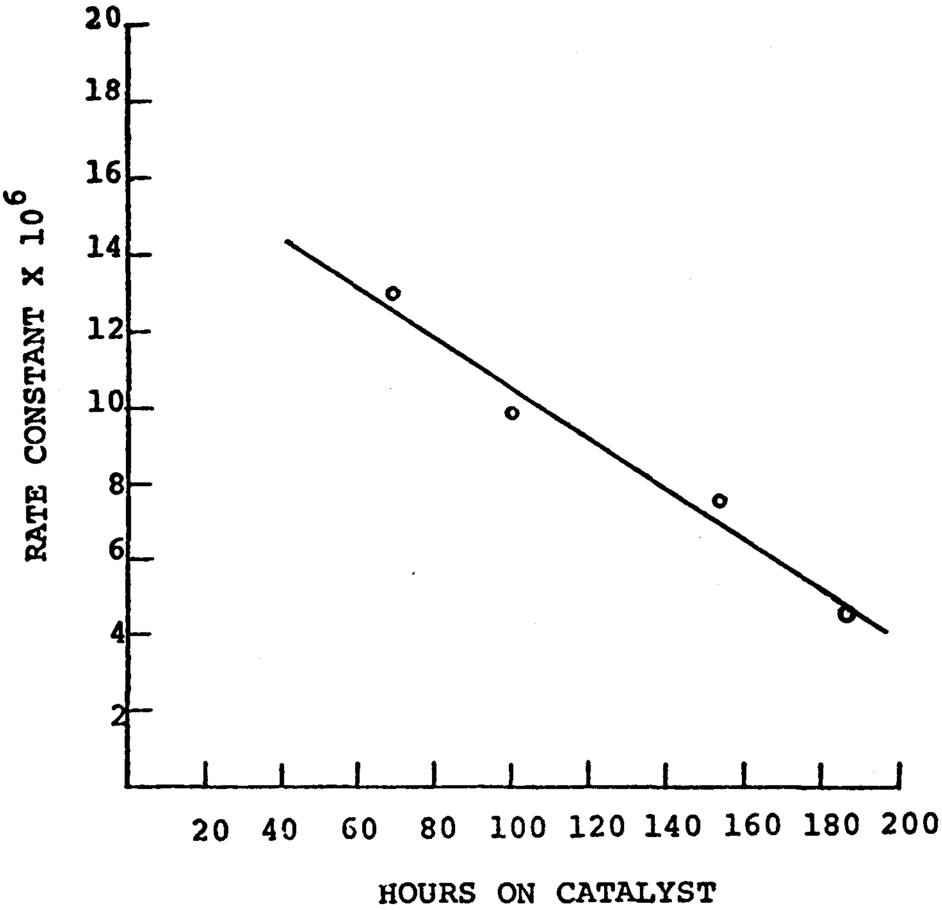
The data also indicates that catalyst activity declined during these hydrocracking experiments. The catalyst deactivation rate is shown in Figure 3 which is a plot of the first order rate constant versus catalyst hours. The rate constant was calculated from the equation:

$$\ln(1-C) = -ke^{\frac{-E}{RT}} P_{H_2} \text{ LHSV}^{-1.0}$$

where - C = $C_1 - C_9$ yield, wt. fraction
k = rate constant
E = 38,000 cal/g mole
R = 1.987 cal/g °K
T = reactor temperature, °K
P_{H_2} = pressure psia
LHSV = liquid space velocity, vol/vol - hr

Figure 3

PLOT OF RATE CONSTANT VERSUS HOURS ON CATALYST FOR VACUUM GAS OIL HYDROCRACKING



Simplified results from the H-Coal mid-distillate and gas oil hydrocracking experiments are presented in Table 6. Included are the operating conditions, C_1-C_9 yield expressed as weight %, a componential analysis of the C_1-C_9 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 H-Coal straight run naphtha fraction 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

TABLE 6

HYDROCRACKING H-COAL MID-DISTILLATE AND GAS OIL FRACTIONS
SIMPLIFIED DATA

RUN NO.	TEMP. °F	PRESS. PSIG	LHSV HR^{-1}	PPM O C_5+	PPM N C_5+	PPM S C_5+	C_1-C_9 YIELD WT. %	H_2 YIELD G/100G FEED	COMPONENTIAL ANALYSIS WT. %				
									METHANE	C_2-C_4 LPG'S	C_5-C_9 PARAF.	NAPH.	AROM.
STRAIGHT RUN MID-DISTILLATE				5800	440	1700							
1	870	2500	0.35	7720	<1	13	24.0	-2.24	5.5	27.7	12.4	33.0	21.3
2	960	2500	0.36	10200	<1	42	76.5	-3.70	7.6	30.6	13.0	28.8	20.1
3	962	2500	1.04	5660	<1	41	59.0	-1.60	6.6	29.0	11.2	23.2	30.1
4	965	2500	1.45	10300	<1	74	53.6	-1.43	6.7	29.2	11.2	21.3	31.5
5	976	2500	0.67	7500	<1	111	67.3	-2.10	7.6	24.5	11.5	26.0	30.3
6	1008	2500	0.67	4310	<1	137	81.8	-3.05	8.4	36.9	7.3	16.6	30.7
HYDROCRACKED MID-DISTILLATE				840	<1								
7	934	2500	1.00	12800	<1	23	28.6	-2.05	6.0	29.2	10.8	22.5	31.4
8	1015	2500	0.99	490	<1	26	78.3	-3.32	11.0	31.3	6.7	9.8	41.0
STRAIGHT RUN VACUUM GAS OIL				7900	820	1700							
1006	840	2500	0.69	780	18	59	13.4	-0.83	6.5	37.9	13.0	24.4	18.2
1009	925	2500	0.71	1440	11	94	41.3	-3.11	8.8	42.4	10.4	16.5	21.8
1016	964	2500	1.30	925	132	41	36.4	-1.70	12.0	47.2	9.8	12.6	18.5
1020	996	2500	1.68	1120	172	75	31.2	-0.82	12.6	44.5	7.8	15.0	20.2

with an excess of hydrogen which passed through once and was vented with the LPG's produced. Runs were carried out over a fixed bed of Harshaw HT-100 E 1/8" or HT-400 E 1/16" extrudate hydrotreating catalyst. These catalysts consisted of nickel and molybdenum or cobalt and molybdenum on an alumina support and had the following physical characteristics:

HT-100 E 1/8"

Composition - 3.8% nickel oxide and 16.8% molybdenum trioxide on alumina
Average Bulk Density - 38 lb/cu ft
Surface Area - 190 m^2/g
Crush Strength - 14 to 20 lb
Pore Volume - 0.54 cc/g

HT-400 E 1/16"

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

The nickel-molybdate catalyst was used because of its demonstrated high activity toward nitrogen, which was expected to be present in the coal naphthas in relatively large concentrations. 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 cobalt-molybdate catalyst was used in an attempt to achieve better sulfur removal from this feedstock than was accomplished using the nickel-molybdate catalyst. Catalyst was loaded in the reactor in the same manner as for the hydrocracking catalyst, described in the previous section. Presulfiding with 1% CS_2 in light naphtha to develop maximum catalyst activity was also performed according to the procedure outlined in the previous section for hydrocracking catalyst. Reactor conditions of 600-780°F, 500-900 psig, and LHSV's of 1.95 to 2.67 were used for the first pass, while 662°F, 800 psig, and a LHSV of 3.4 were employed for the second pass.

Several problems were encountered during these hydrotreating runs. In addition to the analytical difficulties, which were not recognized until after some time had been spent attempting to correct processing conditions, the possibility of sulfur contamination of the product resulting from the method of presulfiding did not become apparent until long after these hydrotreating runs were completed. For these reasons most of the data generated for heteroatom conversions is suspect. Due to the expected high concentration of heteroatoms in the feed, a componential analysis was expected to be in error and was not obtained. Gas make data and hydrogen consumptions calculated from analytical carbon-hydrogen data were determined from these runs and are presented in Table 7.

The limited amount of material available did not allow repeating these inspections. None of the difficulties described above would lead to data which would indicate more success than was realized. On the contrary, these effects would indicate a less active catalyst and that hydrotreating this naphtha may be much easier than the data indicates. As a result, the need for two stage hydrotreating of the H-Coal straight run naphtha was not absolutely established.

The naphtha produced from the two pass hydrocracked mid-distillate was combined and hydrotreated in two passes. A fresh load of the previously described Harshaw HT-100 E 1/8" catalyst, diluted with 2 volumes of 6-10 mesh tabular alumina to prevent back mixing, was used. A load of Cyanamid Aeroform HDS-9A 1/16" extrudate catalyst was also used. The Cyanamid Aeroform catalyst consisted of nickel molybdate on alumina with the following physical characteristics:

Composition - 3% nickel oxide and 18% molybdenum trioxide on alumina
Average Bulk Density - 45 to 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 NiMo catalysts. The HT-100 E catalyst was loaded in the reactor in the same manner as described for the hydrocracking catalysts in the previous section. Presulfiding was accomplished using the 1% CS_2 in Stoddard Solvent technique. In addition, the catalyst load was "washed" overnight with ethyltoluene at nominal reactor run conditions prior to the first run on the hydrocrackate naphtha. Nevertheless, sulfur contamination of the product was again observed. For this reason the presulfiding procedure was changed. The HDS-9A catalyst was diluted with 16-20 mesh silicon carbide and was presulfided with hydrogen sulfide 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°C/15 min to 400°C and held for two hours. The temperature was then reduced to 360°C and the H_2S flow was stopped. While maintaining the hydrogen flow, the reactor pressure was increased to 1000 psig.

Results from the hydrotreating runs performed after this presulfiding procedure indicate that although contamination of the product still occurred, it was to a lesser degree. The

TABLE 7

HYDROTREATING H-COAL STRAIGHT RUN NAPHTHA
SIMPLIFIED DATA

RUN NO.	1st PASS FEED	702	730	804	805	2nd PASS FEED	828
TEMP., °F		662	600	680	780		662
PRESS., PSIG		705	500	900	900		800
LHSV, HR^{-1}		1.95	2.30	2.67	2.42		3.40
O PPM	3900	410	790	2000	1890	400	400
N PPM	470	30	80	30	5	38	5
S PPM	2600	60	70	120	105	93	4
H_2 CONSUMPTION, G/100G FEED		-0.43	-0.23	-0.36	-0.01		-0.11
GAS MAKE G/100G FEED		17.12	3.96	1.85	6.10		2.44
GAS COMPOSITION G/100G FEED							
C_1		0.01	0.01	0.01	0.06		--
C_2		0.01	0.04	0.06	0.28		--
C_3		0.10	0.04	0.04	0.28		0.01
IC_4		0.08	0.01	0.02	0.04		0.02
NC_4		0.63	0.18	0.20	0.40		0.07
IC_5		0.51	0.15	0.10	0.24		0.08
NC_5		1.04	0.38	0.23	0.58		0.21
CYCLO C_5		0.81	0.18	0.08	0.25		0.11
IC_6		0.24	0.16	0.07	0.25		0.10
NC_6		0.52	0.38	0.17	0.58		0.26
METHYL CYCLO C_5		1.31	0.31	0.13	0.46		0.22
BENZENE		1.11	0.10	0.04	0.19		0.09
CYCLO C_6		3.78	0.88	0.34	1.12		0.63
IC_7		0.98	0.18	0.06	0.23		0.12
NC_7		0.62	0.11	0.03	0.12		0.08
METHYL CYCLO C_6		4.07	0.67	0.20	0.74		0.34
TOLUENE		1.29	0.19	0.05	0.26		0.10

analytical problems encountered with the straight run naphtha hydrotreating runs were reduced for this naphtha with the use of improved sulfur analysis techniques and the Antek Pyroreactor for nitrogen analyses. The composite first pass hydrotreated hydrocrackate naphtha was hydrotreated a second time over the same catalyst load of HDS-9A as was used for some of the first pass runs. The resulting 2 pass hydrotreated naphtha contained heteroatoms at low enough levels to be reformed successfully using a bifunctional reforming catalyst. The results of the hydrocrackate naphtha hydrotreating experiments are presented in Table 8.

TABLE 8

HYDROTREATING H-COAL HYDROCRACKATE NAPHTHA
SIMPLIFIED DATA

RUN NUMBER	1st PASS FEED	6-7-3	6-9-2	6-12-2	2nd PASS FEED	8-11-4
TEMPERATURE, °F		756	752	686		683
PRESSURE, psig		1500	1500	1040		980
LHSV, hr^{-1}		1.90	4.01	2.01		2.06
YIELD G/100G FEED						
HYDROGEN		-0.51	-1.13	-0.06		-0.95
C_1 - C_4 GAS		0.27	0.21	0.14		0.05
C_5 - C_{10}+ LIQUID		100.24	100.92	99.92		100.90
AROMATIC SATURATION G/100G FEED		20.00	13.39	9.35		10.20
OXYGEN, ppm	300	170	150	150	350	50
NITROGEN, ppm	8	2	5	4	1	<1
SULFUR, ppm	100	4	1	69	25	5

This data shows that the hydrogen consumed went mainly to saturate aromatics to naphthenes.

Reforming

The H-Coal hydrotreated naphthas were reformed over a conventional bifunctional platinum reforming catalyst to maximize aromatics. A hydrogen ratio of 2000 SCF/BBL of feed for the straight run naphtha and 4000 SCF/BBL of feed for the hydrocrackate naphtha 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 reformate 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 reformate 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 an equal volume of 6-8 mesh tabular alumina for the straight run naphtha and two volumes of 16-20 mesh silicon carbide for the hydrocrackate naphtha 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 N 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 straight run hydrotreated naphtha was reformed at 932 to 977°F and 250 psig with a LHSV of 2. The initial activity was very encouraging, but catalyst activity declined very rapidly as the naphthene conversion data in Table 9 indicates.

TABLE 9

REFORMING H-COAL HYDROTREATED STRAIGHT RUN NAPHTHA
SIMPLIFIED DATA

RUN NUMBER	FEED	103075	110375	112075	112475
TEMP., °F		932	968	968	977
PRESS., psig		250	250	250	240
LHSV, hr^{-1}		1.59	1.66	2.24	2.09
OXYGEN, ppm	420				
NITROGEN, ppm	5				
SULFUR, ppm	4				
YIELD, G/100G FEED					
HYDROGEN		5.47	3.24	3.43	1.29
C_1 - C_5 GAS	0.8	4.7	10.5	15.0	11.4
C_6 - C_9 LIQUID					
PARAFFIN	13.8	8.4	6.7	9.8	11.9
NAPHTHENE	41.3	3.3	1.7	6.4	13.8
AROMATIC	33.9	69.3	72.4	59.5	54.9
C_{10}+	10.2	8.8	5.4	5.9	6.8
% NAPHTHENE CONVERSION		92.0	95.9	84.5	66.6
% AROMATIC C_6 - C_9	38.1	85.6	89.6	78.6	68.1

The hydrocrackate hydrotreated naphtha was reformed at 968°F and 500 psig with a LHSV of 2 over a fresh load of calcined reforming catalyst. The data presented in Table 10 would seem to indicate that doubling the pressure significantly decreased the deactivation rate. The limited amount of this hydrocrackate naphtha allowed for only a 50 hour run at these conditions, making it difficult to determine if the catalyst was "breaking in" or if the decreased deactivation rate would continue.

TABLE 10

REFORMING H-COAL HYDROTREATED HYDROCRACKATE NAPHTHA
SIMPLIFIED DATA

RUN NUMBER	FEED	6-27-2	6-27-3
TEMP., °F		968	968
PRESS., psig		495	495
LHSV, hr^{-1}		2.06	2.07
CHEM. OXYGEN, ppm	80		
WATER, ppm	60		
NITROGEN, ppm	6		
SULFUR, ppm	3		
YIELD, G/100G FEED			
HYDROGEN		2.40	0.70
$C_1 - C_5$ GAS	0.3	10.9	11.5
$C_6 - C_9$ LIQUID			
PARAFFIN	10.8	6.7	7.7
NAPHTHENE	36.8	1.8	2.4
AROMATIC	35.0	72.2	70.5
C_{10}^+	17.4	5.2	5.4
% NAPHTHENE CONVERSION		95.1	93.5
% AROMATIC $C_6 - C_9$	42.4	89.5	87.5

Steam Coil Cracking

The H-Coal straight run naphtha and straight run mid-distillate were subjected to steam coil cracking experiments to evaluate these materials for direct olefin production. The liquid hydrocarbons and water were pumped to a vaporizer preheater. The vaporized feed entered a tubular steel reactor. The reaction products were condensed and the gas was separated and analyzed with a gas chromatograph. The liquid feed and product were analyzed using another gas chromatograph. Using a proprietary in-house correlative technique, the analyses collected were used as inputs to a computer program which adjusted each feed to the same cracking severity, mathematically recycled LPG's, and hydrodealkylated toluene and C_8 aromatics to yield the simplified data in Table 11 below.

TABLE 11

STEAM COIL CRACKING VARIOUS H-COAL FRACTIONS
SIMPLIFIED DATA

YIELD, G/100G FEED

PRODUCT	STRAIGHT RUN NAPHTHA	STRAIGHT RUN MID-DISTILLATE
HYDROGEN	0.8	0.7
METHANE	16.3	12.1
ETHYLENE	23.4	14.4
PROPYLENE	8.5	5.9
BUTADIENE	3.0	1.5
BENZENE	23.6	18.5
FUEL	24.4	46.9

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. Each of the three fractions from the distillation step was analyzed individually as a feedstock to the conceptual plant. The product patterns presented in the tables following are therefore based on 100.00 mass units of each fraction. From this data, the relative value of each 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 H-Coal 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:

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

where - $C = C_1-C_9$ yield, wt. fraction

k = rate constant

E = 38000 cal/g mole (first pass), 43400 cal/g mole (second pass)

R = 1.987 cal/g mole °K

T = reactor temperature, °K

P_{H_2} = pressure, psia

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. A plot of experimental versus the calculated conversions computed from the first and second pass average rate constants is presented in Figure 4. The straight line 45° plot confirms the assumed first order kinetics for mid-distillate hydrocracking conversions. Table 12 includes the reactor conditions, rate constants, and selectivities used to make recycle hydrocracking calculations.

Hydrocracking Vacuum Gas Oil

The single pass data obtained for hydrocracking H-Coal straight run vacuum gas oil was also converted to recycle hydrocracking data. Because of the rapid catalyst deactivation observed for hydrocracking runs on this feedstock, the first order rate constants derived for individual runs were not in agreement. The rate constants varied from 13.0×10^6 to 4.7×10^6 for the four runs. In order to estimate conversions and selectivities for recycle hydrocracking the vacuum gas oil, several assumptions were made. The conversion reaction for virgin material was assumed to be noncompetitive with the conversion reaction for recycle material. The conversion to C_1-C_9 and to C_{10}-650°F was assumed to be 40% for both for all passes. The selectivities observed for the single pass hydrocracked vacuum gas oil, averages of the selectivities for the four experimental runs, were assumed to be valid for all recycle passes. Reaction rates for the laboratory data were calculated according to the following equation:

$$\ln (1-C) = -ke^{-\frac{E}{RT}} P_{H_2} \; LHSV^{-1}$$

where C = conversion to naphtha or mid-distillate, wt. fraction
k = rate constant
E = 38000 cal/g mole
R = 1.987 cal/g mole °K
T = reactor temperature, °K
P_{H_2} = pressure, psia
$LHSV$ = liquid hourly space velocity, vol/vol-hr

Table 13 includes the reactor conditions, reaction rates for naphtha and mid-distillate conversions, and C_1-C_9 selectivities used to make recycle hydrocracking calculations.

Figure 4

PLOT OF EXPERIMENTAL VERSUS
CALCULATED CONVERSIONS

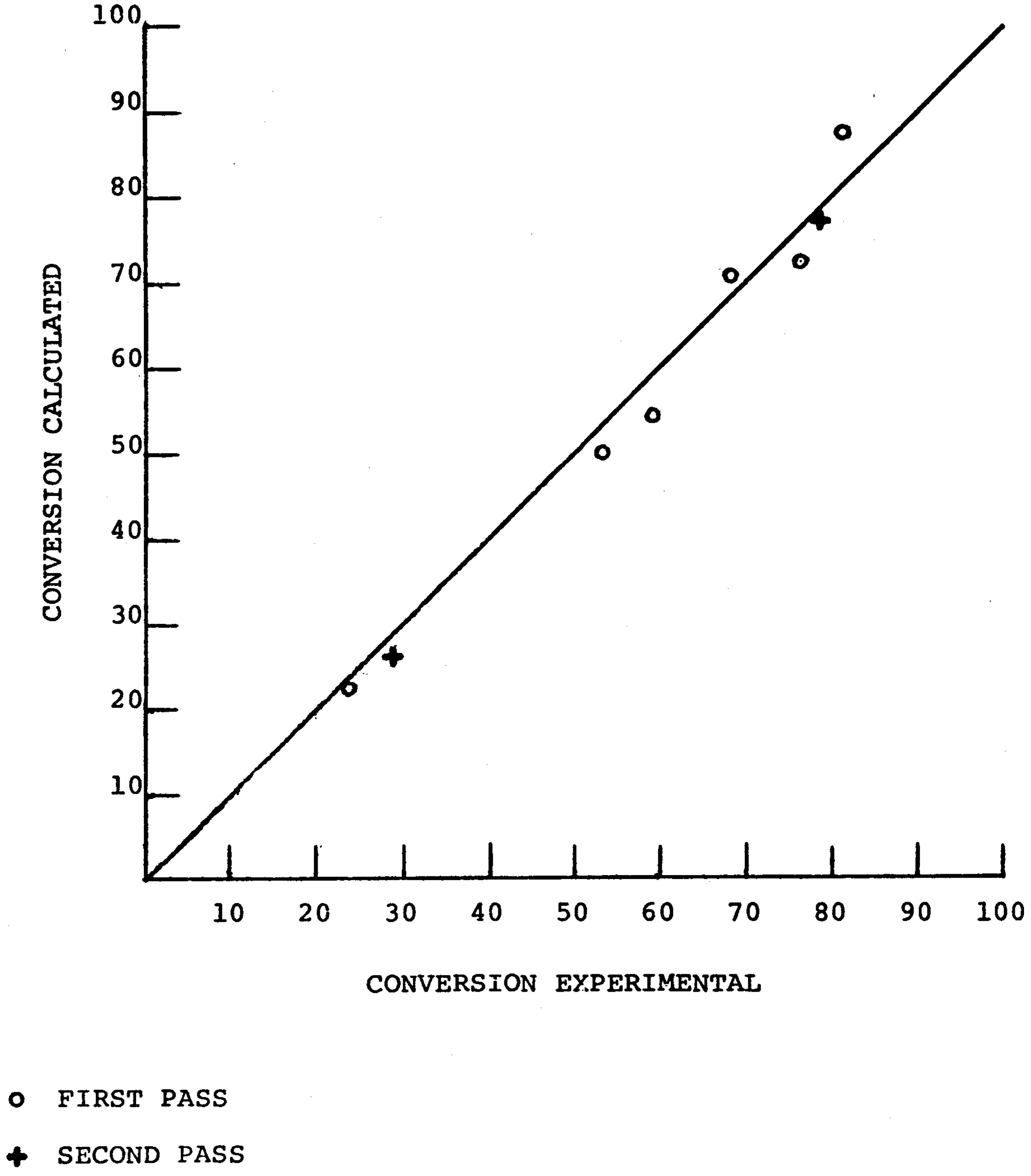


TABLE 12

MID-DISTILLATE RECYCLE HYDROCRACKING DATA

REACTOR CONDITIONS

962 °F
2500 psig
LHSV 0.75 volumes/volume-hr

RATE CONSTANTS

1st PASS	1.04×10^{7} hr^{-1}	E = 38000 cal/g - mole
2nd PASS	2.20×10^{8} hr^{-1}	E = 43400 cal/g - mole
3rd + PASS	1.83×10^{8} hr^{-1}	E = 43400 cal/g - mole - assumed

1st PASS SELECTIVITIES
Wt. percent C_1-C_9

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
Hydrogen	-2.14				
Methane	6.6				
Ethane	8.8				
Propane	11.0				
C_4	8.0	1.2			
C_5	2.3	1.1	2.0		
C_6	1.5	0.6	5.4	4.2	6.5
C_7	1.2	2.3	3.1	4.0	11.7
C_8	0.8	0.5	2.4	1.4	7.6
C_9	0.4	0.5	0.1	0.6	4.3

TABLE 12 (Continued)

2nd PASS + SELECTIVITIES
Wt. percent C_1-C_9

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
Hydrogen	-2.26				
Methane	7.7				
Ethane	8.9				
Propane	11.6				
C_4	8.1	1.3			
C_5	1.9	1.1	2.0		
C_6	1.1	0.8	4.4	3.5	8.3
C_7	0.8	1.9	3.0	2.5	14.0
C_8	0.5	0.3	2.2	0.7	7.8
C_9	0.4	0.6	0.0	0.1	4.6

TABLE 13

VACUUM GAS OIL RECYCLE HYDROCRACKING DATA

REACTOR CONDITIONS

945°F
2500 psig
LHSV 1.0 volume/volume-hr

RATE CONSTANTS

ALL PASSES - C_1-C_9 - 11.0×10^6 hr^{-1}
ALL PASSES - C_{10}-650°F - 11.0×10^6 hr^{-1}

SELECTIVITY TO C_1-C_9

Wt. percent C_1-C_9

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
Hydrogen	-4.14				
Methane	8.8				
Ethane	13.8				
Propane	15.9				
C_4	11.6	1.6			
C_5	2.4	1.4	0.9		
C_6	1.9	0.6	3.2	4.2	4.1
C_7	1.3	1.4	1.1	4.1	7.2
C_8	0.7	0.3	0.9	0.7	4.1
C_9	0.1	0.4	0.4	0.8	6.2

Hydrotreating Naphthas

The selectivity data for the liquid product from hydrotreating the straight run naphtha was not obtained. Analytical carbon-hydrogen data provided the hydrogen consumption data. The product pattern used for the conceptual process calculations is the result of combining gas make data from both passes with the liquid recovery rates and a componential analysis of the composite two-pass hydrotreated product.

Laboratory data from single pass hydrotreating the H-Coal 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. The selectivity data for hydrotreating H-Coal hydrocrackate naphtha is presented in Table 14 below.

TABLE 14

HYDROTREATING H-COAL HYDROCRACKATE NAPHTHA SELECTIVITY DATA

REACTOR CONDITION

750°F
1500 psig
LHSV 4 volumes/volume-hr

SELECTIVITY, lb/100 lb FEED

H_2	-1.13
C_1	0.01
C_2	0.01
C_3	0.04

CONVERSION OF AROMATIC IN FEED, wt. percent

C_6	24.2
C_7	29.3
C_8	34.8
C_9	19.7

The C_4-C_9 paraffins and C_5 naphthenes were assumed to be unchanged during the hydrotreating step.

Reforming Naphthas

The laboratory data for reforming the hydrotreated straight run naphtha was reduced to give conversion and selectivity data for the conceptual process. Conversions of both paraffins and C_5 and C_6 naphthenes were calculated and are presented in the following tables. Paraffin production as weight percent on the feed is also reported for C_1-C_6. The paraffin product normal/iso ratio for C_6-C_9 hydrocarbons is also presented in Tables 14 and 15. Hydrogen production was then calculated from analytical carbon-hydrogen data collected from analyses of the feed and product streams. The same data reduction from laboratory results to conversion and selectivity data for the conceptual process was completed for the reforming of the hydrotreated hydrocrackate naphtha. Tables 15 and 16 contain the reforming data for the conceptual process.

TABLE 15

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

	PARAFFIN	NAPHTHENE	
		CYCLO PENT	CYCLO HEXANE
C_6	-0-	44	97.3
C_7	37	86	97
C_8	85	99	96
C_9	96	99.5	94
C_{10}^+	44		

PARAFFIN PRODUCTION
WT. % ON FEED

	PARAFFIN	CYCLO PENT	NORM/ISO RATIO
C_1	0.9		
C_2	1.8		
C_3	2.5		
C_4	2.4		1.4
C_5	2.1	0.1	0.8
C_6	0.6		0.9
C_7	-0-		0.5
C_8	-0-		0.5
C_9	-0-		0.1

TABLE 16

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

	PARAFFIN	NAPHTHENE CYCLO PENT	 CYCLO HEXANE
C_6	-0-	61	98
C_7	24	94	99
C_8	73	99.8	99.5
C_9	92	100	98
C_{10}^+	70		

PARAFFIN PRODUCTION WT. % ON FEED

	PARAFFIN	CYCLO PENT	NORM/ISO RATIO
C_1	1.2		
C_2	2.2		
C_3	2.8		
C_4	2.3		1.7
C_5	2.0	0.1	0.8
C_6	2.2		0.9
C_7	-0-		0.5
C_8	-0-		0.3
C_9	-0-		0.5

Hydrodealkylating Reformates

The reformates, whether straight run or hydrocrackate were 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 17.

TABLE 17

REFORMATE HYDRODEALKYLATION SELECTIVITY DATA

	C_6	C_7	C_8	C_9
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 FOR INDIVIDUAL DISTILLATE FRACTIONS

Straight Run Naphtha

The H-Coal straight run naphtha was subjected to the mathematical calculations for hydrotreating, reforming, and hydrodealkylation. Componential data for the product from each hydroprocessing step is presented in the tables following. The basis for the componential data is 100.00 lb of naphtha from distillation. Therefore, the values reported for each component are the actual mass values in pounds of the component based on the feed. Table 18 is the result of the conceptual hydrotreating step, Table 19 the result of conceptual reforming, Table 20 the result of conceptual hydrodealkylation, and Table 21 is the total conceptual product pattern from the straight run naphtha. The values for the products were derived from those published by Spitz and Ross[1]. Hydrogen was estimated at $2.10/MCF from a methane reformer operating on $3.25/MM BTU gas.

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[1] Spitz, P. H. and Ross, G. N., "What is Feedstock Worth?" Hydrocarbon Processing, April, 1976.

TABLE 18

CONCEPTUAL HYDROTREATING
H-COAL STRAIGHT RUN NAPHTHA

Basis 100.00 lb
Naphtha from Distillation

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
Hydrogen	- .54				
Methane	.01				
Ethane	.01				
Propane	.11				
C_4	.70	.10			
C_5	1.53	.65	1.23		
C_6	2.09	1.04	3.31	11.71	1.95
C_7	2.95	3.19	2.44	14.15	5.62
C_8	2.25	1.43	3.71	3.22	8.29
C_9	.47	0.93	1.22	3.43	13.93
C_{10}^+	8.93				

TABLE 19

CONCEPTUAL REFORMING
H-COAL STRAIGHT RUN NAPHTHA

Basis 96.20 lb C_5+
from Hydrotreating

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
Hydrogen	2.03				
Methane	.87				
Ethane	1.73				
Propane	2.41				
C_4	1.35	.96			
C_5	.90	1.12	.10		
C_6	2.16	1.54	2.18	.32	13.49
C_7	1.29	2.58	.34	.42	20.37
C_8	.18	.37	.04	.13	14.64
C_9	.01	.05	.01	.21	18.12
C_{10}+	5.89				

TABLE 20

CONCEPTUAL HYDRODEALKYLATION
H-COAL STRAIGHT RUN NAPHTHA

Basis 84.37 lb C_6+
from Reforming

Hydrogen	- 3.07
Methane	18.20
Ethane	9.71
Benzene	51.28
Liquid Fuel	8.25

TABLE 21

CONCEPTUAL PROCESS PRODUCTS
H-COAL STRAIGHT RUN NAPHTHA

	Basis 100 lb from Distillation
Hydrogen	-1.58
Methane	19.08
Ethane	11.45
Propane	2.52
Butanes	3.11
Pentanes	5.53
Benzene	51.28
Liquid Fuel	8.25
Value/100 lb Distillate (1980)	$10.06

Straight Run Mid-Distillate

The H-Coal straight run mid-distillate was subjected to mathematical recycle hydrocracking, hydrotreating, reforming, and hydrodealkylation. Componential data for each step is reported based on 100.00 lb of mid-distillate from distillation. Table 22 lists the componential product pattern for recycle hydrocracking, Table 23 the product from hydrotreating, Table 24 the product from reforming, Table 25 the product from hydrodealkylation, and Table 26 the total conceptual product pattern from the straight run mid-distillate with the product value.

TABLE 22

CONCEPTUAL RECYCLE HYDROCRACKING H-COAL MID-DISTILLATE

Basis 100.00 lbs from Distillation

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
Hydrogen	-4.34				
Methane	7.34				
Ethane	9.20				
Propane	11.73				
C_4	8.36	1.30			
C_5	2.23	1.15	2.08		
C_6	1.39	.69	5.23	4.07	7.57
C_7	1.06	2.23	3.20	3.51	13.18
C_8	.73	.45	2.38	1.17	8.04
C_9	.40	.53	.06	.42	4.61
C_{10}^+	.48				

TABLE 23

CONCEPTUAL HYDROTREATING H-COAL MID-DISTILLATE HYDROCRACKATE NAPHTHA

Basis 66.87 lb C_5+
from Recycle Hydrocracking

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
Hydrogen	-.75				
Methane	.01				
Ethane	.01				
Propane	.03				
C_4	---	---			
C_5	2.23	1.15	2.08		
C_6	1.39	.69	5.23	6.36	5.44
C_7	1.06	2.23	3.20	8.31	8.68
C_8	.73	.45	2.38	4.63	4.77
C_9	.40	.53	.06	1.53	3.55
C_{10}^+	.48				

TABLE 24

CONCEPTUAL REFORMING
H-COAL MID-DISTILLATE HYDROCRACKATE NAPHTHA

Basis 62.10 lbs
C_6+ from Hydrotreating

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
Hydrogen	1.50				
Methane	.75				
Ethane	1.37				
Propane	1.74				
C_4	.90	.53			
C_5	.55	.69	.06		
C_6	1.63	1.81	2.04	.13	12.52
C_7	.83	1.67	.19	.08	16.96
C_8	.07	.25	.00	.02	10.04
C_9	.02	.05	.00	.03	4.45
C_{10}+	.14				

TABLE 25

CONCEPTUAL HYDRODEALKYLATION
H-COAL MID-DISTILLATE HYDROCRACKATE NAPHTHA

Basis 52.93 lb
C_6+ from Reforming

Hydrogen	-1.77
Methane	10.45
Ethane	6.55
Benzene	36.32
Liquid Fuel	1.37

TABLE 26

CONCEPTUAL PROCESS PRODUCTS
H-COAL STRAIGHT RUN MID-DISTILLATE

	Basis 100 lb from Distillation
Hydrogen	-5.36
Methane	18.55
Ethane	17.13
Propane	13.50
Butanes	11.09
Pentanes	6.76
Benzene	36.32
Liquid Fuel	1.37
Value/100 lb Distillate (1980)	$8.12

Straight Run Vacuum Gas Oil

The H-Coal straight run vacuum gas oil was first subjected to mathematical recycle hydrocracking to naphtha and C_{10}-650°F mid-distillate. The componential data from these calculations is presented in Table 27. The C_{10}-650°F mid-distillate from the gas oil hydrocracking was then recycle hydrocracked mathematically to produce naphtha, for which the componential data is presented in Table 28. The naphtha produced from the gas oil was combined and mathematically hydrotreated. The conceptual product pattern from hydrotreating is presented in Table 29. Following hydrotreating, the naphtha was mathematically reformed and hydrodealkylated. Tables 30 and 31 respectively, contain the componential product patterns for these processing steps. Table 32 lists the total conceptual product pattern from the straight run vacuum gas oil with the product value.

TABLE 27

CONCEPTUAL RECYCLE HYDROCRACKING
H-COAL VACUUM GAS OIL

Basis 100 lbs from Distillation

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
Hydrogen	-5.44				
Methane	4.62				
Ethane	7.25				
Propane	8.36				
C_4	6.07	.87			
C_5	1.26	.74	.49		
C_6	.97	.29	1.67	2.19	2.18
C_7	.69	.76	.57	2.17	3.76
C_8	.35	.17	.49	.37	2.14
C_9	.05	.18	.18	.43	3.26
C_{10}^+	52.89				

TABLE 28

CONCEPTUAL RECYCLE HYDROCRACKING
H-COAL MID-DISTILLATE FROM VACUUM GAS OIL

Basis 52.89 lbs C_{10}-650°F
From Vacuum Gas Oil Hydrocracking

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
Hydrogen	-2.30				
Methane	3.88				
Ethane	4.87				
Propane	6.20				
C_4	4.42	.69			
C_5	1.18	.61	1.10		
C_6	.74	.36	2.77	2.15	4.00
C_7	.56	1.18	1.69	1.86	6.97
C_8	.39	.24	1.26	.62	4.25
C_9	.21	.28	.03	.22	2.44
C_{10}^+	.25				

TABLE 29

CONCEPTUAL HYDROTREATING HYDROCRACKATE
H-COAL NAPHTHA FROM VACUUM GAS OIL & MID-DISTILLATE

Basis 60.72 lbs C_5+ from
Recycle Hydrocrack Vacuum Gas Oil
Plus Recycle Hydrocrack Mid-
Distillate from Vacuum Gas Oil

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
Hydrogen	- .64				
Methane	.01				
Ethane	.01				
Propane	.02				
C_4	---	---			
C_5	2.44	1.35	1.59		
C_6	1.71	.65	4.44	6.39	4.28
C_7	1.25	1.94	2.26	8.25	6.77
C_8	.74	.41	1.75	3.95	3.59
C_9	.26	.46	.21	2.13	4.29
C_{10}^+	.25				

TABLE 30

CONCEPTUAL REFORMING
H-COAL VACUUM GAS OIL HYDROCRACKATE NAPHTHA

Basis 55.98 lbs C_6+ from Hydrotreating

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
Hydrogen	1.19				
Methane	.67				
Ethane	1.23				
Propane	1.57				
C_4	.81	.48			
C_5	.50	.62	.06		
C_6	1.70	1.89	1.73	.13	11.29
C_7	.81	1.62	.14	.08	14.69
C_8	.07	.24	.00	.02	8.03
C_9	.02	.04	.00	.04	5.80
C_{10}^+	.08				

TABLE 31

CONCEPTUAL HYDRODEALKYLATION H-COAL VACUUM GAS OIL HYDROCRACKATE NAPHTHA

	Basis 48.42 lb C_6+ from Reforming
Hydrogen	-1.68
Methane	9.94
Ethane	6.35
Benzene	32.58
Liquid Fuel	1.24

TABLE 32

CONCEPTUAL PROCESS PRODUCTS H-COAL STRAIGHT RUN VACUUM GAS OIL

	Basis 100 lbs from Distillation
Hydrogen	8.87
Methane	19.12
Ethane	19.71
Propane	16.15
Butanes	13.34
Pentanes	6.56
Benzene	32.58
Liquid Fuel	1.24
Value/100 lb Distillate (1980)	$6.91

Conceptual Plant Balance

With the pattern and value known for the products of each distillate fraction, the remaining step is to calculate the mass balance for a conceptual plant using the whole crude as the primary feedstock. From this data, the preliminary capital requirements and operating costs for a commercial plant can be estimated. The basis for the mass balance data is a flow of 100.00 lb/hr of the whole crude to the distillation step. With the fuel value of a crude distillate feedback ranging from $6.25 to $6.75 per 100 pounds, it would appear, from the conceptual process product values presented for each fraction in Tables 21, 26, and 32, that mid-distillate processing could be only marginally attractive. With the added processing charges for gas oil hydroprocessing, it is unlikely to be economically attractive as a petrochemical feedstock. For this reason, the gas oil hydroprocessing sequence was not included in the overall conceptual plant mass balance. A schematic diagram of the conceptual plant with selected streams identified by number is included in Figure 5. Tables 33 through 36 include mass flow rates, elemental, and, where known, the componential analysis of the various streams identified in the schematic diagram. The componential data for each stream identified is presented as weight percent of each component by carbon number. Note that part of the process derived methane is converted to hydrogen in an oil fired methane reformer. Enough hydrogen is produced to supply hydroprocessing needs.

Figure 5

CONCEPTUAL PLANT

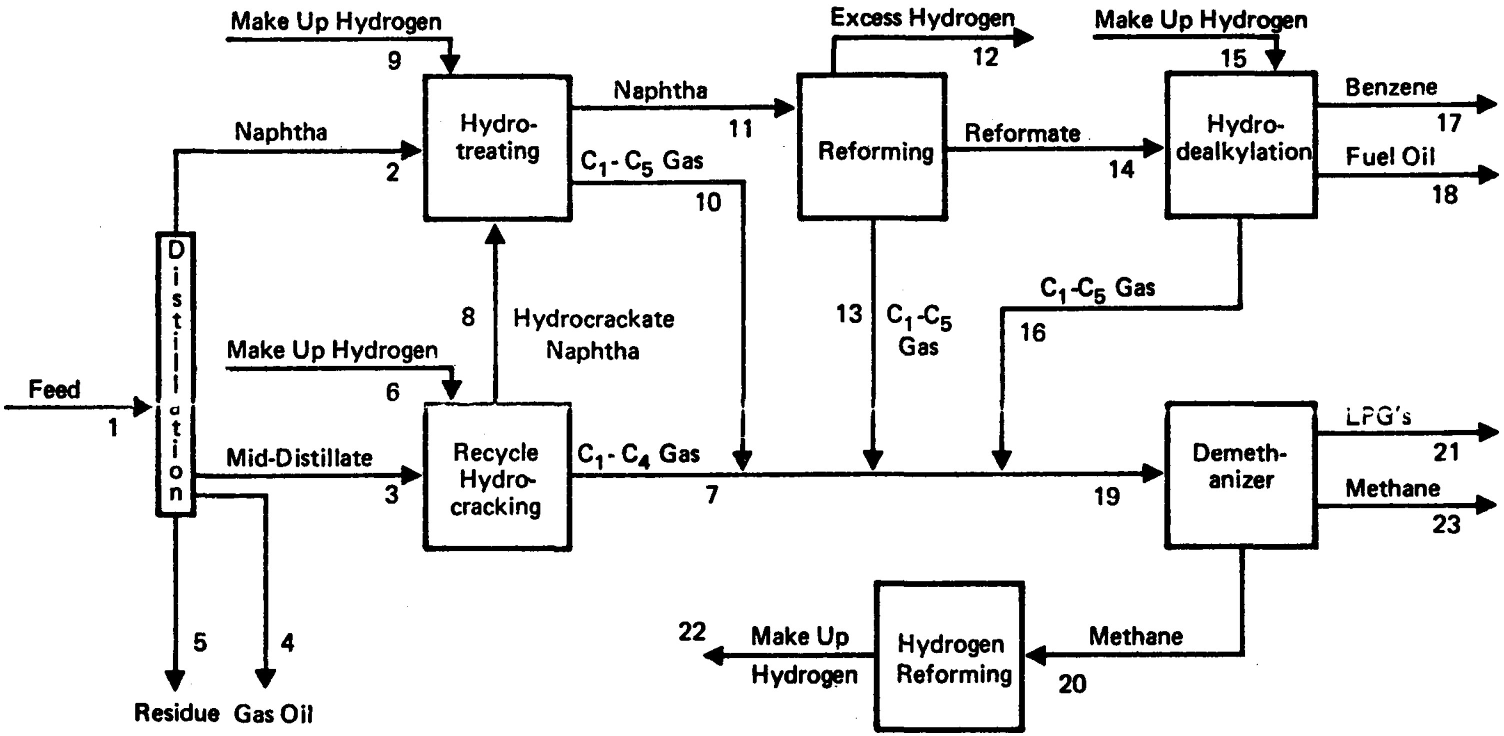

TABLE 33

DISTILLATION

Full Range Oil Including Unreacted Coal and Ash

Stream Identification No. 1
Flow Rate 100 lb/hr

Naphtha

Stream Identification No. 2
Flow Rate 19.8 lb/hr
API Gravity, 60°F - 49.9

	Wt. %
Carbon	86.4
Hydrogen	12.9
Nitrogen	0.047
Oxygen	0.39
Sulfur	0.26

Mid-Distillate

Stream Identification No. 3
Flow Rate 12.1 lb/hr
API Gravity, 60°F - 25.9

	Wt. %
Carbon	88.0
Hydrogen	11.2
Nitrogen	0.044
Oxygen	0.58
Sulfur	0.17

Gas Oil 800°F E.P.

Stream Identification No. 4
Flow Rate 11.5 lb/hr
API Gravity, 60°F - 7.9

	Wt. %
Carbon	89.6
Hydrogen	10.4
Nitrogen	0.083
Oxygen	0.08
Sulfur	0.17

Residue

Stream Identification No. 5
Flow Rate 56.6 lb/hr

	Wt. %
Unreacted Coal	13.4
Ash	25.3

TABLE 34

CONCEPTUAL PLANT HYDROPROCESSING LIQUID STREAMS

Hydrocrackate Naphtha

Stream Identification No. 8
Flow Rate 8.05 lb/hr

	Wt. %
Carbon	87.88
Hydrogen	12.12

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
C_5	3.36	1.73	3.13		
C_6	2.09	1.04	7.88	6.13	11.40
C_7	1.60	3.36	4.82	5.29	19.85
C_8	1.10	.68	3.58	1.76	12.11
C_9	.60	.80	.09	.63	6.94
C_{10}^+	.72				

Hydrotreated Naphtha

Stream Identification No. 11
Flow Rate 26.52 lb/hr

	Wt. %
Carbon	87.36
Hydrogen	12.64

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
C_6	2.19	1.09	4.84	11.63	3.92
C_7	2.68	3.39	3.27	14.33	8.13
C_8	2.01	1.27	3.85	4.50	8.35
C_9	.53	.93	.94	3.25	12.01
C_{10}^+	6.88				

TABLE 34 (Cont'd)

Reformate C_6+

Stream Identification No. 14
Flow Rate 23.28 lb/hr

	Wt. %
Carbon	89.89
Hydrogen	10.11

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
C_6	2.67	2.24	2.91	.34	18.11
C_7	1.52	3.06	.39	.40	26.34
C_8	.19	.44	.03	.13	17.80
C_9	.02	.07	.01	.19	17.87
C_{10}+	5.08				

TABLE 35

CONCEPTUAL PLANT HYDROPROCESSING GAS STREAMS

Hydrocracking Gas Make

Stream Identification No. 7
Flow Rate 4.60 lb/hr

	Wt. %
Carbon	80.10
Hydrogen	19.90

Methane	19.45
Ethane	23.85
Propane	31.09
Butane	22.16
Isobutane	3.45

Hydrotreating Gas Make

Stream Identification No. 10
Flow Rate 1.52 lb/hr

	Wt. %
Carbon	83.83
Hydrogen	16.17

	NORM PARAF	ISO PARAF	CYCLO PENT
Methane	0.21		
Ethane	0.20		
Propane	1.67		
C_4	9.10	1.30	
C_5	37.53	17.55	32.44

Reformer Gas Make

Stream Identification No. 13
Flow Rate 2.66 lb/hr

	Wt. %
Carbon	84.03
Hydrogen	15.97

	NORM PARAF	ISO PARAF	CYCLO PENT
Methane	9.77		
Ethane	19.17		
Propane	25.94		
C_4	14.29	9.40	
C_5	9.02	11.28	1.13

TABLE 36

CONCEPTUAL PLANT HYDRODEALKYLATOR STREAMS

Hydrodealkylator Gas Make

Stream Identification No. 16
Flow Rate 7.57 lb/hr

	Wt. %
Carbon	76.59
Hydrogen	23.41

Methane	64.19
Ethane	35.81

Benzene Product

Stream Identification No. 17
Flow Rate 14.52 lb/hr

	Wt. %
Carbon	92.2
Hydrogen	7.8

Benzene	100.0

Hydrodealkylator Bottoms

Stream Identification No. 18
Flow Rate 1.80 lb/hr

	Wt. %
Carbon	93.6
Hydrogen	6.4

C_{10}^{+}	100.0

TABLE 37

CONCEPTUAL PLANT DEMETHANIZER STREAMS

Feed to Demethanizer

Stream Identification No. 19
Flow Rate 16.35 lb/hr

	Wt. %
Carbon	78.98
Hydrogen	21.02

	NORM PARAF	ISO PARAF	CYCLO PENT
Methane	36.80		
Ethane	26.53		
Propane	13.12		
C_4	9.41	2.62	
C_5	4.96	3.47	3.20

Methane to Hydrogen Production (Reformer)

Stream Identification No. 20
Flow Rate 2.00 lb/hr

	Wt. %
Carbon	74.8
Hydrogen	25.2

Methane	100.0

LPG's

Stream Identification No. 21
Flow Rate 10.33 lb/hr

	Wt. %
Carbon	81.41
Hydrogen	18.59

	NORM PARAF	ISO PARAF	CYCLO PENT
Ethane	41.98		
Propane	20.76		
C_4	14.89	4.15	
C_5	7.85	5.49	5.06

Methane to Export

Stream Identification No. 23
Flow Rate 4.02 lb/hr

	Wt. %
Carbon	74.8
Hydrogen	25.2

Methane	100.0

TABLE 38

HYDROGEN

Flow Rate

to Hydrocracking	-0.53 lb/hr	6
to Hydrotreating	-0.20 lb/hr	9
from Reforming	+0.58 lb/hr	12
to Hydrodealkylator	-0.82 lb/hr	14
from Methane Reformer	+0.97 lb/hr	22

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APPENDICES TO PART I

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

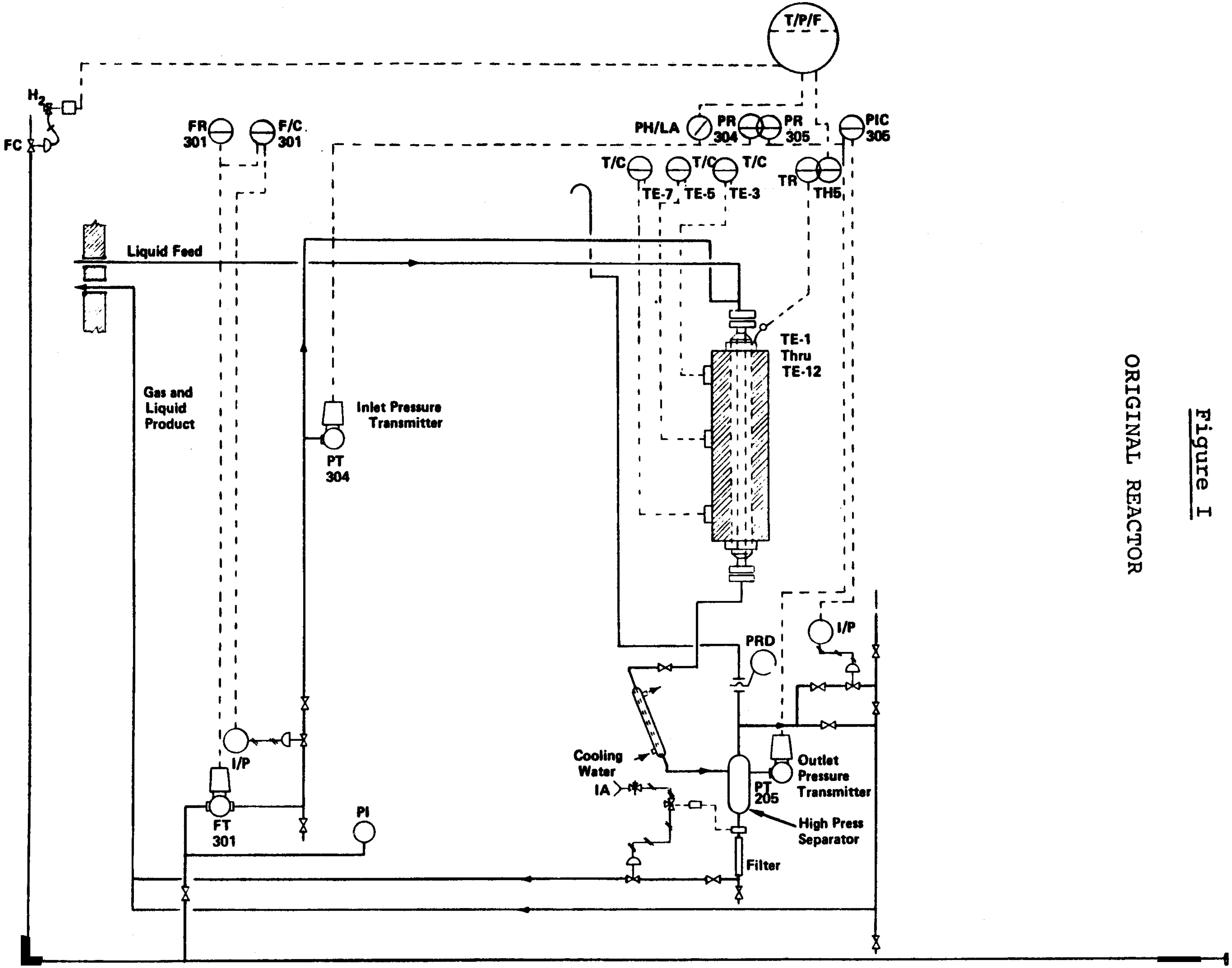
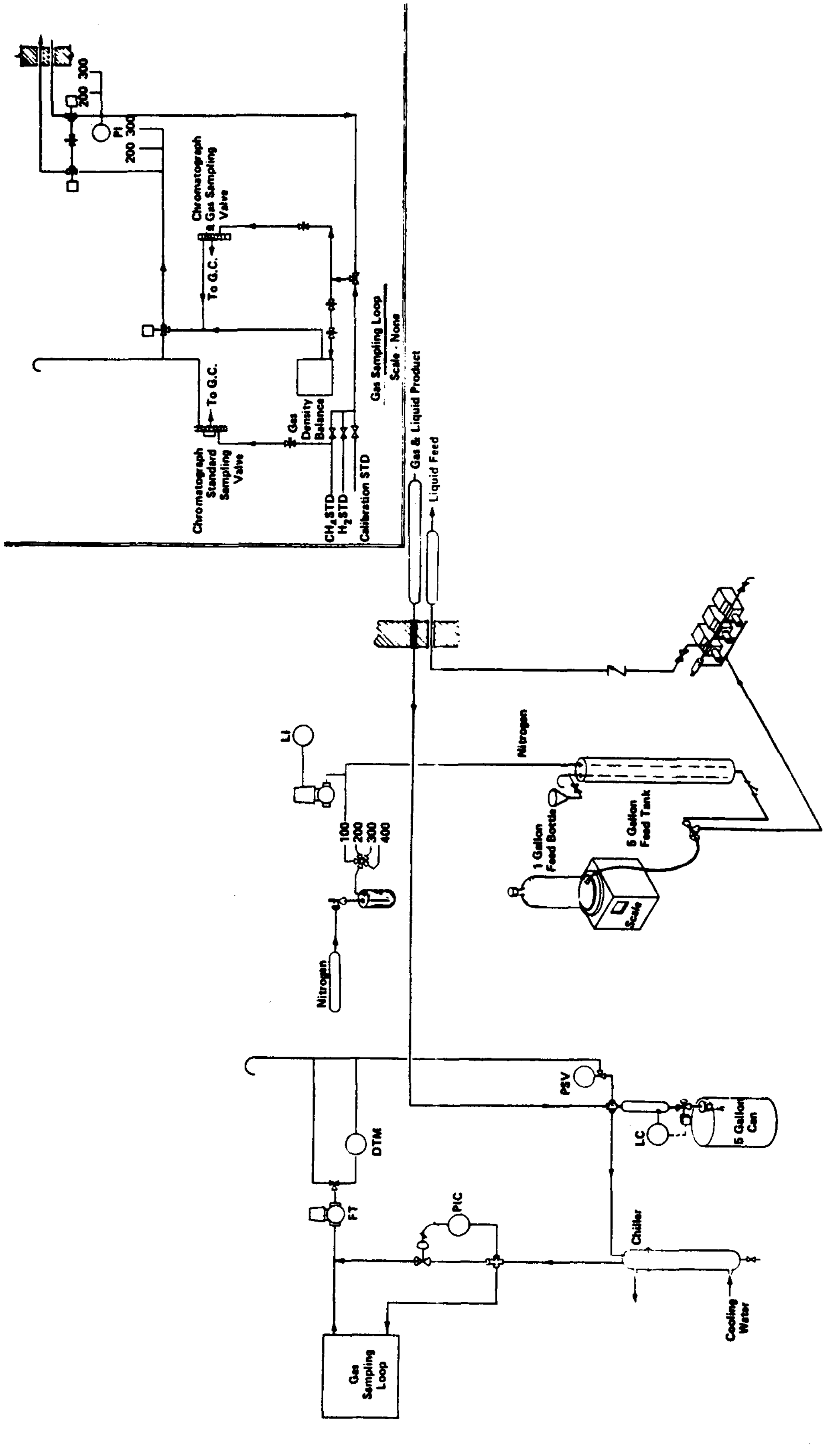


Figure I

ORIGINAL REACTOR

Figure II

ORIGINAL FEED AND PRODUCT RECOVERY EQUIPMENT



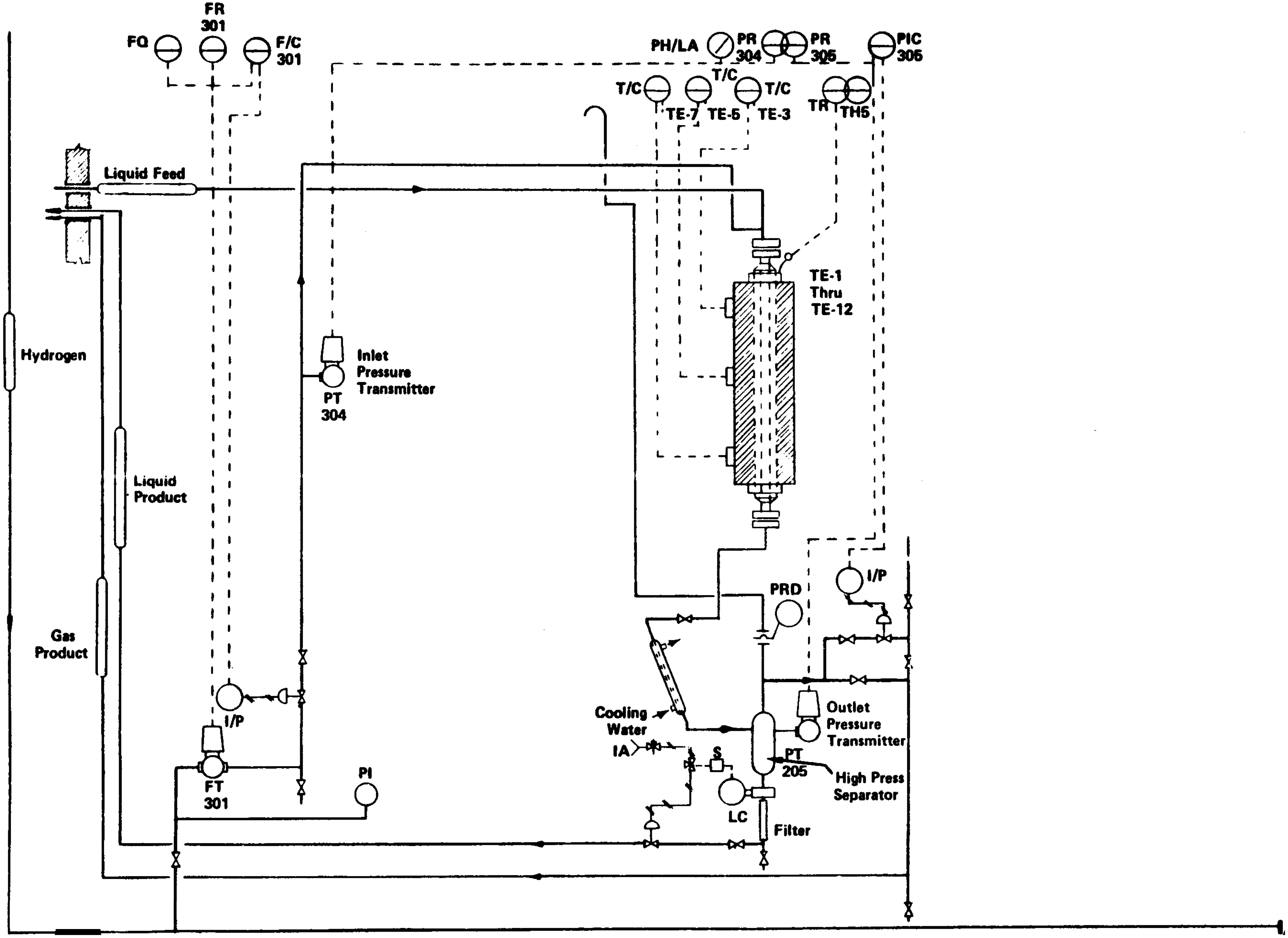
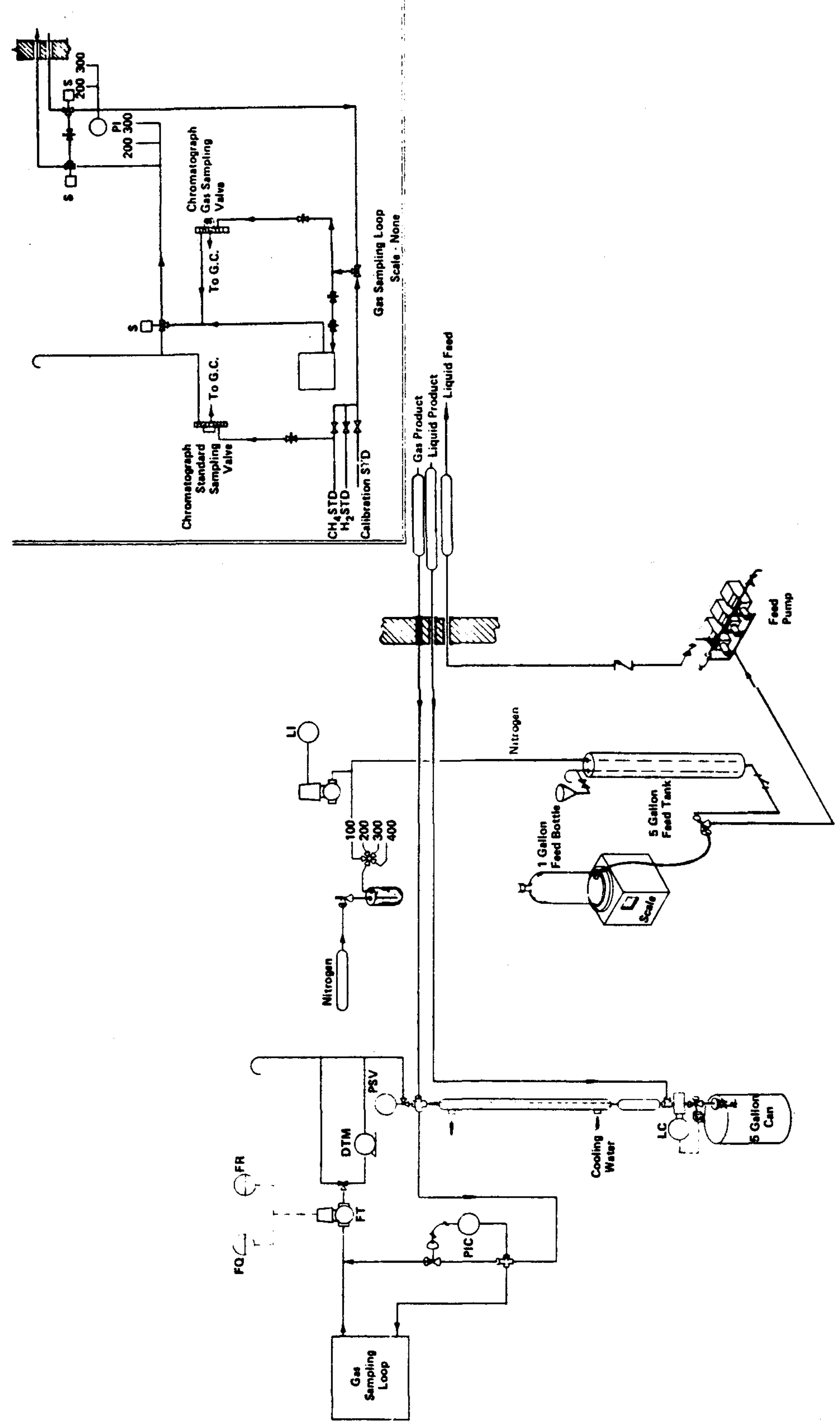


Figure III

MODIFIED REACTOR

Figure IV

MODIFIED FEED AND PRODUCT RECEOVERY 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 hydrotreating 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.

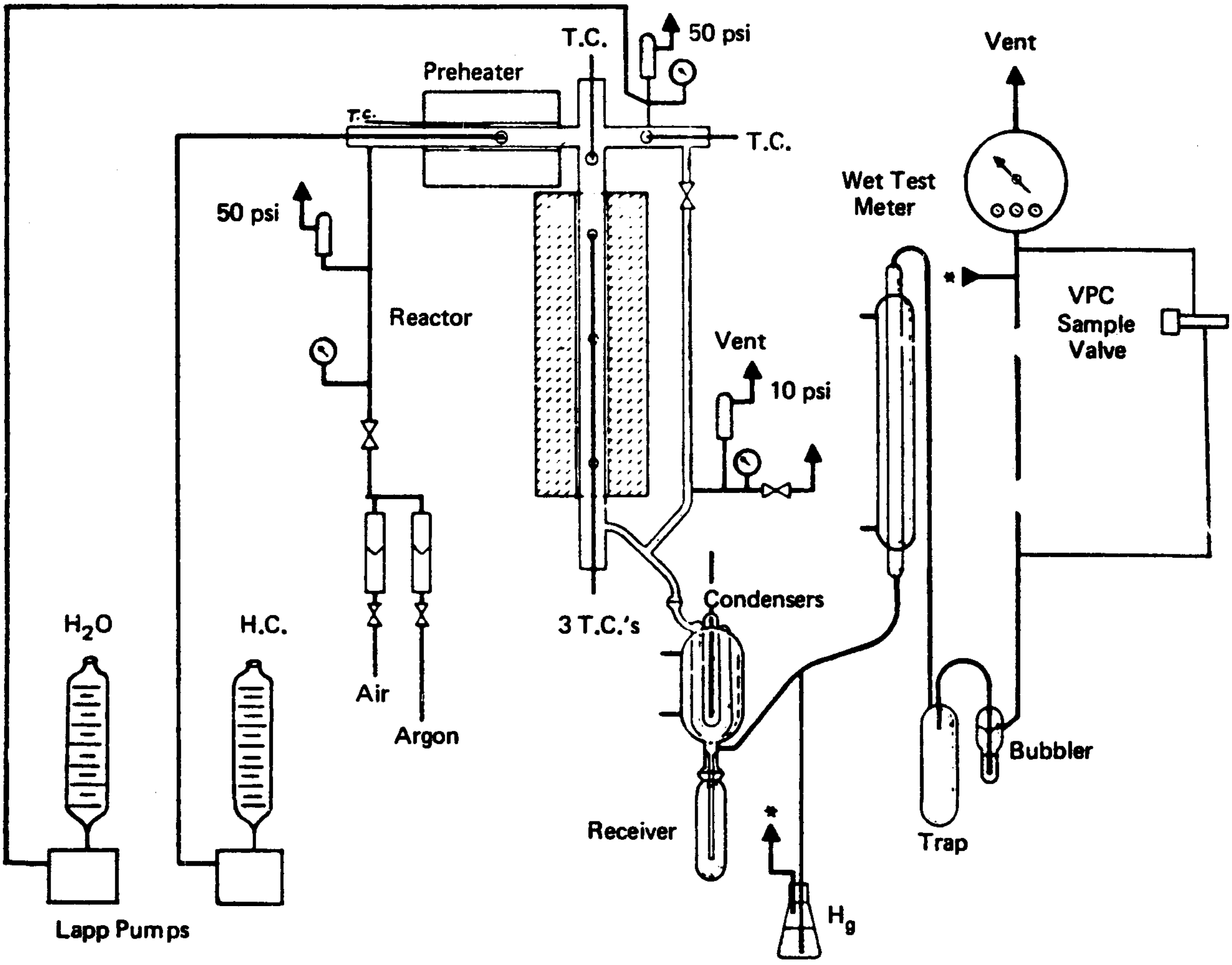
The cold trap provided for condensing very light materials can only be used for atmospheric distillations.

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_4 to C_{12} 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_{10}+ 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_1-C_9 compounds classified by carbon number and structural type and the weight percent C_{10}+ 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_3-C_9 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_2 and H_2O 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_x 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 Microcoulemetric Reactor. Sulfur present in the samples is converted to SO_2. 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 x 10^6 electron volts) produces the necessary activation energy. Samples are conveyed to and from source and detector via a pneumatic transfer system. A scinilation detector equipped with a sodium iodide crystal detects the induced radioactive isotope (Nitrogen 16) at energies of 6.1 and 7.3 x 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% $NaNo_3$ 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. The steam coil cracking data presented is a combination of reactor conditions and analytical and computer data reduction.

HYDROPROCESSING DATA

DATE 2-18-75 DATA BOOK NO. 103-3-21
RUN, SAMPLE NO. H-COAL 1 REV
PROCESS: HYDROCRACKING MID-DISTILLATE
CATALYST: HARSHAW HT-400-1/8-E
FEED: H-COAL ST. RUN MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	870
LHSV - VOL/VOL-HR	.35	CATALYST VOLUME CC	200
MATERIAL BALANCE %	99.71	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	7850	OIL PRODUCT RATE G/HR	55.40
OIL FEED RATE G/HR	63.41	TAIL GAS RATE G/HR	16.89
HYDROGEN FEED RATE G/HR	8.88	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + 47.8 500°F + 100.0

YIELD: G/100G OIL FEED

HYDROGEN	-1.42[A]	-2.24[B]	WATER	---
METHANE	1.33			
ETHANE	2.13			
PROPANE	2.32			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	1.98	.21				2.19
C_5	.64	.42	.36			1.42
C_6	.35	.18	.89	1.50	.50	3.41
C_7	.22	.44	.43	2.44	1.20	4.74
C_8	.34	.10	.77	1.16	.86	3.24
C_9	.05	.25	.05	.33	2.57	3.24
TOTAL	3.57	1.61	2.50	5.42	5.12	18.23

UNIDENTIFIED C_4-C_9 --- C_{10}+ 77.4

HYDROGEN YIELD SCF/BBL -797[A] -1255[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.98	11.23	.044	.576	.169	100.00
HYDROGEN		14.00				14.00
TOTAL	87.98	25.23	.044	.576	.169	114.00
PRODUCTS						
LIQUID	76.35	11.02	.000	.722	.001	88.09
HC GAS	11.63	2.43				14.06
HYDROGEN		12.58				12.01
NH_3		.009	.044			.053
H_2O		NA		NA		NA
H_2S		.011			.168	.1
TOTAL	87.98	26.05	.044	.722	.169	114.40

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 2-20-75 DATA BOOK NO. 103-3-22
RUN, SAMPLE NO. H-COAL 2
PROCESS: HYDROCRACKING MID-DISTILLATE
CATALYST: HARSHAW HT-400-1/8-E
FEED: H-COAL ST. RUN MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	960
LHSV - VOL/VOL-HR	.36	CATALYST VOLUME CC	200
MATERIAL BALANCE %	102.92	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	7170	OIL PRODUCT RATE G/HR	32.27
OIL FEED RATE G/HR	64.17	TAIL GAS RATE G/HR	40.11
HYDROGEN FEED RATE G/HR	8.21	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + 86.5 500°F + 100.0

YIELD: G/100G OIL FEED

HYDROGEN	-2.92 [A]	-3.70 [B]	WATER	---
METHANE	5.85			
ETHANE	7.77			
PROPANE	8.76			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	5.94	.98				6.92
C_5	1.60	.94	1.90			4.44
C_6	1.10	.45	6.46	3.83	3.57	15.40
C_7	1.28	2.84	2.11	4.98	6.37	17.58
C_8	.54	.31	1.56	.91	2.65	5.97
C_9	.29	.62	.05	.27	2.80	4.03
TOTAL	10.74	6.14	12.09	9.99	15.38	54.35

UNIDENTIFIED C_4-C_9 .02 $C_{10}+$ 26.38

HYDROGEN YIELD SCF/BBL -1640 [A] -2070 [B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.98	11.23	.044	.576	.169	100.00
HYDROGEN		12.79				12.79
TOTAL	87.98	24.02	.044	.576	.169	112.79
PRODUCTS						
LIQUID	44.36	5.90	.0000	.69	.022	50.95
HC GAS	43.62	9.01				52.63
HYDROGEN		9.87				9.87
NH_3		.009	.044			.053
H_2O				NA		NA
H_2S		.010			.167	.177
TOTAL	87.98	24.80	.044	.69	.169	113.68

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE	3-4-75	DATA BOOK NO.	103-3-25

RUN, SAMPLE NO. H-COAL 3 REV
PROCESS: HYDROCRACKING MID-DISTILLATE
CATALYST: HARSHAW HT-400-1/8-E
FEED: H-COAL ST. RUN MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	962
LHSV - VOL/VOL-HR	1.04	CATALYST VOLUME CC	200
MATERIAL BALANCE %	104.72	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	2510	OIL PRODUCT RATE G/HR	134.46
OIL FEED RATE G/HR	186.42	TAIL GAS RATE G/HR	60.30
HYDROGEN FEED RATE G/HR	8.34	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + 70.8 500°F + 85.6

YIELD: G/100G OIL FEED

HYDROGEN	-0.74 A	-1.60 B	WATER	---
METHANE	3.88			
ETHANE	5.18			
PROPANE	6.49			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	4.71	.70				5.41
C_5	1.37	.65	1.17			3.19
C_6	.88	.35	3.21	2.46	3.85	10.75
C_7	.69	1.36	1.85	2.37	6.90	13.18
C_8	.49	.30	1.39	.83	4.50	7.51
C_9	.24	.27	.05	.36	2.55	3.46
TOTAL	8.38	3.62	7.68	6.02	17.80	43.51

UNIDENTIFIED C_4-C_9 .07 $C_{10}+$ 41.70

HYDROGEN YIELD SCF/BBL -415 A -897 B

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.98	11.23	.044	.576	.169	100.00
HYDROGEN		4.47				4.47
TOTAL	87.98	15.70	.044	.576	.169	104.47
PRODUCTS						
LIQUID	64.48	7.68	.0000	.51	.002	72.67
HC GAS	23.50	5.12				28.62
HYDROGEN		3.73				3.73
NH_3		.009	.044			.053
H_2O		.007		.06		.067
H_2S		.010			.167	.17
TOTAL	87.98	16.56	.044	.57	.169	105.32

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 3-6-75 DATA BOOK NO. 103-3-27
RUN, SAMPLE NO. H-COAL 4 REV
PROCESS: HYDROCRACKING MID-DISTILLATE
CATALYST: HARSHAW HT-400-1/8-E
FEED: H-COAL ST. RUN MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	965
LHSV - VOL/VOL-HR	1.45	CATALYST VOLUME CC	200
MATERIAL BALANCE %	99.53	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	2610	OIL PRODUCT RATE G/HR	194.90
OIL FEED RATE G/HR	261.10	TAIL GAS RATE G/HR	78.34
HYDROGEN FEED RATE G/HR	12.14	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + 64.2 500°F + 70.9

YIELD: G/100G OIL FEED

HYDROGEN	- .79[A]	-1.43[B]	WATER	---
METHANE	3.57			
ETHANE	4.91			
PROPANE	6.03			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	4.08	.62				4.70
C_5	.97	.57	1.01			2.55
C_6	.81	.33	2.67	2.06	3.26	9.13
C_7	.62	1.11	1.16	2.14	6.21	11.24
C_8	.48	.26	1.29	.85	4.42	7.29
C_9	.27	.62	.04	.18	2.99	4.10
TOTAL	7.21	3.52	6.16	5.24	16.88	39.01

UNIDENTIFIED C_4-C_9 .10 C_{10}+ 47.15

HYDROGEN YIELD SCF/BBL -447[A] -801[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.98	11.23	.044	.576	.169	100.00
HYDROGEN		4.65				4.65
TOTAL	87.98	15.88	.044	.576	.169	104.65
PRODUCTS						
LIQUID	66.58	7.90	.0000	.94	.006	75.43
HC GAS	21.40	4.74				26.14
HYDROGEN		3.86				3.86
NH_3		.009	.044			.053
H_2O		NA		NA		NA
H_2S		.010			.163	.173
TOTAL	87.98	16.52	.044	.94	.169	105.65

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 3-11-75 DATA BOOK NO. 103-3-28
RUN, SAMPLE NO. H-COAL 5 REV
PROCESS: HYDROCRACKING MID-DISTILLATE
CATALYST: HARSHAW HT-400-1/8-E
FEED: H-COAL ST. RUN MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	976
LHSV - VOL/VOL-HR	.67	CATALYST VOLUME CC	200
MATERIAL BALANCE %	99.11	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	3370	OIL PRODUCT RATE G/HR	84.10
OIL FEED RATE G/HR	119.90	TAIL GAS RATE G/HR	42.31
HYDROGEN FEED RATE G/HR	7.21	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + 78.2 500°F + 97.2

YIELD: G/100G OIL FEED

HYDROGEN	-2.19[A]	-2.10[B]	WATER	---
METHANE	5.13			
ETHANE	5.69			
PROPANE	6.07			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	4.05	.63				4.68
C_5	1.33	.71	1.71			3.76
C_6	1.02	.45	4.90	3.08	4.65	14.09
C_7	.90	1.88	2.35	2.97	8.18	16.28
C_8	.55	.33	1.45	.82	4.53	7.67
C_9	.27	.30	.05	.17	3.02	3.81
TOTAL	8.12	4.30	10.46	7.03	20.38	50.28

UNIDENTIFIED C_4-C_9 0.06 C_{10}+ 34.90

HYDROGEN YIELD SCF/BBL -1200[A] -1180[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.98	11.23	.044	.58	.169	100.00
HYDROGEN		6.01				6.01
TOTAL	87.98	17.24	.044	.58	.169	106.01
PRODUCTS						
LIQUID	62.14	7.68	.0000	.65	.008	70.48
HC GAS	25.84	5.63				31.47
HYDROGEN		3.82				3.82
NH_3		.009	.044			.053
H_2O		NA		NA		
H_2S		.010			.161	.1[illegible]
TOTAL	87.98	17.15	.044	.65	.169	105.99

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 3-13-75 DATA BOOK NO. 103-3-29
RUN, SAMPLE NO. H-COAL 6 REV
PROCESS: HYDROCRACKING MID-DISTILLATE
CATALYST: HARSHAW HT-400-1/8-E
FEED: H-COAL ST. RUN MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	1008
LHSV - VOL/VOL-HR	.67	CATALYST VOLUME CC	200
MATERIAL BALANCE %	105.36	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	3390	OIL PRODUCT RATE G/HR	62.44
OIL FEED RATE G/HR	119.52	TAIL GAS RATE G/HR	64.31
HYDROGEN FEED RATE G/HR	7.23	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + 87.7 500°F + 100.0

YIELD: G/100G OIL FEED

HYDROGEN	-2.44 [A]	-3.05 [B]	WATER	---
METHANE	6.89			
ETHANE	10.14			
PROPANE	12.43			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	6.15	1.48				7.64
C_5	1.46	.77	3.03			5.26
C_6	1.04	.43	5.88	1.78	8.45	17.59
C_7	.63	1.10	1.18	1.06	9.18	13.15
C_8	.24	.11	.39	.19	3.90	4.82
C_9	.16	.04	.04	.04	3.56	3.83
TOTAL	9.68	3.94	10.52	3.07	25.09	52.29

UNIDENTIFIED C_4-C_9 --- C_{10}^+ 20.69

HYDROGEN YIELD SCF/BBL -1370 [A] -1710 [B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.98	11.23	.044	.58	.169	100.00
HYDROGEN		6.05				6.05
TOTAL	87.98	17.28	.044	.58	.169	106.05
PRODUCTS						
LIQUID	46.81	5.20	.000	.34	.014	52.36
HC GAS	41.17	9.03				50.20
HYDROGEN		3.61				3.61
NH_3		.009	.044			.053
H_2O		.03		.24		.27
H_2S		.01			.155	.155
TOTAL	87.98	17.89	.044	.58	.169	106.66

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 3-20-75 DATA BOOK NO. 103-3-30
RUN, SAMPLE NO. H-COAL 7 REV
PROCESS: HYDROCRACKING MID-DISTILLATE
CATALYST: HARSHAW HT-400-1/8-E
FEED: H-COAL 2nd PASS MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	934
LHSV - VOL/VOL-HR	1.00	CATALYST VOLUME CC	200
MATERIAL BALANCE %	98.47	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	2960	OIL PRODUCT RATE G/HR	161.74
OIL FEED RATE G/HR	182.58	TAIL GAS RATE G/HR	30.31
HYDROGEN FEED RATE G/HR	9.47	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + 29.4 500°F + 63.1

YIELD: G/100G OIL FEED

HYDROGEN	-1.89 [A]	-2.05 [B]	WATER	---
METHANE	1.72			
ETHANE	2.07			
PROPANE	3.13			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	2.76	.36				3.12
C_5	.60	.33	.54			1.47
C_6	.40	.18	1.43	1.04	1.77	4.82
C_7	.26	.65	.91	1.16	3.39	6.37
C_8	.25	.15	.79	.42	2.10	3.71
C_9	.11	.17	.02	.11	1.70	2.11
TOTAL	4.37	1.84	3.69	2.73	8.96	21.60

UNIDENTIFIED C_4-C_9 .03 C_{10}+ 73.34

HYDROGEN YIELD SCF/BBL 1080 [A] 1170 [B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	89.56	10.44	.0000	.0840	.0070	100.09
HYDROGEN		5.19				5.19
TOTAL	89.56	15.63	.0000	.0840	.0070	105.28
PRODUCTS						
LIQUID	78.66	10.09	.0000	.0890	.0023	88.84
HC GAS	10.90	2.40				13.30
HYDROGEN		3.30				3.30
NH_3		.000				.000
H_2O		.000		.0000		.000
H_2S		.000			.0047	.00[illegible]
TOTAL	89.56	15.79	.0000	.0890	.0070	105.44

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 3-25-75 DATA BOOK NO. 103-3-31
RUN, SAMPLE NO. H-COAL 8
PROCESS: HYDROCRACKING MID-DISTILLATE
CATALYST: HARSHAW HT-400-1/8-E
FEED: H-COAL 2nd PASS MID-DISTILLATE

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	1015
LHSV - VOL/VOL-HR	.99	CATALYST VOLUME CC	200
MATERIAL BALANCE %	99.01	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	2980	OIL PRODUCT RATE G/HR	105.30
OIL FEED RATE G/HR	180.90	TAIL GAS RATE G/HR	85.06
HYDROGEN FEED RATE G/HR	9.46	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + 76.2 500°F + 88.8

YIELD: G/100G OIL FEED

HYDROGEN	-3.48[A]	-8.32[B]	WATER	---
METHANE	8.62			
ETHANE	9.41			
PROPANE	9.98			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	3.70	1.39				5.10
C_5	.98	.79	1.69			3.46
C_6	.76	.39	3.45	.53	9.04	14.17
C_7	.45	1.02	.91	.54	13.73	16.65
C_8	.14	.09	.40	.11	6.85	7.59
C_9	.53	.11	.01	.03	2.49	3.16
TOTAL	6.56	3.79	6.46	1.21	32.11	50.13

UNIDENTIFIED C_4-C_9 .13 C_{10}+ 25.22

HYDROGEN YIELD SCF/BBL -1995[A] -1900[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	89.56	10.44	.0000	.0840	.0070	100.09
HYDROGEN		5.23				5.23
TOTAL	89.56	15.67	.0000	.0840	.0070	105.32
PRODUCTS						
LIQUID	52.50	5.54	.0000	.0410	.0040	58.08
HC GAS	37.06	8.21				45.27
HYDROGEN		1.75				1.75
NH_3		.000				.000
H_2O		.005		.043		.048
H_2S		.000			.0030	.003
TOTAL	89.56	15.50	.0000	.084	.0070	105.16

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 10-6-75 | DATA BOOK NO. 103-2-31

RUN, SAMPLE NO. H-COAL 1006 REV
PROCESS: HYDROCRACKING GAS OIL
CATALYST: HARSHAW HT-400-1/8-E
FEED: H-COAL ST. RUN GAS OIL

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	840
LHSV - VOL/VOL-HR	.69	CATALYST VOLUME CC	150
MATERIAL BALANCE %	99.13	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	7910	OIL PRODUCT RATE G/HR	95.53
OIL FEED RATE G/HR	105.14	TAIL GAS RATE G/HR	22.75
HYDROGEN FEED RATE G/HR	13.14	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

650°F + 55.4 | 750°F + 55.8

YIELD: G/100G OIL FEED

HYDROGEN	- .83 A	-2.04 B	WATER ---
METHANE	.88		
ETHANE	1.66		
PROPANE	1.67		

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	1.61	.18				1.79
C_5	.42	.24	.19			.84
C_6	.69	.0	.54	.97	.40	2.59
C_7	.14	.15	.13	.99	.59	1.99
C_8	.05	.01	.12	.12	.36	.65
C_9	.01	.04	.05	.21	1.13	1.44
TOTAL	2.92	.62	1.02	2.28	2.46	9.30

UNIDENTIFIED C_4-C_9 .02 | C_{10}+ 87.28

HYDROGEN YIELD SCF/BBL -534 A -1290 B

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	89.73	9.23	.082	.79	.166	100.00
HYDROGEN		12.50				12.50
TOTAL	89.73	21.73	.082	.79	.166	112.50
PRODUCTS						
LIQUID	81.50	9.41	.002	.075	.005	90.99
HC GAS	8.23	1.74				9.97
HYDROGEN		11.67				11.67
NH_3		.017	.080			.097
H_2O		.089		.715		.804
H_2S		.010			.161	.1[illegible]
TOTAL	89.73	22.94	.082	.79	.166	113.70

A From Hydrogen Mass Balance | B From Elemental Balance

HYDROPROCESSING DATA

DATE 10-9-75 DATA BOOK NO. 103-2-33
RUN, SAMPLE NO. H-COAL 1009 REV
PROCESS: HYDROCRACKING GAS OIL
CATALYST: HARSHAW HT-400-1/8-E
FEED: H-COAL ST. RUN GAS OIL

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	925
LHSV - VOL/VOL-HR	.71	CATALYST VOLUME CC	150
MATERIAL BALANCE %	99.47	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	7740	OIL PRODUCT RATE G/HR	77.50
OIL FEED RATE G/HR	107.40	TAIL GAS RATE G/HR	43.04
HYDROGEN FEED RATE G/HR	13.14	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

650°F + 83.3 750°F + 79.3

YIELD: G/100G OIL FEED

HYDROGEN	-3.11[A]	-3.69[B]	WATER	---
METHANE	3.76			
ETHANE	4.76			
PROPANE	6.76			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	5.81	.72				6.53
C_5	1.02	.60	.40			2.02
C_6	.79	.24	1.37	1.80	1.78	5.98
C_7	.56	.62	.47	1.78	3.08	6.52
C_8	.28	.14	.40	.30	1.75	2.88
C_9	.04	.15	.15	.35	2.67	3.37
TOTAL	8.50	2.47	2.79	4.24	9.29	27.29

UNIDENTIFIED C_4-C_9 0.0 C_{10}+ 60.54

HYDROGEN YIELD SCF/BBL -1980[A] -2335[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	89.73	9.23	.082	.79	.166	100.00
HYDROGEN		12.23				12.23
TOTAL	89.73	21.46	.082	.79	.166	112.23
PRODUCTS						
LIQUID	64.29	7.30	.001	.128	.007	71.73
HC GAS	25.44	5.51				30.95
HYDROGEN		9.12				9.12
NH_3		.017	.081			.098
H_2O		.083		.662		.745
H_2S		.010			.159	.169
TOTAL	89.73	22.04	.082	.79	.166	112.81

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 10-16-75 DATA BOOK NO. 103-2-37
RUN, SAMPLE NO. H-COAL 1016 REV
PROCESS: HYDROCRACKING GAS OIL
CATALYST: HARSHAW HT-400-1/8-E
FEED: H-COAL ST. RUN GAS OIL

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	964
LHSV - VOL/VOL-HR	1.30	CATALYST VOLUME CC	150
MATERIAL BALANCE %	102.22	FORCE BALANCED ON	OIL FEED
HYDROGEN RATIO SCF/BBL	4220	OIL PRODUCT RATE G/HR	145.96
OIL FEED RATE G/HR	197.99	TAIL GAS RATE G/HR	65.22
HYDROGEN FEED RATE G/HR	13.19	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

650°F + 75.0 750°F + 76.4

YIELD: G/100G OIL FEED

HYDROGEN	-1.70[A]	-2.76[B]	WATER	---
METHANE	4.44			
ETHANE	5.76			
PROPANE	6.93			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	4.12	.68				4.80
C_5	.86	.46	.36			1.69
C_6	.49	.42	1.24	1.12	1.23	4.51
C_7	.36	.67	.23	1.02	2.44	4.72
C_8	.17	.08	.23	.16	1.54	2.17
C_9	.06	.04	.07	.21	1.63	2.00
TOTAL	6.06	2.35	2.14	2.51	6.84	19.89

UNIDENTIFIED C_4-C_9 0.0 C_{10}+ 64.68

HYDROGEN YIELD SCF/BBL -1080[A] -1750[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	89.73	9.23	.082	.79	.166	100.00
HYDROGEN		6.66				6.66
TOTAL	89.73	15.89	.082	.79	.166	106.66
PRODUCTS						
LIQUID	66.95	6.68	.010	.086	.003	73.73
HC GAS	22.78	5.20				27.98
HYDROGEN		4.96				4.96
NH_3		.015	.072			.087
H_2O		.088		.704		.792
H_2S		.010			.163	.1[illegible]
TOTAL	89.73	16.95	.082	.79	.169	107.72

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 10-20-75 DATA BOOK NO. 103-2-38
RUN, SAMPLE NO. COED 1020 REV
PROCESS: HYDROCRACKING GAS OIL
CATALYST: HARSHAW HT-400-1/8-E
FEED: H-COAL ST. RUN GAS OIL

REACTOR CONDITIONS

PRESSURE - PSIG	2500	TEMPERATURE °F	996
LHSV - VOL/VOL-HR	1.68	CATALYST VOLUME CC	150
MATERIAL BALANCE %	111.18	FORCE BALANCED ON	OIL FEED
HYDROGEN RATIO SCF/BBL	3260	OIL PRODUCT RATE G/HR	201.50
OIL FEED RATE G/HR	256.06	TAIL GAS RATE G/HR	67.73
HYDROGEN FEED RATE G/HR	13.17	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

650°F + 77.8 750°F + 75.3

YIELD: G/100G OIL FEED

HYDROGEN - .82[A] -1.76[B] WATER ---
METHANE 3.95
ETHANE 5.04
PROPANE 5.67

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	2.70	.57				3.27
C_5	.59	.31	.32			1.21
C_6	.32	.35	1.20	.71	1.17	3.76
C_7	.28	.26	.37	.62	2.61	4.15
C_8	.05	.07	.22	.19	1.01	1.55
C_9	.17	.03	.23	.86	1.54	2.83
TOTAL	4.12	1.59	2.34	2.39	6.34	16.78

UNIDENTIFIED C_4-C_9 0.0 C_{10}+ 69.37

HYDROGEN YIELD SCF/BBL -519[A] -1110[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	89.73	9.23	.082	.79	.166	100.00
HYDROGEN		5.14				5.14
TOTAL	89.73	14.37	.082	.79	.166	105.14
PRODUCTS						
LIQUID	71.77	6.71	.014	.11	.006	78.61
HC GAS	17.96	4.17				22.13
HYDROGEN		4.32				4.32
NH_3		.015	.068			.083
H_2O		.085		.68		.765
H_2S		.010			.160	.170
TOTAL	89.73	15.31	.082	.79	.166	106.08

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 7-2-75 DATA BOOK NO. 103-4-14
RUN, SAMPLE NO. H-COAL 702
PROCESS: HYDROTREATING
CATALYST: HARSHAW HT-100-1/8-E
FEED: H-COAL ST. RUN NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	705	TEMPERATURE °F	662
LHSV - VOL/VOL-HR	1.95	CATALYST VOLUME CC	100
MATERIAL BALANCE %	97.07	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	1630	OIL PRODUCT RATE G/HR	127.83
OIL FEED RATE G/HR	152.21	TAIL GAS RATE G/HR	29.47
HYDROGEN FEED RATE G/HR	5.09	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	- 1.11[A]	-0.43[B]
GAS	17.12	
	NORMPARAF	
METHANE	0.01	
ETHANE	0.01	
PROPANE	0.10	ISOPARAF
C_4	0.63	0.08
LIQUID	83.31	

HYDROGEN YIELD SCF/BBL -157[A] -138[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.0	13.3	.0470	.3900	.2600	100.00
HYDROGEN		3.34				3.34
TOTAL	86.0	16.64	.0470	.3900	.2600	103.34
PRODUCTS						
LIQUID	72.6	11.25	.0030	.0410	.0060	83.90
HC GAS	14.7	2.42				17.12
HYDROGEN		2.23				2.23
NH_3		.008	.0440			.052
H_2O		.039		.3490		.388
H_2S		.015			.2540	.269
TOTAL	87.3	15.96	.0470	.3900	.2600	103.96

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 7-30-75 DATA BOOK NO. 103-4-20
RUN, SAMPLE NO. H-COAL 730
PROCESS: HYDROTREATING
CATALYST: HARSHAW HT-400-1/16-E
FEED: H-COAL ST. RUN NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	500	TEMPERATURE °F	600
LHSV - VOL/VOL-HR	2.30	CATALYST VOLUME CC	100
MATERIAL BALANCE %	100.93	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	595	OIL PRODUCT RATE G/HR	172.50
OIL FEED RATE G/HR	180.00	TAIL GAS RATE G/HR	9.70
HYDROGEN FEED RATE G/HR	2.20	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	0.19 [A]	-0.23 [B]
GAS	3.96	
	NORMPARAF	
METHANE	0.01	
ETHANE	0.04	
PROPANE	0.04	ISOPARAF
C_4	0.18	0.01
LIQUID	99.30	

HYDROGEN YIELD SCF/BBL -81 [A] -62 [B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.0	13.3	.0470	.3900	.2600	100.00
HYDROGEN		1.22				1.22
TOTAL	86.0	14.52	.0470	.3900	.2600	101.22
PRODUCTS						
LIQUID	82.80	12.94	.0080	.0790	.0070	95.83
HC GAS	3.37	0.59				3.96
HYDROGEN		1.41				1.41
NH_3		.007	.0390			.046
H_2O		.035		.3110		.346
H_2S		.015			.2530	.268
TOTAL	86.17	15.00	.0470	.3900	.2600	101.87

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 8-4-75 DATA BOOK NO. 103-4-23
RUN, SAMPLE NO. H-COAL 804
PROCESS: HYDROTREATING
CATALYST: HARSHAW HT-400-1/16-E
FEED: H-COAL ST. RUN NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	900	TEMPERATURE °F	680
LHSV - VOL/VOL-HR	2.67	CATALYST VOLUME CC	100
MATERIAL BALANCE %	101.74	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	511	OIL PRODUCT RATE G/HR	204.90
OIL FEED RATE G/HR	208.00	TAIL GAS RATE G/HR	5.28
HYDROGEN FEED RATE G/HR	2.18	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	-0.36 [A]	-0.09 [B]
GAS	1.85	
	NORMPARAF	
METHANE	0.01	
ETHANE	0.06	
PROPANE	0.04	ISOPARAF
C_4	0.20	0.02
LIQUID	98.24	

HYDROGEN YIELD SCF/BBL -35 [A] -21 [B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.0	13.3	.0470	.3900	.2600	100.00
HYDROGEN		1.05				1.05
TOTAL	86.0	14.35	.0470	.3900	.2600	101.05
PRODUCTS						
LIQUID	85.21	13.10	.0030	.2000	.0120	98.53
HC GAS	1.56	0.29				1.85
HYDROGEN		0.69				0.69
NH_3		.008	.0440			.052
H_2O		.021		.1900		.211
H_2S		.015			.2480	.263
TOTAL	86.77	14.26	.0470	.3900	.2600	101.73

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 8-5-75 DATA BOOK NO. 103-4-23
RUN, SAMPLE NO. H-COAL 805
PROCESS: HYDROTREATING
CATALYST: HARSHAW HT-400-1/16-E
FEED: H-COAL ST. RUN NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	900	TEMPERATURE °F	780
LHSV - VOL/VOL-HR	2.42	CATALYST VOLUME CC	100
MATERIAL BALANCE %	91.11	FORCE BALANCED ON	OIL PRODUCT
HYDROGEN RATIO SCF/BBL	562	OIL PRODUCT RATE G/HR	175.80
OIL FEED RATE G/HR	189.00	TAIL GAS RATE G/HR	15.38
HYDROGEN FEED RATE G/HR	2.18	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	0.88[A]	-0.01[B]
GAS	6.10	
	NORMPARAF	
METHANE	0.06	
ETHANE	0.28	
PROPANE	0.28	ISOPARAF
C_4	0.40	0.04
LIQUID	93.91	

HYDROGEN YIELD SCF/BBL -31[A] -3[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.0	13.3	.0470	.3900	.2600	100.00
HYDROGEN		1.15				1.15
TOTAL	86.0	14.45	.0470	.3900	.2600	101.15
PRODUCTS						
LIQUID	80.45	12.37	.0005	.1890	.0105	93.02
HC GAS	5.16	0.94				6.10
HYDROGEN		2.03				2.03
NH_3		.008	.0465			.054
H_2O		.022		.2010		.223
H_2S		.015			.2495	.264
TOTAL	85.61	15.39	.0470	.3900	.2600	101.70

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 8-25-75 DATA BOOK NO. 103-4-27
RUN, SAMPLE NO. H-COAL 828
PROCESS: HYDROTREATING
CATALYST: HARSHAW HT-100-1/8-E
FEED: H-COAL 1 PASS HYDROTREATED ST. RUN NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	800	TEMPERATURE °F	662
LHSV - VOL/VOL-HR	3.40	CATALYST VOLUME CC	100
MATERIAL BALANCE %	90.96	FORCE BALANCED ON	OIL PRODUCT
HYDROGEN RATIO SCF/BBL	437	OIL PRODUCT RATE G/HR	256.18
OIL FEED RATE G/HR	265.00	TAIL GAS RATE G/HR	11.20
HYDROGEN FEED RATE G/HR	2.38	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	0.86[A]	-0.11[B]
GAS	2.44	
	NORMPARAF	
METHANE	---	
ETHANE	---	
PROPANE	0.01	ISOPARAF
C_4	0.07	0.02
LIQUID	97.67	

HYDROGEN YIELD SCF/BBL -22[A] -20[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.7	13.3	.0038	.0400	.0093	100.05
HYDROGEN		0.90				0.90
TOTAL	86.7	14.20	.0038	.0400	.0093	100.95
PRODUCTS						
LIQUID	83.62	13.05	.0005	.0400	.0004	96.71
HC GAS	2.08	0.36				2.44
HYDROGEN		1.76				1.76
NH_3		.001	.0033			.004
H_2O		.000		.0000		.000
H_2S		.001			.0089	.010
TOTAL	85.70	15.17	.0038	.0400	.0093	100.92

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 3-4-76 DATA BOOK NO. 103-6-7
RUN, SAMPLE NO. H-COAL 103-6-7-3
PROCESS: HYDROTREATING
CATALYST: HARSHAW HT-100-1/8-E
FEED: H-COAL HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	1500	TEMPERATURE °F	756
LHSV - VOL/VOL-HR	1.90	CATALYST VOLUME CC	50
MATERIAL BALANCE %	99.59	FORCE BALANCED ON	OIL PRODUCT
HYDROGEN RATIO SCF/BBL	2157	OIL PRODUCT RATE G/HR	73.24
OIL FEED RATE G/HR	75.50	TAIL GAS RATE G/HR	5.50
HYDROGEN FEED RATE G/HR	3.24	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	-0.51[A]	-1.19[B]	-1.17[C]
GAS	3.49		
	NORMPARAF		
METHANE	0.01		
ETHANE	0.02		
PROPANE	0.06	ISOPARAF	
C_4	0.16	0.02	
LIQUID	97.70		

AROMATIC SATURATION:

	G/100 G OIL FEED	% OF FEED
C_6	3.30	39.3
C_7	7.73	47.8
C_8	5.78	52.5
C_9	3.19	22.5
TOTAL	20.00	40.2

HYDROGEN YIELD SCF/BBL -256[A] -597[B] -587[C]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.8	12.2	.0008	.0300	.0100	100.04
HYDROGEN		4.29				4.29
TOTAL	87.8	16.49	.0008	.0300	.0100	104.33
PRODUCTS						
LIQUID	84.10	12.90	.0002	.0170	.0004	97.02
HC GAS	3.00	0.49				3.49
HYDROGEN		3.78				3.78
NH_3		.000	.0006			.001
H_2O		.001		.0130		.014
H_2S		.001			.0096	.011
TOTAL	87.10	17.17	.0008	.0300	.0100	104.31

A From Hydrogen Mass Balance B From Elemental Balance
C From Aromatic Saturation

HYDROPROCESSING DATA

DATE	3-5-76	DATA BOOK NO.	103-6-9

RUN, SAMPLE NO. 103-6-9-2
PROCESS: HYDROTREATING
CATALYST: HARSHAW HT-100-1/8-E
FEED: H-COAL HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	1500	TEMPERATURE °F	752
LHSV - VOL/VOL-HR	4.01	CATALYST VOLUME CC	50
MATERIAL BALANCE %	98.74	FORCE BALANCED ON	OIL FEED
HYDROGEN RATIO SCF/BBL	2009	OIL PRODUCT RATE G/HR	156.20
OIL FEED RATE G/HR	160.90	TAIL GAS RATE G/HR	11.16
HYDROGEN FEED RATE G/HR	6.46	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	-1.13 [A]	-1.06 [B]	-0.79 [C]
GAS	4.03		
	NORMPARAF		
METHANE	0.01		
ETHANE	0.01		
PROPANE	0.04	ISOPARAF	
C_4	0.14	0.01	
LIQUID	97.03		

AROMATIC SATURATION:	G/100G OIL FEED	% OF FEED
C_6	2.03	24.2
C_7	4.74	29.3
C_8	3.83	34.8
C_9	2.79	19.7
TOTAL	13.39	26.9

HYDROGEN YIELD SCF/BBL	-565 [A]	-530 [B]	-395 [C]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.8	12.2	.0008	.0300	.0100	100.04
HYDROGEN		4.01				4.01
TOTAL	87.8	16.21	.0008	.0300	.0100	104.05
PRODUCTS						
LIQUID	84.36	12.72	.0005	.0150	.0001	97.10
HC GAS	3.49	.54				4.03
HYDROGEN		2.88				2.88
NH_3		.000	.0003			.000
H_2O		.002		.0150		.017
H_2S		.001			.0099	.011
TOTAL	87.85	16.14	.0008	.0300	.0100	104.04

A From Hydrogen Mass Balance B From Elemental Balance

C From Aromatic Saturation

HYDROPROCESSING DATA

DATE 6-15-76 DATA BOOK NO. 103-6-12
RUN, SAMPLE NO. 103-6-12-2
PROCESS: HYDROTREATING
CATALYST: CYANAMID AERO HDS-9A
FEED: H-COAL HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	1040	TEMPERATURE °F	686
LHSV - VOL/VOL-HR	2.01	CATALYST VOLUME CC	50
MATERIAL BALANCE %	97.85	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	1929	OIL PRODUCT RATE G/HR	75.00
OIL FEED RATE G/HR	80.67	TAIL GAS RATE G/HR	8.78
HYDROGEN FEED RATE G/HR	3.11	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	-0.06[A]	0.24[B]	-0.55[C]
GAS	7.02		
	NORMPARAF		
METHANE	0.01		
ETHANE	0.03		
PROPANE	0.05	ISOPARAF	
C_4	0.03	0.02	
LIQUID	93.53		

AROMATIC SATURATION:	G/100G OIL FEED	% OF FEED
C_6	2.25	26.8
C_7	2.53	15.6
C_8	1.80	16.3
C_9	2.77	19.6
TOTAL	9.35	18.8

HYDROGEN YIELD SCF/BBL -30[A] 120[B] -276[C]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.8	12.2	.0008	.0300	.0100	100.04
HYDROGEN		3.86				3.86
TOTAL	87.8	16.06	.0008	.0300	.0100	103.90
PRODUCTS						
LIQUID	81.91	11.06	.0004	.0150	.0069	92.99
HC GAS	6.12	.90				7.02
HYDROGEN		3.80				3.80
NH_3		.000	.0004			.000
H_2O		.002		.0150		.017
H_2S		.000			.0031	.003
TOTAL	88.03	15.76	.0008	.0300	.0100	103.83

A From Hydrogen Mass Balance B From Elemental Balance
C From Aromatic Saturation

HYDROPROCESSING DATA

DATE 9-1-76 DATA BOOK NO. 103-8-11
RUN, SAMPLE NO. 103-8-11-4
PROCESS: HYDROTREATING
CATALYST: CYANAMID AERO HDS-9A
FEED: H-COAL 1 PASS HYDROTREATED HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	980	TEMPERATURE °F	683
LHSV - VOL/VOL-HR	2.06	CATALYST VOLUME CC	50
MATERIAL BALANCE %	94.61	FORCE BALANCED ON	OIL PRODUCT
HYDROGEN RATIO SCF/BBL	1942	OIL PRODUCT RATE G/HR	81.94
OIL FEED RATE G/HR	81.84	TAIL GAS RATE G/HR	3.10
HYDROGEN FEED RATE G/HR	3.20	WATER PRODUCT G/HR	---

YIELD: G/100G OIL FEED

HYDROGEN	-0.95[A]	-1.33[B]	-0.50[C]
GAS	0.81		
	NORMPARAF		
METHANE	0.00		
ETHANE	0.01		
PROPANE	0.02	ISOPARAF	
C_4	0.01	0.01	
LIQUID	100.90		

AROMATIC SATURATION: G/100G OIL FEED

	G/100G OIL FEED	% OF FEED
C_6	0.83	29.0
C_7	3.28	31.1
C_8	3.30	42.0
C_9	2.79	21.7
TOTAL	10.20	29.9

HYDROGEN YIELD SCF/BBL -577[A] -807[B] -303[C]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.7	12.3	.0001	.0350	.0025	100.04
HYDROGEN		3.91				3.91
TOTAL	87.7	16.21	.0001	.0350	.0025	103.95
PRODUCTS						
LIQUID	86.61	13.52	.0000	.0050	.0005	100.14
HC GAS	.70	.11				.81
HYDROGEN		2.96				2.96
NH_3		.000	.0001			.000
H_2O		.003		.0300		.033
H_2S		.000			.0020	.002
TOTAL	87.31	16.59	.0001	.0350	.0025	103.95

A From Hydrogen Mass Balance B From Elemental Balance

C From Aromatic Saturation

H-COAL
STRAIGHT RUN NAPHTHA FEED TO REFORMING

Carbon	87.3
Hydrogen	12.7

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
C_5	0.3	0.1	0.4		
C_6	1.6	0.9	2.2	9.1	0.9
C_7	1.8	2.6	3.0	12.1	5.3
C_8	2.8	1.8	4.6	4.0	10.3
C_9	0.6	1.2	1.5	4.3	17.4
C_{10}^+	11.0				

HYDROPROCESSING DATA

DATE 10-30-75 DATA BOOK NO. 103-4-50
RUN, SAMPLE NO. 103075
PROCESS: REFORMING ST. RUN NAPHTHA
CATALYST: CYANAMID AERO PHF-4
FEED: H-COAL HYDROTREATED ST. RUN NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	250	TEMPERATURE °F	932
LHSV - VOL/VOL-HR	1.59	CATALYST VOLUME CC	100
MATERIAL BALANCE %	97.26	FORCE BALANCED ON	OIL PRODUCT
HYDROGEN RATIO SCF/BBL	2520	OIL PRODUCT RATE G/HR	98.30
OIL FEED RATE G/HR	125.20	TAIL GAS RATE G/HR	33.30
HYDROGEN FEED RATE G/HR	6.40	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + --- 500°F + ---

YIELD: G/100G OIL FEED

HYDROGEN	5.47[A]	2.77[B]	WATER	---
METHANE	.38			
ETHANE	.66			
PROPANE	.96			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	.54	.34				.89
C_5	.63	.70	.47			1.80
C_6	1.67	1.47	1.99	.10	9.84	15.08
C_7	1.36	2.24	.64	.00	20.58	24.82
C_8	.00	.81	.02	.34	18.11	19.28
C_9	.00	.57	.12	.00	20.79	21.48
TOTAL	4.21	6.14	3.24	.44	69.32	83.35

UNIDENTIFIED C_4-C_9 .32 $C_{10}+$ 8.80

HYDROGEN YIELD SCF/BBL 2690[A] 1360[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.31	12.69				100.00
HYDROGEN		5.11				5.11
TOTAL	87.31	17.80				105.11
PRODUCTS						
LIQUID	70.67	7.84				78.51
HC GAS	13.88	2.08				15.96
HYDROGEN		10.59				10.59
NH_3						
H_2O						
H_2S						
TOTAL	84.55	20.51				105.06

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 11-3-75 DATA BOOK NO. 103-4-51
RUN, SAMPLE NO. 110375
PROCESS: REFORMING ST. RUN NAPHTHA
CATALYST: CYANAMID AERO PHF-4
FEED: H-COAL HYDROTREATED ST. RUN NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	250	TEMPERATURE °F	968
LHSV - VOL/VOL-HR	1.66	CATALYST VOLUME CC	100
MATERIAL BALANCE %	100.86	FORCE BALANCED ON	OIL PRODUCT
HYDROGEN RATIO SCF/BBL	2420	OIL PRODUCT RATE G/HR	98.92
OIL FEED RATE G/HR	130.70	TAIL GAS RATE G/HR	38.20
HYDROGEN FEED RATE G/HR	6.42	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + --- 500°F + ---

YIELD: G/100G OIL FEED

HYDROGEN	3.24 [A]	2.32 [B]	WATER	---
METHANE	.87			
ETHANE	1.76			
PROPANE	2.47			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	1.43	.98				2.42
C_5	1.11	1.40	.50			3.00
C_6	1.50	1.61	1.24	0	12.45	16.79
C_7	.95	1.84	.43	0	25.85	28.41
C_8	.23	.48	.05	0	19.98	20.75
C_9	.00	.07	.00	0	14.77	14.84
TOTAL	5.23	6.38	2.21	0	72.38	86.20

UNIDENTIFIED C_4-C_9 0.0 C_{10}+ 5.40

HYDROGEN YIELD SCF/BBL 1590 [A] 1140 [B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.31	12.69				100.00
HYDROGEN		4.91				4.91
TOTAL	87.31	17.60				104.91
PRODUCTS						
LIQUID	68.32	7.36				75.68
HC GAS	18.05	3.00				21.05
HYDROGEN		8.15				8.15
NH_3						
H_2O						
H_2S						
TOTAL	86.37	18.51				104.88

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 11-20-75 DATA BOOK NO. 103-4-56
RUN, SAMPLE NO. 112075
PROCESS: REFORMING ST. RUN NAPHTHA
CATALYST: CYANAMID AERO PHF-4
FEED: H-COAL HYDROTREATED ST. RUN NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	250	TEMPERATURE °F	968
LHSV - VOL/VOL-HR	2.24	CATALYST VOLUME CC	100
MATERIAL BALANCE %	98.41	FORCE BALANCED ON	OIL PRODUCT
HYDROGEN RATIO SCF/BBL	1790	OIL PRODUCT RATE G/HR	124.50
OIL FEED RATE G/HR	176.40	TAIL GAS RATE G/HR	58.30
HYDROGEN FEED RATE G/HR	6.40	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + --- 500°F + ---

YIELD: G/100G OIL FEED

HYDROGEN	3.43[A]	1.32[B]	WATER	---
METHANE	1.62			
ETHANE	2.86			
PROPANE	3.48			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	2.07	1.30				3.37
C_5	1.38	1.62	.67			3.67
C_6	1.95	1.97	2.49	.50	8.71	15.63
C_7	1.35	2.06	.89	.74	18.52	23.57
C_8	.55	1.14	.69	.32	16.28	18.98
C_9	.39	.32	.30	.51	15.94	17.46
TOTAL	7.69	8.43	5.04	2.06	59.46	82.68

UNIDENTIFIED C_4-C_9 0.0 C_{10}+ 5.88

HYDROGEN YIELD SCF/BBL 1690[A] 650[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.31	12.69				100.00
HYDROGEN		3.63				3.63
TOTAL		16.32				103.63
PRODUCTS						
LIQUID	63.23	7.35				70.58
HC GAS	21.95	4.02				25.97
HYDROGEN		7.06				7.06
NH_3						
H_2O						
H_2S						
TOTAL	85.18	18.43				103.61

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 11-24-75 DATA BOOK NO. 103-4-57
RUN, SAMPLE NO. 112475
PROCESS: REFORMING ST. RUN NAPHTHA
CATALYST: CYANAMID AERO PHF-4
FEED: H-COAL HYDROTREATED ST. RUN NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	240	TEMPERATURE °F	977
LHSV - VOL/VOL-HR	2.09	CATALYST VOLUME CC	100
MATERIAL BALANCE %	102.2	FORCE BALANCED ON	TAIL GAS
HYDROGEN RATIO SCF/BBL	1890	OIL PRODUCT RATE G/HR	131.00
OIL FEED RATE G/HR	165.00	TAIL GAS RATE G/HR	40.33
HYDROGEN FEED RATE G/HR	6.33	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + --- 500°F + ---

YIELD: G/100G OIL FEED

HYDROGEN	1.29[A]	.84[B]	WATER	---
METHANE	1.35			
ETHANE	2.23			
PROPANE	2.56			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	1.72	0.91				2.63
C_5	1.11	1.18	.34			2.63
C_6	1.95	1.58	3.70	1.46	6.73	15.43
C_7	1.53	3.13	1.88	2.50	16.08	25.12
C_8	1.02	1.56	1.42	1.08	15.87	20.96
C_9	.37	.74	.60	1.12	16.16	18.99
TOTAL	7.70	9.10	7.95	6.16	54.85	85.76

UNIDENTIFIED C_4-C_9 0.0 C_{10}+ 6.80

HYDROGEN YIELD SCF/BBL 633[A] 413[B]

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	87.31	12.69				100.00
HYDROGEN		3.84				3.84
TOTAL	87.31	16.53				103.84
PRODUCTS						
LIQUID	70.62	8.77				79.39
HC GAS	16.23	3.08				19.31
HYDROGEN		5.12				5.12
NH_3						
H_2O						
H_2S						
TOTAL	86.85	16.97				103.82

A From Hydrogen Mass Balance B From Elemental Balance

H-COAL
HYDROCRACKATE NAPHTHA
HYDROTREATED FEED TO REFORMING

Carbon	86.5
Hydrogen	13.5

	NORM PARAF	ISO PARAF	CYCLO PENT	CYCLO HEXANE	AROMATIC
C_5	---	---	0.3		
C_6	0.6	0.2	3.2	4.2	2.4
C_7	1.2	2.3	5.0	9.1	8.0
C_8	2.6	0.5	5.0	7.7	5.9
C_9	0.8	2.6	0.3	2.4	18.7
C_{10}^+	17.1				

HYDROPROCESSING DATA

DATE 9-15-76 DATA BOOK NO. 103-6-27
RUN, SAMPLE NO. 103-6-27-2
PROCESS: REFORMING HYDROCRACKATE NAPHTHA
CATALYST: CYANAMID AERO-PHF-4
FEED: H-COAL HYDROTREATED HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	495	TEMPERATURE °F	968
LHSV - VOL/VOL-HR	2.06	CATALYST VOLUME CC	50
MATERIAL BALANCE %	99.18	FORCE BALANCED ON	NOT DONE
HYDROGEN RATIO SCF/BBL	3840	OIL PRODUCT RATE G/HR	58.82
OIL FEED RATE G/HR	81.95	TAIL GAS RATE G/HR	28.74
HYDROGEN FEED RATE G/HR	6.33	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + --- 500°F + ---

YIELD: G/100G OIL FEED

HYDROGEN	2.40 A	2.98 B	WATER	---
METHANE	1.18			
ETHANE	2.21			
PROPANE	2.78			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	1.48	.85				2.33
C_5	.84	1.12	.40			2.36
C_6	1.39	1.60	1.22	.08	9.10	13.39
C_7	.87	1.80	.32	.09	26.38	29.46
C_8	.19	.65	.01	.00	17.76	18.61
C_9	.09	.17	.00	.06	18.93	19.24
TOTAL	4.86	6.17	1.97	.24	72.16	85.40

UNIDENTIFIED C_4-C_9 0.0 C_{10}+ 5.15

HYDROGEN YIELD SCF/BBL 1190 A 1480 B

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.5	13.5				100
HYDROGEN		7.72				7.72
TOTAL	86.5	21.22				107.72
PRODUCTS						
LIQUID	64.74	7.03				71.77
HC GAS	21.46	3.49				24.95
HYDROGEN		10.12				10.12
NH_3						
H_2O						
H_2S						
TOTAL	86.2	20.64				106.84

A From Hydrogen Mass Balance B From Elemental Balance

HYDROPROCESSING DATA

DATE 9-16-76 DATA BOOK NO. 103-6-27
RUN, SAMPLE NO. 103-6-27-3
PROCESS: REFORMING HYDROCRACKATE NAPHTHA
CATALYST: CYANAMID AERO-PHF-4
FEED: H-COAL HYDROTREATED HYDROCRACKATE NAPHTHA

REACTOR CONDITIONS

PRESSURE - PSIG	495	TEMPERATURE °F	968
LHSV - VOL/VOL-HR	2.07	CATALYST VOLUME CC	50
MATERIAL BALANCE %	98.61	FORCE BALANCED ON	NOT DONE
HYDROGEN RATIO SCF/BBL	3810	OIL PRODUCT RATE G/HR	58.70
OIL FEED RATE G/HR	82.17	TAIL GAS RATE G/HR	28.54
HYDROGEN FEED RATE G/HR	6.30	WATER PRODUCT G/HR	---

CONVERSIONS WEIGHT PERCENT

400°F + --- 500°F + ---

YIELD: G/100G OIL FEED

HYDROGEN	.70 A	3.01 B	WATER	---
METHANE	2.07			
ETHANE	2.34			
PROPANE	2.24			

	PARAFFIN		NAPHTHENE		AROMATIC	TOTAL
	NORMAL	ISO	CYCLO C_5	CYCLO C_6		
C_4	1.51	1.11				2.62
C_5	.77	1.07	.41			2.25
C_6	1.61	1.67	1.73	.09	9.38	14.47
C_7	1.04	2.04	.40	.12	25.67	29.27
C_8	.24	.84	.01	.00	17.00	18.09
C_9	.09	.21	.00	.07	18.47	18.85
TOTAL	5.25	6.95	2.55	.28	70.53	85.56

UNIDENTIFIED C_4-C_9 0.0 C_{10}+ 5.38

HYDROGEN YIELD SCF/BBL 346 A 1495 B

ELEMENTAL MATERIAL BALANCE - WEIGHT

FEED	CARBON	HYDROGEN	NITROGEN	OXYGEN	SULFUR	TOTAL
OIL	86.5	13.5				100.00
HYDROGEN		7.67				7.67
TOTAL		21.17				107.67
PRODUCTS						
LIQUID	64.72	6.72				71.44
HC GAS	22.60	3.77				26.37
HYDROGEN		8.37				8.37
NH_3						
H_2O						
H_2S						
TOTAL	87.32	18.86				106.18

A From Hydrogen Mass Balance B From Elemental Balance

H-COAL STEAM COIL CRACKING DATA

	H-COAL STRAIGHT RUN NAPHTHA			
Temperature, °F	1436	1472	1517	1562
Res. Time, sec.	1.52	1.49	1.59	14.9
Steam/Oil Ratio	0.31	0.30	0.30	0.29
Product Pattern, wt. %				
Hydrogen	0.7	0.8	1.0	1.2
Methane	9.6	11.5	13.2	14.8
Ethylene	14.9	17.7	20.0	20.7
Ethane	3.7	3.8	3.4	2.7
Propylene	8.2	7.9	6.5	4.9
Propane	0.4	0.4	0.2	0.1
1,3 Butadiene	3.3	2.7	1.8	1.7
Other C_4's	2.7	2.1	1.0	0.9
C_5 - 410°F Non-Aromatic	18.9	13.7	8.3	6.1
Benzene	9.5	10.5	13.9	17.0
Toluene	9.3	8.5	8.7	8.1
C_8 Aromatics	8.3	7.9	7.1	6.5
C_9 - 410°F Aromatics	5.4	4.7	5.2	4.0
C_{10}^+	4.8	7.3	8.8	11.2

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