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U.S. Department of Energy
Pittsburgh Energy Technology Center

Refining and End Use Study of Coal Liquids

Contract No. DE-AC22-93PC91029

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Quarterly Report
April - June 1995

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Introduction and Summary

This report is Bechtel's seventh quarterly technical progress report and covers the period of March 27, 1995 through June 30, 1995.

1.1 Introduction

Bechtel, with Southwest Research Institute, Amoco Oil R&D, and the M.W. Kellogg Co. as subcontractors, initiated a study on November 1, 1993, for the U.S. Department of Energy's (DOE's) Pittsburgh Energy Technology Center (PETC) to determine the most cost effective and suitable combination of existing petroleum refinery processes needed to make specification transportation fuels or blending stocks, from direct and indirect coal liquefaction product liquids. This 47-month study, with an approved budget of $4.4 million dollars, is being performed under DOE Contract Number DE-AC22-93PC91029.

A key objective is to determine the most desirable ways of integrating coal liquefaction liquids into existing petroleum refineries to produce transportation fuels meeting current and future, e.g. year 2000, Clean Air Act Amendment (CAAA) standards. An integral part of the above objectives is to test the fuels or blends produced and compare them with established ASTM fuels. The comparison will include engine tests to ascertain compliance of the fuels produced with CAAA and other applicable fuel quality and performance standards.

The final part of the project includes a detailed economic evaluation of the cost of processing the coal liquids to their optimum products. The cost analyses is for the incremental processing cost; in other words, the feed is priced at zero dollars. The study reflects costs for operations using state of the art refinery technology; no capital costs for building new refineries is considered. Some modifications to the existing refinery may be required. Economy of scale dictates the minimum amount of feedstock that should be processed.

To enhance management of the study, the work has been divided into two parts, the Basic Program and Option 1.

The objectives of the Basic Program are to:

- Characterize the coal liquids
- Develop an optimized refinery configuration for processing indirect and direct coal liquids
- Develop a LP refinery model with the Process Industry Modeling System (PIMS) software.

Introduction and Summary

The work has been divided into six tasks.

Task 1 -	Development of a detailed project management plan for the Basic Program
Task 2 -	Characterization of four coal liquid feeds supplied by DOE
Task 3 -	Optimization of refinery processing configurations by linear programming
Task 4 -	Pilot plant analysis of critical refinery process units to determine yield, product quality and cost assumptions. Petroleum cuts, neat coal liquids, and coal liquids/petroleum blends will be processed through the following process units: reforming, naphtha and distillate hydrotreating, catalytic cracking and hydrocracking.
Task 5 -	Development of the project management plan for Option 1
Task 6 -	Project management of the Basic Program and Option 1

The objectives of Option 1 are to:

- Confirm the validity of the optimization work of the Basic Program
- Produce large quantities of liquid transportation fuel blending stocks
- Conduct engine emission tests
- Determine the value and the processing costs of the coal liquids

This will be done by processing the coal liquids as determined by the optimization work, blending and characterizing the product liquids, and running engine emission tests of the blends. Option 1 has been divided into three tasks.

Task 1 -	Based on the pilot plant and linear programming optimization work of the Basic Program, production runs of pilot plants (hydrotreating, reforming, catalytic cracking, and hydrocracking) will be conducted to produce sufficient quantities for blending and engine testing.
Task 2 -	The pilot plant products will be blended, characterized, and engine tested
Task 3 -	An economic analysis will be conducted to determine the costs of processing the coal liquids through the existing refinery

Table 1-1 shows which organization has the primary responsibility for each task.

1.2 Summary

The major efforts conducted during the second quarter of 1995 were in the areas of:

Introduction and Summary

- DL1 catalytic cracking - Pilot plant and micro activity tests showed that the DL1 heavy distillate was an excellent catalytic cracking feedstock with good gasoline production properties. Gasoline yield increased with higher hydrotreating severity.
- IL catalytic cracking - Pilot plant tests showed that the indirect liquid (IL) wax was also an excellent catalytic cracker feed.
- IL wax hydrocracking - Pilot plant hydrocracking tests on the IL wax are in progress
- Indirect wax cleanup - Approximately 240 gallons of clean FT wax was produced for future processing tests.

Table 1-1 Project Task Primary Responsibility Chart

Task	Description	Bechtel	SwRI	Amoco	Kellogg
1	Project Management Plan (PMP) development	x			
2	Feed characterization		x		
3	Linear programming	x			
4	Pilot plant analysis -				
	Cat cracking of DL liquids				x
	Cat cracking of indirect wax			x	
	Hydrocracking of wax			x	
	Fractionation, reforming, hydrotreating, etc.		x		
5	Option 1 PMP development	x			
6	Project management	x			
Option 1 - Task 1	Pilot plant production -				
	Cat cracking of DL liquids and wax				x
	All other production work		x		
Option 1 - Task 2	Fuel blending, characterizing, engine testing		x		
Option 1 - Task 3	Economic analysis	x			

x = key participant

Section 2

SwRI Activities

2.0 Wax Cleanup and Blending

2.1 Background

The LaPorte Alternative Fuels Division Unit (AFDU) produced Fischer-Tropsch indirect coal liquids as three related products: hydrocarbon liquid, light wax (an overhead product), and heavy wax. These materials will be used in future processing experiments on Indirect Coal Liquids (ICL).

The three as-received products required some processing before they could be integrated into the ICL testing scheme. The "light" wax was distilled at an equivalvent separation temperature of 650°F. The 650°F+ material was then combined with clean heavy wax.

The black wax (heavy wax prior to cleaning) was contaminated with catalyst fines during its production. The concentration of iron from the iron oxide fines in this "black" wax was about 5000 ppm. The presence of iron in the wax presents a problem for later processing and analysis. Fines in concentrations above 500 ppm iron may cause catalyst fouling during fixed bed cracking experiments. One hundred and ninety-two (192) gallons of the clean heavy wax are required for testing in the End Use Study.

SwRI was asked to clean the heavy wax to within acceptable limits and then blend it with the heavy portion of the light wax. The objectives of the cleanup effort were to:

1) Remove iron contaminant in the wax down to 500 ppm

2) Produce a finished wax containing a representative sample of the full boiling range of the heavy portion of the original wax

3) Clean and blend sufficient quantities of the waxes to satisfy the needs of the indirect coal liquid testing requirements (a total of 240 gallons) as shown in Table 2-1.

2.2 Wax Cleaning

2.2.1 Approach

A practical and effective means of reducing the iron oxide contaminent to acceptable levels was systematically determined. A simple processing procedure was proposed: 1) the wax would be dissolved in a suitable solvent; 2) the wax/solvent mixture would then be passed through a filter, removing the iron contaminant; and, 3) solvent would be removed from the wax by distillation. The development of the wax cleaning process was conducted in three steps as shown in Figure 2.1. The first step was to conduct laboratory tests to determine if the procedure was feasible on a small scale. The second step was to work out the problems of extending the cleaning technique to a full scale operation capable of treating hundreds of gallons of wax. The final step was to process the quantity of clean heavy wax required.

2.2.2 Laboratory Testing

Wax cleaning was first investigated with laboratory experiments. The primary objective of the experiments was to find a suitable solvent. The solvent to be used had three requirements:

1) It must be capable of dissolving black wax without altering the hydrocarbon distribution as the wax

2) The solvent boiling range must be outside the range of the wax so the mixture could be separated by distillation

3) The solvent/dissolved wax mixture should permit filtering at a temperature safely below the flash point of the solvent

The solubility of ten solvents were examined by placing black wax chips in the solvent, followed by heating and shaking. The solvents tested were: mixed xylenes; methylethylketone; heptane; carbon disulfide; petroleum naphtha; toluene; methylpyrolidone; Isopar M; pyridine; and C14-C16 solvent. The black wax readily dissolved in the carbon disulfide and midboiling range paraffin solvents.

Filtering tests were conducted with mixtures of wax and carbon disulfide, Isopar G, and Isopar M. Paper and gel filters were examined. The paper filter tests gave promising results. Solvent/wax mixtures passed through 1.5 micron porosity Miliport filters (under vacuum), producing a light colored product. This was an indication that the black contaminant content of the wax had been greatly reduced. At this point, no tests were conducted to quantify the iron content in either the black wax (contaminated heavy wax) or the filtered heavy wax.

The unfiltered and filtered heavy waxes were examined by TGA (Thermo-gravitational Analysis) and high temperature chromotography. The results of these tests showed that the filtered wax from the Isopar M solution had a boiling range similar to the parent material. Isopar K and carbon disulfide skewed the boiling curve of the filtered wax.

The filtration yield was approximately 30%. That is, about 30% of the wax in the solvent solution was recovered. The remainder was trapped in the filter cake. The experiments showed that the yield increased at higher temperatures and at decreasing concentrations of wax in the solution.

Isopar M was selected as the solvent for the full scale experiments because it produced a relatively clean product and its boiling range falls safely below that of the wax. Isopar M has a boiling range between 401 and 490°F, while the wax begins to boil at about 550°F.

2.2.3 Full Scale Experiments

Full scale experiments, based on scaling up the laboratory filtrations, were conducted. In addition to achieving satisfactory contaminent removal, the full scale separation technique needed to be able to produce filtered wax at a sufficient rate to complete the wax cleanup within the time and budget available. The overall approach was to mix the black wax with hot Isopar M, and filter the mixture to remove the iron oxide contaminant. The wax and solvent were then heated to 220°F, mixed thoroughly, and filtered.

Filtration tests of the black wax suggest that the iron oxide particles were on the order of one micron in size. (A 1.5 micron filter was shown to be able to remove the contaminent in the lab studies). Filter sizes were selected accordingly. Six test series were conducted to explore a number of filtration methods.

Test Series A. Bag Filtration

The first approach was to clean the wax using bag filters. Filters with pore sizes from 10 micron down to 0.1 micron were tested with limited success. Some of the bags simply would not filter out the iron oxide. Others would remove the particulates, but only with a low output (less than one gallon per hour). Attempts to increase the flow tended to breach the filter cake and result in contaminated output.

Test Series B. Paper Filtration

Since preliminary laboratory tests showed the wax could be successfully filtered with paper filters, large scale tests were conducted. Sheets of 24 inch diameter laboratory filter paper were placed over screens set in funnels and the wax was filtered under gravity. The technique produced clean wax, but only at a trickle. A wax/solvent mixture was then forced through the paper at 40 psi with a slightly higher flow rate of clean product but the system would clog within 15 minutes. A 30" x 30" tray of filter press paper filled with a solvent/wax mixture was placed in an oven at 190°F. Relatively clean wax (600 ppm iron) dripped through the paper into a tray below. Unfortunately, the solvent boiled off in the process, creating an unacceptable hazard in the oven, so the method was abandoned.

Test Series C. Cartidge Filters

Several types of cartridge filters were tested including oil filters and fiber filters. None of the cartidges showed any apparent filtering.

Test Series D. Gravity Settling

As the drums of solvent and wax were heated and cooled for the filtration testing, regions of brown wax could be seen in the drum. Analysis of the wax from the lighter areas shown they had distinctly lower iron concentrations (about 200 ppm). A beaker of a 2:1 solvent/wax mixture was placed in an oven at 200°F. Within 12 hours a distinct gravity separation was noticed. Eleven drums of wax at a 2:1 solvent/wax ratio were then placed in an environmental chamber at 176°F (the upper limit of the chamber) for 3 days. The drums were removed and inspected. The first 2 inches of some of the drums were brown (the remainder was black). The test was repeated at a higher temperature for a single drum. Following heating to 200°F for 2 days, the drum developed a brown layer within the top 3 inches. The lower 20 inches were black.

Test Series E. Continuous Centrifuge

In an effort to accelerate the gravity settling, a solvent/wax mixture was passed through a small, continuous centrifuge. There was no observable separation. This was likely due to the short residence time of the mixture in the separation chamber.

Test Series F. Filter Press

A filter press was considered because it provides a high filtering area under high pressure. The plate and frame press allowed the wax mixture to flow through 20" by 20" filters arranged in parallel. As many as 12 filters could be passed through simultaneously. The wax was first successfully filtered using two 4 micron filters and a 20 micron outer layer. The product wax/solvent mix was a tan color (indicating contaminent removal). X-ray analysis of the wax portion of the product showed the iron concentration near 500 ppm. The production rate of filter press was much better than the previous alternatives. Flow rates of about 5 gallons an hour were achieved during the early portion of filtering. The flow rate through the filters would decrease sharply as the filtration progressed, and the contaminent accumulated in the filter.

Early filter press trials were plagued by tears in the paper that permitted product contamination. The press would also cake up with wax. Further testing on the filter press was necessary to correct those problems.

Having concluded that the filter press is the most appropriate technique for this application, the challenge was to define the conditions needed for sustained filtration with a high quality product. Four key parameters were then optimized: temperature; dilution; filter pore size; and pressure.

Temperature

The most important factor in developing a sustainable flow is creating a filter press temperature that will prevent the wax from solidifying and suppressing the flow. Modifications were made to the press to increase the heat up rate. A preheater and strip heaters on the plates were added to the filter press. The press was heated by recirculating hot solvent through it for several hours before filtering. The 3000 pound filter press had a high heat capacity and required thorough heating before filtering. It was found that the press needed to be heated to about 200°F for an hour so that the entire machine could be brought up to temperature. Insufficient heating caused the wax to accumulate in the filter paper, which slowed down the flow, reduced yield, and accelerated the cooling by reducing the flow of hot feedstock to the press.

Dilution

The filter press test runs examined solvent/wax mixtures ranging from 2:1 to 10:1. The mixtures with higher wax concentrations generally fouled sooner. In a typical filtration run, the effluent from the press comes out dark (filled with iron oxide) immediately after the solvent/wax mixture is introduced. The flow is initially strong, but begins to decrease with time as the filter cake builds on the filters. The quality of the product then increases, changing to brownish color. The outlet temperature then decreases as the flow gradually slows to a trickle.

Filter Pore Size

A number of sizes of filter paper were used. The wax has been filtered with 4 micron paper, but with inconsistancy and with great difficulty. Multiple (1 to 4) layers of 1.5 micron paper were used with better results.

Pressure

A centrifugal pump was used to maintain a pressure of about 40 psi on the filters. A diaphragm pump was added in series with the centrifugal pump to create pressures up to 80 psi. The increased pressure has significantly increased the flow through the system and helped maintain the temperature. The incidence of filter failure, however, was high with the two-pump system. The production filtering relied on a single gear pump with pressures up to 60 psi.

2.2.4 Production Cleaning and Blending

The processing for the light and heavy waxes is shown in Figure 2.2. Drums of light and heavy waxes were received at SwRI and stored until required for processing. Samples of the waxes were submitted for testing. The light wax was distilled in batches in the DOE Synthetic Fuels Center at SwRI. The material was processed in a batch distillation unit. Seven ten-gallon batches of light wax were distilled, yielding a bottoms portion of 48 gallons of light wax (650°F+). Samples of the light wax were submitted for Thermogravitational Analysis following the distillation.

The heavy wax drums were opened with an air-driven chisel, and the wax was broken into small chunks. The wax was then mixed with Isopar M solvent in a ratio of roughly 7 pounds of Isopar per pound of wax and heated to 220°F.

Filtration

The wax/solvent mixture was passed through a plate and frame filter press to remove the iron oxide contaminent in the wax. A double layer of 1.5 micron filter paper was used. The wax and solvent mixture recovered from the press was inspected for color to assure that an adequate amount of contaminent had been removed. A light brown or tan sample would indicate that the wax contained approximately 500 ppm. This criteria was verified with x-ray testing of the sample products and gravimetrically by ashing. Dark brown samples would be rejected as possibly having too much iron, and returned to the feed drum until a light effluent was obtained.

Filtered wax spanned the sequence of drums from the runs at LaPorte. Wax was drawn from drums 32, 34, 42, 43, 49, 51, and 57. Each of the three batches of finished wax (for Amoco, Kellogg, and SwRI) contains some wax from the 30, 40, and 50 series. SwRI was able to collect an acceptably clean product from the drums, with the exception of the material in drum 55. It is suspected that that drum, produced near the end of the run, had a greater amount of fines than the earlier drums.

Experiments were conducted to estimate the yield of the filtration operation. The experimental setup involved weighing both the feed and product drums as a wax/solvent solution was passed through the filter press. The increase in weight of the product drum was compared to the loss in weight of the feed drum. Approximately 43% of the solvent/wax mixture was recovered. Of the first three drums processed (32, 42, and 57), approximately half of the 150 gallons were recovered. The slightly higher yield of the full scale experiments may be due to the fact that higher temperatures (around 200°F) were used.

The filtered wax/solvent was collected in open top, 55 gallon drums and allowed to settle. Solvent was decanted from the upper layer of the drums and returned to the filtering process. The concentrated wax/solvent mixture continued on to the solvent removal step.

Distillation

Solvent was removed from the wax in a Wiped Film Evaporator (WFE). A WFE is a continuous distillation apparatus. Wax/solvent mixture was pumped through a preheater into an evacuated chamber. The mixture was spread along the surface of the chamber by a rotating wiper blade. In this operation, the WFE was maintained at 270 F and 4 Torr, which is an equivalent atmospheric temperature of 550°F. Isopar M boils at temperatures below this point, while the wax requires higher temperatures for distillation. The wax and solvent separate, with the solvent boiling off, recondensed, and then collected in the overhead accumulator. The wax was collected in the bottoms accumulator. Recovered solvent was returned to the filtering step.

Solvent was removed in two passes through the WFE. The first pass, at about 7 gallons per hour was able to remove most of the solvent. The product from the first pass contained approximately 30% solvent. A second pass at roughly 2 gallons per hour reduced the solvent concentration to less than 9%. Samples were drawn from the product wax to measure the iron content by x-ray analysis. Solvent removal was confirmed and boiling point distribution was determined with ASTM D-2887 high temperature simulated distillation. Any residue of solvent was chemically of the same hydrocarbon type as the wax product and made little perturbation of the start of the boiling curve.

Wax Blending

Following filtration and solvent removal, the heavy wax was blended with the light wax heavy fraction. The waxes were mixed in a proportion of 4.97 pounds of heavy wax per pound of light wax heavy fraction. Blended wax batches were prepared for further testing at Amoco, Kellogg, and SwRI.

2.3 Wax Properties Before and After Cleaning

The success of the wax cleanup is measured in three ways: 1) the iron content; 2) the boiling point distribution of the filtered wax (and its similarity to the parent black wax); and 3) the quantity of material produced.

2.3.1 Iron Content

The iron content of the original black wax contained was between 5000 and 7000 ppm, varying from drum to drum. The iron content of the processed heavy wax is shown in Table 2-2 for the batches of wax to be tested at Amoco, Kellogg, and SwRI. Each of the heavy wax samples shows an iron concentration of slightly above 500 ppm. When the heavy wax was blended with the inherently iron-free light wax, the overall iron concentration falls to slightly below the targeted 500 ppm. The exception is the 70 gallon batch prepared for Kellogg which contains 576 ppm. This batch will be blended with the SwRI batch to lower the iron content to just below 500 ppm.

2.3.2 Boiling Point Distribution

The second requirement was for the filtered wax to retain a paraffin distribution similar to the parent material. Samples of the black wax and heavy wax from each of the product batches was analyzed with a high temperature, simulated distillation per ASTM D-2887. The boiling point distribution has been determined for each sample as shown in Table 2-3. Comparing the treated waxes to the black wax shows a close similarity over most of the boiling range. The differences between the values are due mainly to variability in the properties of the black wax from drum to drum and the presence of small amounts of solvent in the wax.

Figure 2.3 shows high temperature gas chromatograms for the black wax (top trace) and the clean heavy wax. The two traces show a similar distribution of paraffins over a wide range of molecular weights. The solvent was not completely removed and is visable as the plateau at the left of the lower trace.

2.3.3 Production Summary

Ample quantities of the wax were filtered and blend as required for the Work Plan. A total of 240 gallons of wax have been processed as denoted in Table 2-4. The three batches were produced from source drums in the 30, 40, and 50 series. These batches will be provided for processing experiments.

Table 2-1. Wax Production Requirements

Testing by:	Total Wax, gal	Heavy Wax, gal	Light Wax, gal
Amoco	10	8	2
Kellogg	70	56	14
SwRI	160	128	32
TOTAL	240	192	48

Table 2-2 Iron Content of Wax Samples

	Amoco	Kellogg	SwRI
Sample ID Number	FL-2442	LN 772	LN 773
Heavy Wax Iron Conc, ppm	579	721	530
Blended Wax Conc, ppm	463	576	424

Table 2-3 Boiling Point Distributions per ASTM D-2887

	Black Wax (°F)	Heavy Wax (°F)		
		Amoco	Kellogg	SwRI
IBP	517	369	443	437
10	792	523	502	488
20	875	878	695	510
50	1101	1113	882	984
70	1217	1228	1066	1154
80	1271	1272	1165	1226
90	1310	1302	1253	1286
FBP	1340	1326	1304	1325

Table 2-4 Wax Production Summary

Source Drum Numbers	Testing by:	Total Wax, gal	Heavy Wax, gal	Light Wax, gal
32,42,57	Amoco	10	8	2
32,42,57	Kellogg	70	56	14
34,43,49,51	SwRI	160	128	32
	TOTAL	240	192	48

Figure 2-1 Wax Cleaning Process Development

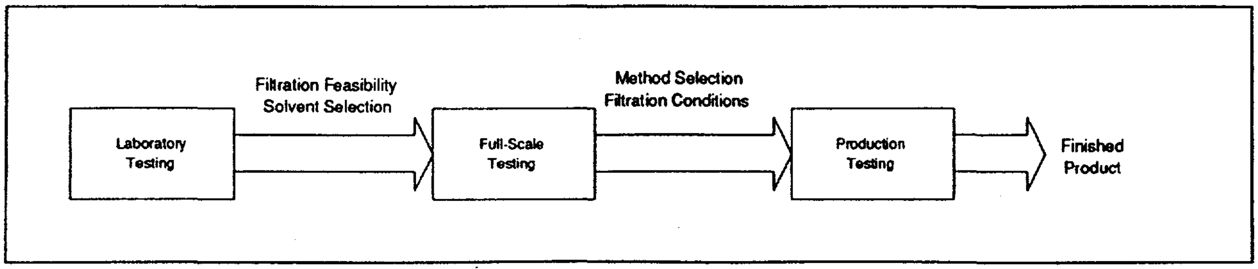


Figure 2-2 Wax Cleanup and Blending

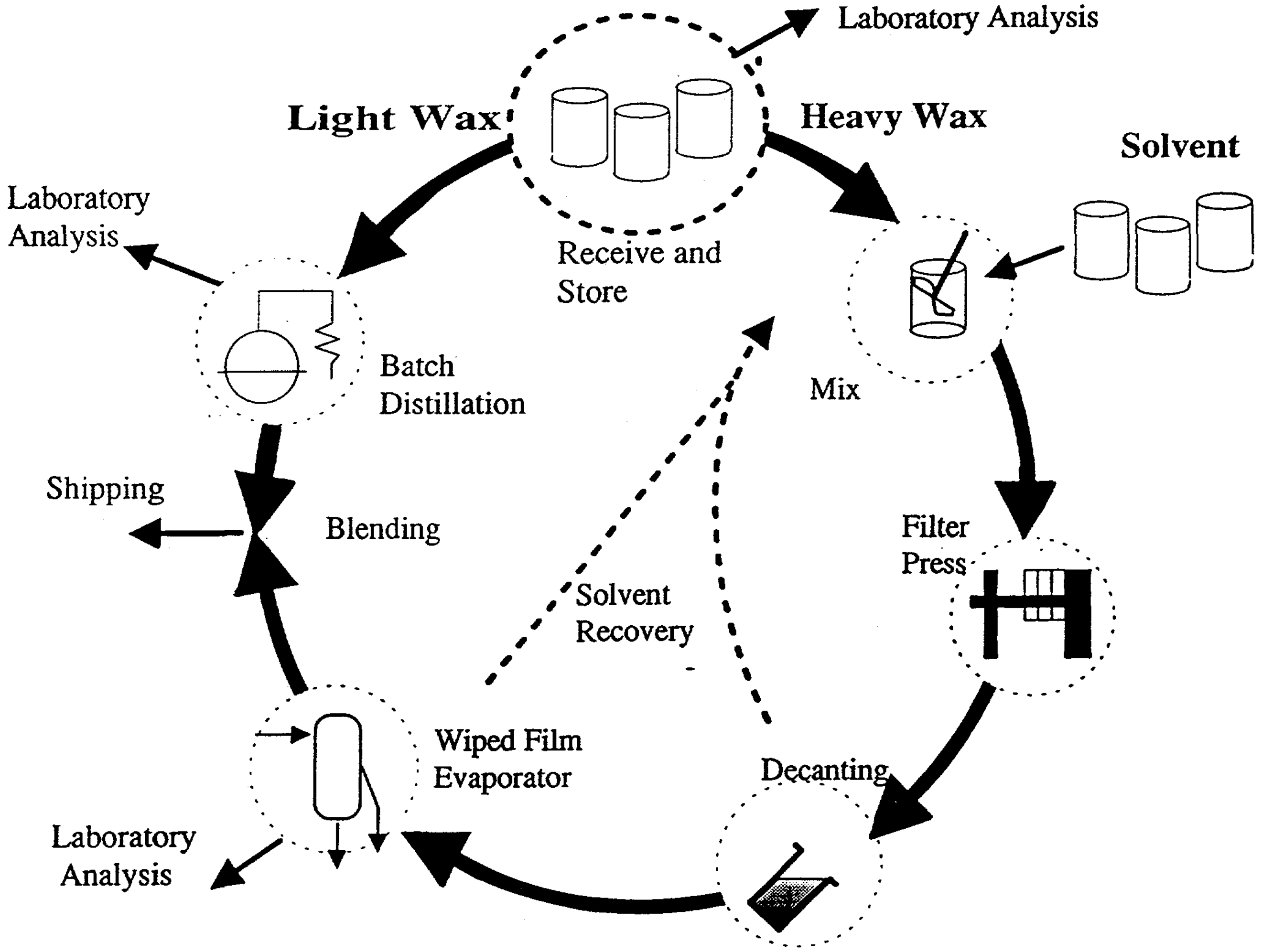
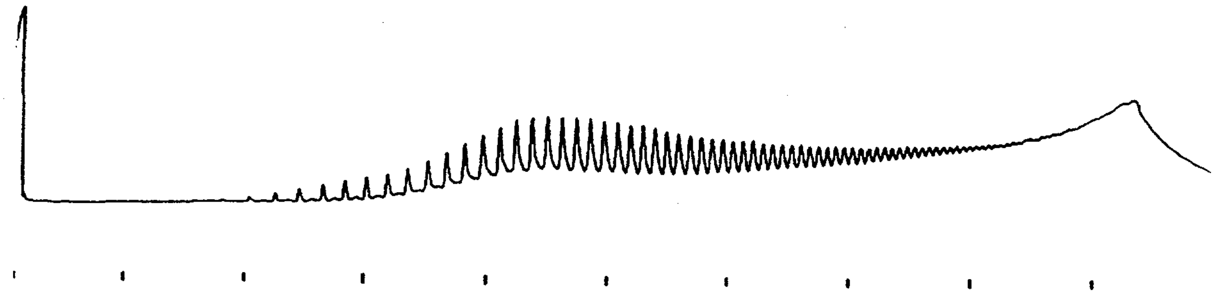
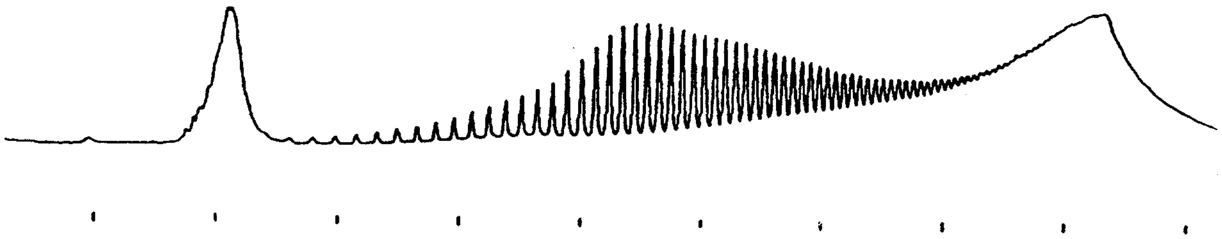


Figure 2-3 High Temperature Chromatograms of Black Wax (top) and Heavy Wax (below)



Black Wax



Heavy Wax

Section 3

Bechtel Activities

3.1 Linear Programming Model - Task 3

A report on the design basis of the linear programming model for direct coal liquids is being developed.

Section 4

Amoco Activities

4.1 Indirect wax catalytic cracking

A report summarizing the bench scale wax catalytic cracking tests is being developed and will be issued in the next quarterly report.

Section 5

M.W. Kellogg Activities

5.0 FCC CRACKING OF DIRECT COAL LIQUID IN MAT AND PILOT PLANT

5.1 SUMMARY

The M.W. Kellogg Company conducted both laboratory and pilot plant catalytic cracking tests with feedstocks derived from both coal and petroleum. The purpose of these tests is to supply basic yield and property information to be used by Bechtel in a linear model of a petroleum refinery wherein the coal-derived feeds are processed along with existing petroleum feeds in conventional refining units.

A bituminous coal was processed by direct liquefaction and the resulting syn-crude distilled to produce a material with a boiling range similar to many diesel oils. Alternate processing choices for this material are to use it in diesel blending, possibly after hydrotreating, or to feed it to the fluid catalytic cracking unit (FCCU) again, with or without hydrotreating. To provide data to explore the hydrotreating options, portions of coal-derived material were hydrotreated at various severities. Samples received by Kellogg for testing included two drums of a hydrotreated product obtained at moderate severity and one drum of a typical petroleum-based FCCU feed, along with small laboratory samples representing products obtained at a variety of hydrotreating severities. An equilibrium catalyst was obtained from an operating refinery for use in evaluating all feeds on a common basis.

Kellogg used the Microactivity Test unit (MAT) in a matrix of experiments with all of the feeds to establish the effect of hydrotreating severity on the value of the product slate from the FCCU. By varying catalyst-to-oil ratio to change cracking severity, it was possible to construct curves from the data to estimate maximum gasoline yields with each feed. The results showed a benefit of 10 wt% gasoline for the most severe hydrotreatment and a linear relationship between the hydrogen added and the extra gasoline produced.

None of the coal-derived feeds produced much coke during cracking and heat balance calculations indicated that extra heat would have to be supplied to the regenerator to allow operation at optimum conditions. In a typical refinery this heat is readily supplied by blending low value residual material into the feed but, for the linear model, it is more convenient to consider the heat to be supplied by torch oil fed to the regenerator. Accordingly, product yield distributions for every feed were calculated at the same catalyst-to-oil ratio needed by the petroleum feed for heat balance without adding torch oil. Torch oil requirements for the coal liquids and the blend were quoted in terms of BTUs per pound of feed. This parameter can be used directly in the linear model.

M.W. Kellogg Activities

The Kellogg circulating FCC pilot plant was run to produce enough product gasoline for engine octane determination and to calibrate data obtained in the MAT unit. Runs were made with the petroleum feed, the hydrotreated coal-derived feed and a blend containing 33 vol% of the hydrotreated coal feed and 67% petroleum material. Conditions were set so that the petroleum feed produced the required coke for heat balance in a refinery, then held for runs with the other two feeds. The runs went very smoothly and the resulting yield data compared very well with expected yields calculated from the MAT. It was established that the yields with the blend matched the weighted average yields from the pure feeds.

Analytical data were gathered on the gasoline products from MAT runs made near optimum conditions using a chromatographic technique that employs backflushing to separate the gasoline from heavier products. Hydrocarbon type analyses (PIANO) and GCOCTANE analyses were obtained. The GCOCTANE method was also used on the pilot plant liquid products without distillation. The analytical results showed more naphthenes in the FCC gasolines from all coal liquids than in gasolines obtained by cracking petroleum stocks.

The pilot plant liquid products were distilled by Southwest Research Institute and produced gasolines with octane numbers that were almost identical, despite the fact that the feeds represented both a coal liquid and a petroleum liquid, suggesting an easy acceptance for this material in the refinery. Data were obtained for calibration of the MAT/GCOCTANE method for estimating the yield and octane number of gasoline obtainable from a coal-derived feedstock by comparing MAT and pilot plant results for the same feed. These calibrations were then applied in the MAT study of the effect of hydrotreating severity.

The smoothness of operation and consistency of data lead to expectations of efficient performance of the pilot plant in the planned production run.

5.2 INTRODUCTION

Three subject liquids are being evaluated in a study in which coal liquids are used as incremental feed in an expanded refinery. Two of the liquids were produced by direct liquefaction, while one is from indirect (Fischer-Tropsch) processing. Many refining options will be examined by a linear programing model (PIMS) which needs basic yield and product quality information for each of the coal liquids. The present task is concerned only with the product of direct liquefaction of a bituminous coal (DL1) and the value of the heavy distillate and residual portion of this liquid as an FCCU feedstock. A similar study with the direct liquefaction product of a subbituminous coal (DL2) will be carried out and reported at a later date.

Preparation of the DL1 liquid and characterization of the total liquid and the lower-boiling fractions are described elsewhere. The method of preparation involved recycle of high boiling fractions to extinction, which resulted in a product with a distillation end point near 750°F. Accordingly, the "back end" of DL1, which is the subject for FCC testing, has a nominal boiling range of 430°F to 750°F, rather than the 430°F to 1100°F range that is typical of petroleum-derived vacuum gas oils used as FCCU feed.

It was decided to hydrotreat this feedstock to reduce its aromaticity – both for use as a component in diesel and jet fuels and to improve its value as a FCCU feed. Several hydrotreating severity levels were run. Because increasing severity incurs greater cost, the extent of improvement in the gasoline yield and an estimate of the change in octane quality were needed to determine its value.

Since the assumptions used in the linear model involve handling the coal liquids in mixtures with petroleum-derived stocks, there is a need to establish an experimental basis for blending rules. For the present study, a typical gas oil from Amoco's Whiting refinery was characterized and utilized in the test work.

Distillation of the DL1 liquid, hydrotreating of the heavy distillate and residual fraction, and initial characterization of the feeds were performed by Southwest Research Institute (1,2). Several different identifications for the various materials produced have been used along the way. When received by Kellogg for testing, sample numbers were assigned and codes for each sample (or blend of samples) used in setting up the experimental plan. A cross reference between these samples and the identifications used by SwRI and others is given in Table 5-13.

5.3 PURPOSE

The purpose of the work described here is to develop the needed experimental results to support the LP modeling effort with the DL1 liquid and to produce adequate volumes of liquid material for ASTM and compositional testing. A similar program will be carried out with the DL2 liquid when it is available.

Specifically, the work is designed to provide estimates of the extent of change in FCCU product value with severity when the coal liquid is hydrotreated, to establish reliable values for the yields and product octanes for a typical blending situation, and to determine whether linear blending is obtained.

5.4 METHODOLOGY

5.4.1 MAT UNIT

5.4.1.1 EQUIPMENT

A schematic of the MAT test system is shown in Figure 5-1. Typical sample injections to the MAT unit are 1 cc with an injection time of 30 seconds. Actual sample weights are determined by weighing the syringe before and after injection.

Conversion is changed by variation in the amount of catalyst charged to the unit. A practical range is from 3 g to 7.5 g.

The feed is preheated as it flows through a syringe needle within a metal shot-filled "deadman" in the upper furnace zone. Zone temperatures are controlled to produce a time weighted average temperature in the catalyst bed within ±10°F of the specified operating temperature.

Injection of the feed is followed by an extensive flush with nitrogen (not shown) to strip the catalyst and reactor of all hydrocarbons. The total volume of gas is measured by displacement of brine. After mixing the gas, a sample is displaced through a Carle gas chromatograph for analysis. The weight of the liquid product collected is measured and the liquid is transferred to a vial for simulated distillation and other chromatographic analyses. Residual liquid in the bottom of the reactor ("dribble") is removed with a solvent and weighed after solvent evaporation. The dumped catalyst is separated from extraneous material and carbon on catalyst is determined by combustion and measurement of the CO_2 produced.

From the measured weights, the gas volume, and the analyses of gas, liquid and catalyst it is possible to determine the complete product distribution and the material balance for the run. Runs with material balance lower then 95% are discarded. Additionally, the analysis of the gasoline fraction for paraffins, isoparaffins, aromatics, naphthenes and olefins (PIANO) and GCOCTANE is accomplished by use of chromatographs equipped with backflush capability. The run tables (Tables 5-14 through 5-20) provide examples of the data gathering capability of the MAT unit.

5.4.1.2 EXPERIMENTAL PLAN

General

The MAT studies provide initial estimates of yields for both coal liquids and blends with petroleum stocks and give guidance in setting conditions for operation of the pilot plant. Samples to be run in the MAT unit are identified as:

A. Unhydrotreated DL 1 Heavy Distillate and Residual Fraction (F-9827)
B. Slightly Hydrotreated DL 1 Heavy Distillate and Residual Fraction (F-9824)
C. Highest Severity Hydrotreated DL1 Heavy Distillate and Residual Fraction (F-9826)
D. Severely Hydrotreated DL 1 Heavy Distillate and Residual Fraction (F-9823)
E. Amoco-supplied typical refinery gas oil (F-982 1)
F. 50:50 Blend of severely hydrotreated coal liquid and the typical refinery gas oil. (F-9823 & F9821)

An equilibrium FCC catalyst was obtained from Conoco for use in this study.

Experimental Objectives

1. Provide yield data over a range of conversions for each liquid.
2. Obtain knowledge of the gasoline compositions by running PIANO analysis on one product from each liquid.
3. Obtain GCOCTANE information on samples selected to show the effect of hydrotreatment.

Experimental Steps

1. Calcine the equilibrium catalyst at 1000°F for 2 hours in air to remove any residual carbon. Store the calcined catalyst in a tightly fastened bottle.

2. Code the liquids as follows.

   A = F-9827, Unhydrotreated DL1 Heavy Distillate and Residual Fraction
   B = F-9824, Slightly Hydrotreated DL1 Heavy Distillate and Residual Fraction
   C = F-9826, Highest Severity Hydrotreated DL1 Heavy Distillate and Residual Fraction
   D = F-9823, Severely Hydrotreated DLI Heavy Distillate and Residual Fraction
   E = F-9821, Amoco-supplied typical refinery gas oil
   F = 50:50 Blend of F-9823 and F-9821.

3. Using 30 seconds injection time and an average bed temperature of 970°F ± 10°F, carry out two blocks of MAT runs as indicated below, where the letter signifies the feed and the number signifies the catalyst-to-oil ratio. Randomize the order of running within each block. Complete the first block and plot the data before starting the second block to determine whether any adjusttnents in catalyst-to-oil ratio are needed.

Block I	Block II
A6, A4.5, B6, B4.5, C6, C4.5	A3, A4.5, B3, B4.5, C3, C4.5
D3, D4.5, E3, E4.5, F3, F4.5	D6, D4.5, E6, E4.5, F6, F4.5

4. Obtain PIANO analysis on one of the product liquids from each feed, selected on the basis of maximum gasoline yield.

5. Obtain GCOCTANE analysis on product liquids, selected on the same basis, from runs made with feeds A, C and D.

5.4.2 FCC PILOT PLANT

5.4.2.1 EQUIPMENT

General

The pilot plant used in this work (shown in Figure 5-2) is a nominal 1/3 barrel per day Riser FCC/Resid FCC unit consisting of cracking, stripping, and regeneration sections, all operating under pressure with catalyst continuously circulating between these sections. This unit is designed to handle a wide range of operating variables. The temperatures and flow rates are controlled to tight tolerances as required by the specifics of the test program.

Process Flows

Oil feed is introduced into the unit from a heated feed tank by a gear pump. After passing through an electrically-heated preheater. The hot feedstock stream (normal range: 150-700°F) is atomized with dispersion nitrogen in a proprietary injection nozzle and carries into the flowing catalyst stream.

Regenerated catalyst (1100-1450°F) passes through a slide valve which controls the catalyst circulation rate (20-50 lb/hr) and is transported via a short transfer line to the bottom of the riser with a flow of nitrogen. The dispersed feed stream and the catalyst stream mix in the 1/2" SCH 40 injection chamber, designed for use with heavy feeds to avoid coke deposition on the riser walls, and are transported up the riser.

Riser effluent enters the stripper tangentially. The solids are disengaged from the product oil vapors. The solids are then stripped with nitrogen to remove interstitial and adsorbed hydrocarbons from the catalyst. The catalyst then flows to the regenerator where coke is burned off. Upon leaving the unit, the regenerator flue gas is cooled to about 50°F to condense water of combustion. The remaining gas is then measured, analyzed, and vented. It is from these flue gas measurements that coke make is calculated.

From the disengager/stripper, the product oil vapors are partially condensed in two stages of cooling. Product is withdrawn continuously and collected hourly. The syncrude is analyzed off-line for dissolved gases to complete a full set of C_4 & lighter yields. GC Simulated Distillation (GCSD) provides conversion and the yields of heavier fractions.

The uncondensed product gas exiting the low temperature receiver is then analyzed by an on-line G.C., measured by a wet test meter, and, finally, vented to a flare. Other on-line analytical instruments monitor the product gas density and the carbon dioxide and oxygen content of the regenerator flue gas.

Riser Description

The riser is a 1/4" SCH 40 stainless steel pipe, about 30 feet in length with provisions for temperature and pressure measurements at several points along its length. The riser is fitted with three separate heating zones. The electrical heating wires are wound around a layer of insulation surrounding the riser. At the midpoint of each zone, skin thermocouples are welded to the riser outer surface. Internal thermocouples extend inside the riser to measure actual fluid temperatures. Additionally, jacket thermocouples are positioned in the insulation between the riser wall and the electrical windings at about the same elevation as both the skin and internal thermocouples. This design provides the flexibility to simulate adiabatic operation or to run isothermally.

Disengager/Stripper Operation

Product vapors exiting the riser (900-1050°F) enter the stripper tangentially into an annular space created by placing a collar within the stripper body. Catalyst is disengaged from the vapors by cyclonic forces and a change of direction as the vapors move downward in the annulus, then upward into the upper section of the stripper which contains a sintered-metal filter to prevent entrained catalyst particles from leaving the unit.

The catalyst passes downward into the stripping section. A bed of spent catalyst is maintained while stripping nitrogen passes countercurrently from its inlet, which is located by the entrance to the stripper standpipe.

Regenerator Operation

The regenerator controls the level of carbon on regenerated catalyst. The regenerator includes both electrical windings and an air-cooled jacket to permit the riser to run in heat balance independently of coke make. The air jacket also allows operation with higher carbon residue-containing feeds than would otherwise be possible. By adjusting the regenerator temperature to about 1325°F and maintaining oxygen content of the flue gas between about 6 and 12 percent, carbon on regenerated catalyst levels below 0.1 weight percent are produced.

5.4.2.2 EXPERIMENTAL PLAN

Three runs were planned for the FCC1 pilot plant. Feedstocks were Amoco Heavy Vacuum Gas Oil (F-9819), Direct Coal Liquid Distillate (F-9820), and a 33.3 vol% (33.6 wt%) blend of the Coal Liquid with the VGO. The catalyst used in all three runs would be a sample of equilibrium Vektor-50 (F-9804) obtained from Conoco (Billings, MT).

The experimental plan was to use the first run (H-2006-1) with VGO to set the operating conditions for all three runs. Base operating targets set for the pilot plant operators were:

Catalyst rate 48 lbs/hr
Catalyst temperature 1250°F
Riser outlet pressure 35 psig
Riser isothermal temperatures 980°F.

The key target was a calculated coke yield of 5.0 wt%. In seeking this target, the catalyst rate was fixed and the oil feed rate adjusted, higher to lower coke yield or lower to increase coke yield. The catalyst rate was set at a high value to maximize the feed rate, in anticipation of the production run to be made at a later date. A chart of calculated oil preheat temperatures versus oil feed rates was supplied to the operators to assist them in obtaining the targeted coke yield in the least amount of time.

5.4.3 ANALYTICAL METHODS

5.4.3.1 GC SIMULATED DISTILLATION

Analytical Controls/HP 5890
J&W Capillary (DB2887), 10 m x 0.544 mm, 3.0 μ Film Thickness.

ASTM D2887

5.4.3.2 GC OCTANE

Kellogg Method/Varian GC 3700
Main column SGE Capillary(BP-1), 25 m x 0.53 mm, 1.0 μ Film
Back flush column SGE Capillary(BP-1), 0.5 m x 0.53 mm, 1.0 μ Film

(See References 1 through 3.)

5.4.3.3 PIANO

HP 5890 with a SGE Multidimensional Capillary GC System
(**P**araffins, **I**soparaffins, **A**romatics, **N**aphthenes and **O**lefins)
Main column, J&W Capillary (DB-1), 100 m x 0.25 mm, 0.5 μ Film Thickness
Cutting column, SGE Capillary (DB-1), 1 m x 0.25 mm, 1μ Film Thickness

PIANO software program by Analytical Automation Specialists

5.4.3.4 CARLE® REFINERY GAS ANALYSIS

Application 196, E.G. & G. CHANDLER ENGINEERING

Isothermal multicolumn chromatography with hydrogen transfer system and separate TCD for hydrogen analysis. Six different 1/8" packed columns are utilized in this application.

5.4.3.5 CARBON ON CATALYST

DIETERT CARBON ANALYZER (HARRY W. DIETERT CO.)

Gas volumetric method in which carbon on catalyst is burned in pure oxygen and carbon dioxide determined by volume measurements before and after treating product gas with KOH.

5.5 RESULTS AND DISCUSSION

5.5.1 FEEDSTOCK CHARACTERIZATION

In addition to feedstock characterizations previously done by SwRI and Amoco, it was necessary, in this study, to determine the distillation characteristics of each feed, specifically to determine the amount of the feed material boiling below 430°F. These data are included in Table 5-1, which also describes a reference ASTM feed used as a standard benchmark.

5.5.2 MAT STUDIES

Results for all MAT runs are shown in Tables 5-14 through 5-20.

5.5.2.1 CONVERSION AND COKE

Plots of apparent conversion and coke yield versus catalyst-to-oil ratio are given in Figures 5-3 through 5-9. For all of the coal-derived liquids it was observed that the variation of conversion with increasing catalyst-to-oil ratio was very flat compared to petroleum-based stocks. Increases in coke yield appear to follow a linear relationship with catalyst-to-oil ratio for both the coal liquids and the petroleum feeds.

In petroleum work, the kinetic conversion (defined as %conversion / (100 - %conversion)) is used in modeling data because cat cracking appears to follow second order kinetics, making this parameter linearly related to severity. The relationship is not only linear, but regression of the kinetic conversion with catalyst-to-oil ratio usually shows an intercept near zero. Figures 5-10 and 5-11 are plots obtained in past investigations that show typical behavior.

In order to establish the extent of difference between the coal and petroleum derived feeds the true conversion for each run was calculated by taking into account the material in the feed that boiled below 430°F. Kinetic conversions were calculated using these true conversion values and plotted against catalyst-to-oil ratio. Figures 5-12 and 5-13 are the plots for the coal liquids, with and without hydrotreating.

The apparent positive intercept with the coal liquids is an artifact of the plotting; with no catalyst, the true conversion would be zero. The true representation would be a curve and the conversion curve has nearly flattened in the region of the experiment. This implies a kinetic order higher than 2 for the unconverted liquid. The chemical interpretation is that the residual liquid is composed largely of two and three ring aromatic structures which are relatively inert towards cracking.

With the petroleum-derived feeds, a higher boiling back end allows the existence of components with varying reactivity that lead to a simulation of second order behavior. This seems to be precluded by the choice of end point in the preparation of the present group of coal-derived feeds. What we find is a limiting conversion that depends upon the level of hydrotreating, but is relatively insensitive to the FCC operating conditions. There is also a low byproduction of coke.

Since the conventional kinetic conversion plots were not an appropriate model for the coal liquids, a simple power function was used to fit curves of conversion versus catalyst-to-oil ratio. The lines shown in Figures 5-3 through 5-9 were constructed in this manner and the parameters found for each feed are used in the section on heat balance to estimate the conversion obtained at specified coke make.

5.5.2.2 YIELDS SUMMARY

Gasoline

The gasoline yield selectivity for each run is calculated by dividing the wt% gasoline yield by the wt% conversion. When the selectivity is plotted against catalyst-to-oil ratio, a straight line of decreasing slope is produced. Using the regression parameters for the lines found with each feed, along with the previously discussed power function relating conversion to catalyst-to-oil ratio, a new curve expressing gasoline yield as a function of catalyst-to oil ratio is derived. The determined data for gasoline yield fall very close to the curves for every feed examined. Figures 5-14 through 5-20 carry the plots of selectivity and gasoline yield.

There is a maximum gasoline yield for each feed at an associated catalyst-to-oil ratio which is easily observed in the figures. The conversion, coke yield and the distribution of other products under these conditions define the optimum total value of the feedstock. In cases where the C3 and C4 olefins plus isobutane are valued for their use in alkylation and etherification, the sum of the gasoline and these components is considered potential gasoline. The maximum in potential gasoline usually occurs at a higher conversion (greater catalyst-to-oil ratio) than the maximum gasoline yield. Tables 5-2 and 5-3 summarize the conditions and product yield distributions associated with both the maximum gasoline yield and the maximum potential gasoline yield for all of the feeds.

From Tables 5-2 and 5-3, it is obvious that the maximum gasoline yield and the maximum potential gasoline yield are improved by hydrotreating and the extent of improvement can be estimated by putting values on the products. In Figure 5-21, these maximum yields are plotted against the hydrogen content of the coal-derived liquids. The relationship is linear and may be used to interpolate product values to hydrotreating severities not tested in the present work. Feedstocks from a different source will not fit the same line, however, as is evidenced from the fact that the petroleum feeds have more hydrogen than any of the coal liquids, but give lower gasoline yield.

5.5.2.3 HEAT BALANCE

The refinery FCCU operates in heat balanced mode. Usually, this means that the regenerator supplies the heat of combustion of the coke formed in the reactor to make up for the heat required for vaporization, cracking and for various heat losses. Figure 5-22 provides a sketch of the heat balance as applied to a standard Kellogg Orthoflow® FCCU.

Some modern catalytic crackers are equipped with catalyst coolers that remove excess heat from the regenerator with coils that generate steam. This is usually done when residual material is processed through the FCCU to obtain high conversion without exceeding metallurgical limits in the regenerator. This option is provided in making heat balance calculations. To establish conditions for a unit without a catalyst cooler, the heat generated as steam is defined as zero.

In other situations, the coke produced in cracking is not sufficient to supply enough heat to meet the unit needs. For example, if the FCCU is limited in catalyst circulation, the temperature of the regenerated catalyst may not be high enough to allow the maintenance of the desired riser outlet temperature (ROT). Without decreasing the oil feed rate, an option that may be used is to feed torch oil to the regenerator. In a modification to the usual heat balance calculations, the heat value of the torch oil required can also be obtained. Tables 5-21 through 5-23 contains examples of standard heat balance calculations and a heat balance modified to estimate added heat requirements. All calculations use the power function mentioned earlier to relate conversion to catalyst-to-oil ratio.

Similar calculations were made for all feedstocks studied. In summarizing these results, Table 5-4 gives the fixed conditions for making the heat balance and Table 5-5 gives the heat balance for all of the feeds used in this study without supplying extra heat. Table 5-6 gives the results with enough torch oil addition to achieve the desired ROT at the same catalyst-to-oil ratio as was used with the refinery gas oil and provides the heat value of the torch oil used. In all cases these conditions were found to be very close to the conditions for producing maximum potential gasoline.

5.5.2.4 PIANO ANALYSIS

A summary of the PIANO analysis for the products from the MAT tests is shown in Table 5-26. The analytical results showed higher naphthenes in the FCC gasolines from all coal liquids than in gasolines obtained by cracking petroleum stocks.

5.5.3 PILOT PLANT RUNS

5.5.3.1 OPERATING SUMMARY

Table 5-7 lists the key operating variables for the three pilot plant runs. Run H-2006-1 achieved the coke yield target to within 0.1 wt% at a catalyst-to-oil ratio of about 12. Catalyst rates averaged 48.2 lbs/hr and oil rates were 1805 ± 9 g/hr.

Material balances were all around 98.5 wt% with conversions of about 73-74 wt%. The riser outlet pressure held at 35 psig.

Oil preheat temperatures averaged 213°F and catalyst inlet temperatures were 1258 ± 7°F. Riser averages were 985 ± 2°F. All eight riser internal temperatures were within the range of 975-995°F for all three runs. All operating data are tabulated in Tables 5-21 through 5-23.

All three feedstocks ran well. Riser and stripper filter plugging tendencies appear to be low. This experience would indicate that the production run should proceed well.

5.5.3.2 YIELDS SUMMARY

Table 5-8 summarizes the yields of product materials, in weight percent, from all three runs. Because the conversions from the three runs are so close, side-by-side comparisons can be made without the need to extrapolate.

Compared to the run on VGO (H-2006-1), the run with Coal Liquid (H-2006-2) made significantly less coke and less of each of the categories of converted materials (C_2 & lighter, C_3's, and C_4's), except for C_5-430°F gasoline, which increased almost 5 wt% (absolute). It also produced almost 3 wt% (absolute) more light gas oil (430-650°F), at the expense of less valuable heavy gas oil (650°F$^+$).

Also of interest is the comparison between a weighted average of the yields from the two runs with neat feeds and those of the run with a blend of these feeds (H-2006-3). For essentially every component and boiling range, the results of the run are not significantly different from the calculated values. A complete distribution of the products is given in Tables 5-21 through 5-23.

5.5.3.3 GASOLINE OCTANE NUMBERS

Samples of the condensed total liquid product were debutanized and sent to Southwest Research Institute for fractionation and determination of the octane number of the IBP to 430°F gasoline. Sample numbers for the two laboratories corresponding to runs documented in this report are shown in Table 5-9.

Both the Research Octane Number (RON) and the Motor Octane Number (MON) were determined. Previously, by using a backflushing technique the GCOCTANE method also obtained values for the octane numbers of these gasolines. A comparison of the results is given in Table 5-10.

Due to inefficiencies in the condensation of the gasoline in the pilot plant approximately 7-9 wt% of the gasoline remains in the vapor. These $C5^+$ components in the gas are included in calculating yields, but they are absent in the materials tested for octane number. A more accurate evaluation of the octane numbers of these gasolines is made by adding the contribution of the gasoline in the vapor to the values obtained with the liquid. Table 5-11 contains the octane numbers of the gasolines after making this correction.

Comparison of Tables 5-10 and 5-11 shows that addition of the gaseous $C5^+$ components to the recovered gasoline scarcely affects the RON but the MON is increased by more than one unit. The GCOCTANEs, in all these cases, remain about 2 numbers high in RON and 1 number high in MON compared to the engine numbers.

5.5.3.4 COMPARISON TO MAT RESULTS

The pilot plant runs were designed to be run at a severity slightly higher than achieved at the highest catalyst-to-oil ratio used in the MAT unit (6) in order to produce enough coke with the petroleum feed to stay in heat balance. The requirement for a catalyst-to-oil ratio as high as 12 in the pilot plant is an expected consequence of differences in vapor-solids contact in the two units.

Since the MAT conversion, coke and other yields were fit to curves, it was easily possible to extrapolate to a similar severity, which would require an MAT catalyst-to-oil ratio of 6.54. The yield data and octane numbers obtained by GC at a catalyst-to-oil ratio of 6 are shown in Table 5-12 alongside the results from the pilot plant. It is observed that the agreement in yields is excellent. In the single case studied, a deduction of 2 from both the RON and MON appears necessary to predict the actual octane numbers of the pilot plant gasolines from the GC analysis of MAT products.

5.6 CONCLUSIONS

- All of these coal liquids are good gasoline producers. The maximum gasoline yield can be increased from 52 to 65 wt% by very severe hydrotreating. Yield improvement is a linear function of the increase in feed hydrogen content.
- The coal liquids do not behave as typical petroleum feeds and follow a different conversion-severity model. This behavior and the low coke make are probably due to the fact that 2 ring aromatic nuclei are stable and pass into the cycle oil. The end points of these feeds are too low to accommodate appreciable material with larger aromatic clusters.
- Due to the low coke make, the conversion required for heat balance with coal liquid feeds is well past the optimum for product yields. Cracking these liquids at the conditions needed for heat balance with the petroleum feed gives maximum high value product yields and is more representative of the real world. Yields and required heat input for these conditions are available for use in the linear model.
- Liquid product from MAT runs having maximum potential gasoline yield were analyzed by the PIANO method with 3 samples also analyzed for GCOCTANE. These results show a small increase in octane number over the range of hydrotreating considered for the linear model.
- Yield results compare well between MAT and Pilot Plant. Comparison of the actual octane numbers found in the pilot plant, with the GC values for a MAT product made with the same coal-derived feed at the same conversion, showed that MAT overestimated both RON and MON by about 2 numbers. It is recommended that an adjustment of -2 be made to all of the octane values obtained in the effect of hydrotreating study to correct for this difference.

5.7 REFERENCES

1. Bechtel, DOE Project No. DE-AC22-93PC91029, Bechtel Job No. 22439, November, 1994 Monthly Project Status Report and Milestone Schedule .
2. Bechtel, DOE Project No. DE-AC22-93PC91029, Bechtel Job No. 22439, December, 1994 Monthly Project Status Report and Milestone Schedule .

3. Anderson, P.C., Sharkey, J.M., Walsch, R.P., "Calculation of the Research Octane Number of Motor Gasolines from Gas Chromatographic Data and a New Approach to Motor Gasoline Quality Control," J. Inst. of Petrol. 58, (1972) pp.83-93.

4. Cronkright, W.A. and Butler, M.M., "FCC Feedstock Evaluations using the Microactivity Test," paper presented at ACS meeting, August 1984.

5. Cronkright, W.A., Butler, M.M. and Harter D.A. "Getting more information from the microactivity test", paper presented at the Ketjen Catalyst Symposium '86, Scheveningen, The Netherlands, May 1986.

Table 5-1 FEEDSTOCK INSPECTIONS

CODE	A	B	C	D	E	ASTM
DESCR.	UNHYD	SL HYD	V SEV HT	SEV HT	PETR FD	REF FD
	F-9827	F-9824	F-9826	F-9823	F-9821	F-9803
API	22.5	23.3	31.7	24.2	26.4	27.6
% H	12.03	12.13	12.69	12.23	13.10	NA
WT%	DEG. F	DEG. F	DEG. F	DEG. F	DEG. F	DEG. F
0.5	453	396	168	284	336	286
5	499	495	378	484	458	524
10	512	509	464	502	516	577
20	529	528	502	521	579	633
30	544	542	520	537	629	676
40	561	559	536	554	673	716
50	576	575	554	571	710	756
60	593	591	573	587	750	798
70	610	609	591	605	792	841
80	632	631	614	628	840	889
90	663	662	647	659	901	942
95	689	688	674	684	942	973
99	749	742	730	733	993	1004
EP	788	769	758	753	>1014	>1014
Wt%430 °F-	0	0.8	7.6	1.8	3.1	1.3
NOTES:	1) Analysis of coal-driven feeds for hydrogen and gravity by SwRI 2) Analysis of petroleum feed for hydrogen by Amoco 3) Remaining analyses by Kellogg 4) Distillation data obtained by chromatography (ASTM D2887)					

Table 5-2 YIELDS AT CONDITIONS FOR MAXIMUM GASOLINE

FEED	A	B	C	D	E	F	ASTM
CAT/OIL RATIO	4.4	4.4	4.5	2.9	4.5	4.5	5.9
CONV	66.0	67.7	77.2	68.6	69.6	70.7	75.3
C2 & LTR	1.5	1.5	1.5	1.1	2.7	2.3	3.7
TOTAL C3	4.2	4.6	4.9	4.3	5.7	5.4	7.3
TOTAL C4	6.1	6.7	7.5	6.2	8.2	7.6	9.1
GASOLINE	52.0	52.8	61.7	55.9	49.9	52.7	50.8
LCO	30.3	29.0	20.6	28.4	23.7	25.6	19.0
SLURRY OIL	3.7	3.3	2.3	2.9	6.7	3.6	5.7
COKE	2.2	2.0	1.6	1.2	3.1	2.6	4.4

M.W. Kellogg Activities

Table 5-3 YIELDS AT CONDITIONS FOR MAXIMUM POTENTIAL GASOLINE

FEED	A	B	C	D	E	F	ASTM
CAT/OIL RATIO	5.9	4.4	6.2	4.5	6.0	5.9	6.2
CONVERSION	67.9	67.7	79.2	70.4	72.9	73.1	75.9
POT GASOLINE	61.0	61.8	72.5	65.0	63.1	64.4	65.2
C2 & LTR	2.0	1.5	2.0	1.6	3.6	3.1	3.8
TOTAL C3	4.7	4.6	5.5	4.6	6.4	6.0	7.5
TOTAL C4	6.5	6.7	8.0	6.4	8.8	8.2	9.3
GASOLINE	51.5	52.8	61.5	55.6	49.7	52.1	50.7
LCO	28.3	29.0	18.7	26.4	22.6	22.5	19.3
SLURRY OIL	3.9	3.3	2.0	3.2	4.4	4.5	4.8
COKE	3.2	2.0	2.3	2.2	4.4	3.6	4.6

Table 5-4 FIXED CONDITIONS FOR HEAT BALANCE COMPARISONS

FIXED CONDITIONS:	UNITS	VALUE
FEED RATE	BBL/DAY	100,000
FEED RATE	#/HR	1,342,132
WATER IN WET AIR	MOL %	3.0
BLOWER DISCHARGE TEMP	DEG F	355
FLUE GAS CO2/CO RATIO	MOL/MOL	1000
MOLE % O2 IN DRY FLUE GAS	%	1.0
DELTA T DUE TO AFTERBURN	DEG F	0
FEED PREHEAT TEMPERATURE	DEG F	500
RISER OUTLET TEMPERATURE	DEG F	980

Table 5-5 HEAT BALANCED CONVERSIONS AND COKE YIELDS FOR ALL FEEDS

HEAT BALANCED FOR EACH FEED							
		PETC "A"	PETC "B"	PETC "C"	PETC "D"	PETC "E"	PETC "F"
FEED API	API DEG.	22.5	23.3	31.7	24.2	26.4	25.4
CONVERSION	WT %	70.1	70.0	83.4	73.1	74.3	75.5
HEAT OF CRACKING	BTU / #FEED	180	179	188	182	183	184
TOTAL COKE YIELD	WT %	5.0	5.0	5.1	5.1	5.2	5.1
CATALYST TO OIL RATIO	# / #	8.5	8.7	13.2	8.7	6.8	8.0
REGENERATED CAT TEMP.	DEG F	1,206	1,200	1,132	1,204	1,263	1,222

Table 5-6 CONVERSIONS AND COKE YIELDS WITH TORCH OIL ADDED TO HOLD CAT/OIL CONSTANT

HEAT BALANCED FOR PETROLEUM FEED; OTHERS AT SAME CAT/OIL RATIO							
	UNITS	PETC "A"	PETC "B"	PETC "C"	PETC "D"	PETC "E"	PETC "F"
FEED API	API DEG.	22.5	23.3	31.7	24.2	26.4	25.4
CONVERSION	WT %	68.8	69.2	79.8	72.2	74.3	74.2
HEAT OF CRACKING	BTU / #FEED	178	179	187	181	183	183
TOTAL COKE YIELD	WT %	3.8	3.7	2.5	3.8	5.2	4.8
CATALYST TO OIL RATIO	# / #	6.8	6.8	6.8	6.8	6.8	6.8
REGENERATED CAT TEMP.	DEG F	1,269	1,270	1,286	1,271	1,264	1,270
HEAT ADDED TO REGENERATOR	BTU / #FEED	202	201	414	213	0	111

Table 5-7 PILOT PLANT OPERATIONS SUMMARY

RUN NUMBER: H-2006-	1	2	3
CATALYST/OIL RATIO	12.2	12.2	12.0
TEMPERATURES, DEG F:			
OIL PREHEAT	212	212	214
CATALYST INLET	1265	1253	1252
RISER AVERAGE	984	987	983
MATERIAL BALANCE:			
CLOSURE, WT%	98.50	98.49	98.46
GASOLINE, WT%	50.52	55.17	51.01
CONVERSION, WT%	74.13	74.20	73.18
COKE YIELD, WT%	4.90	3.27	4.32

Table 5-8 PILOT PLANT YIELDS SUMMARY

Run Number: H-2006	1	2	3	Avg
Total C2 & Lighter	3.34	2.03	2.83	2.90
Total C3's	5.99	5.18	5.69	5.72
Total C4's	9.38	8.55	9.33	9.10
Total Gasoline	50.52	55.17	51.01	52.07
Total Cycle Oil	25.87	25.80	26.82	25.85
Coke	4.90	3.27	4.32	4.36
Conversion	74.13	74.20	73.18	74.15

Table 5-9 GASOLINE SAMPLE IDENTIFICATIONS

FEED DESCRIPTION	RUN NO. H-	MWK AL #	SwRI FL #
Petroleum	2006-1	498	2470
H.T. Coal Liquid	2006-2	499	2471
33 vol% Blend	2006-3	500	2472

Table 5-10 RECOVERED GASOLINE OCTANE NUMBERS

RUN NO. H-	GCRON	ENGINE RON	GCMON	ENGINE MON
2006-1	93.2	91.0	81.1	80.3
2006-2	92.8	91.0	81.0	80.0
2006-3	92.6	90.7	80.7	80.2

Table 5-11 CORRECTED OCTANE NUMBERS FOR PILOT PLANT GASOLINES

RUN NO. H-	GCRON	ENGINE RON	GCMON	ENGINE MON
2006-1	93.0	91.0	82.1	81.4
2006-2	92.6	90.9	81.9	81.0
2006-3	92.9	91.2	82.2	81.7

Table 5-12 SUMMARY COMPARISON OF MAT AND PILOT PLANT RESULTS

FEED DESCRIPTION	PETROLEUM		SEV. HT COAL LIQUID		67/33 BLND	50/50 BLND
FEED, F-NUMBER	9819	9821	9820	9823	9819/9820	9821/9823
YIELDS, WT%	P. PLANT	MAT	P. PLANT	MAT	P. PLANT	MAT
TOTAL C2 & LIGHTER	3.3	3.9	2.0	2.4	2.8	3.4
TOTAL C3'S	6.0	6.7	5.2	5.0	5.7	6.3
TOTAL C4'S	9.4	9.0	8.5	6.6	9.3	8.5
TOTAL GASOLINE	50.5	49.3	55.2	54.3	51.0	51.7
TOTAL CYCLE OIL	25.9	26.1	25.8	28.0	26.8	26.1
COKE	4.9	4.9	3.3	3.6	4.3	4.0
CONVERSION	74.1	73.9	74.2	72.0	73.2	73.9
CAT/OIL	12.2	6.54	12.2	6.54	12.0	6.54
GASOLINE RON	91	N.A.	90.9	92.6	91.2	N.A.
GASOLINE MON	81.4	N.A.	81	83.7	81.7	N.A.

NOTES:
1) All runs made with cat/oil set to produce 4.9 wt% coke with petroleum feed.
2) Runs made at 980 F +/- 5 deg F.
3) Mat data are extrapolations; pilot plant data are actual run yields.
4) Pilot plant octanes measured with engine, mat octanes with GC.

Table 5-13 CROSS REFERENCE FOR MAT FEEDSTOCKS

KELLOGG IDENTIFICATIONS			SOUTHWEST RESEARCH IDENTIFICATIONS		
CODE	ID	DESCRIPTION	DESIG	ID	DESCRIPTION
A	F 9827	UNHYDROTREATED FEED	HD1c+AT1C	FL-2372	PreFCC HTR FEED, NEAT COAL FEED
B	F 9824	SLIGHTLY HYDROTREATED FEED	J	49J-46	LOW SEVERITY
C	F 9826	VERY SEVERE HYDROTREATED FEED	R*	49R	HIGHEST SEVERITY
D	F 9823	SEVERE HYDROTREATED FEED	C	49C-23	WORK PLAN HIGH SEVERITY
E	F 9821	AMOCO PETROLEUM FEED	CCFpet	FL-2312	PETR CAT CRK FEED
F	F9823/F9821	50:50 BLEND OF "D" AND "E"			
ASTM	F 9603	ASTM REFERENCE FEED			
	F- 9804	CONOCO EQUILIBRIUM CATALYST (ENGELHARD VEKTOR 50)			

Table 5-14 A – UNHYDROTREATED FEED

Run Number	790	786	802	810	814	805
Date (Mon-Day-Yr)	DEC-21-94	DEC-20-94	JAN-05-95	JAN-09-95	JAN-10-95	JAN-06-95
Catalyst F or AL Number	F-9804	F-9804	F-9804	F-9804	F-9804	F-9804
Catalyst Source	CONOCO	CONOCO	CONOCO	CONOCO	CONOCO	CONOCO
Catalyst Trade Name	Vektor 50	Vektor 50	Vektor 50	Vektor 50	Vektor 50	Vektor 50
Catalyst Activity	66	66	66	66	66	66
Oil Feed F# or AL#	F-9827	F-9827	F-9827	F-9827	F-9827	F-9827
Specific Gravity	0.919	0.919	0.919	0.919	0.919	0.919
Feed API	22.5	22.5	22.5	22.5	22.5	22.5
Feed 430 minus, wt%	0.0	0.0	0.0	0.0	0.0	0.0
Company supplying feedstock	SwRI	SwRI	SwRI	SwRI	SwRI	SwRI
Special Features	A-4.5	A-6	A-6	A-6	A-7.5	A-7.5
Catalyst Charge, grams	4.51	6.01	6.00	6.01	7.50	7.50
Feed Charge, grams	1.03	1.02	1.03	1.02	1.02	1.01
Catalyst/Oil Ratio	4.39	5.90	5.85	5.91	7.36	7.41
Initial Bed Temperature, deg F	998	995	999	999	999	999
Average Bed Temperature, deg F	987	970	980	975	980	975
Oil Inject Time, seconds	30	30	30	30	30	30
Conversion, Wt %	66.1	67.8	67.1	68.4	68.8	70.2
Kinetic Conversion	1.95	2.11	2.04	2.16	2.20	2.36
Weight % Yields, normalized: H_2S	0.01	0.00	0.00	0.01	0.03	0.01
H_2	0.15	0.33	0.19	0.18	0.24	0.25
CH_4	0.43	0.59	0.53	0.69	0.95	0.87
C_2H_2	0.00	0.00	0.00	0.00	0.00	0.00
C_2H_4	0.50	0.54	0.54	0.66	0.78	0.74
C_2H_6	0.38	0.49	0.45	0.55	0.72	0.67
C_3H_4	0.00	0.00	0.00	0.00	0.00	0.00
C_3H_6	3.48	3.56	3.29	3.96	3.97	3.75
C_3H_8	0.81	0.87	0.99	1.24	1.53	1.46
C_4H_6	0.00	0.00	0.00	0.00	0.00	0.00
1-C_4H_8	0.69	0.68	0.63	0.66	0.61	0.63
I-C_4H_8	0.41	0.39	0.34	0.39	0.38	0.38
c-2-C_4H_8	0.53	0.53	0.49	0.52	0.46	0.47
t-2-C_4H_8	0.73	0.74	0.67	0.71	0.65	0.67
I-C_4H_{10}	2.88	2.86	2.85	3.69	3.53	3.40
N-C_4H_{10}	1.02	1.03	1.06	1.15	1.18	1.20
C5-430 deg F	51.89	51.61	51.96	51.04	49.49	51.54
430-680 deg F	30.33	28.28	29.05	27.67	27.07	25.87
680-800 deg F	2.93	3.11	3.15	3.18	3.24	3.15
800 deg F+	0.62	0.80	0.72	0.77	0.90	0.77
COKE	2.20	3.60	3.07	2.95	4.28	4.17
Weight Balance, %	96.6	95.5	96.6	97.0	96.5	95.8
True Conversion, wt	66.1	67.8	67.1	68.4	68.8	70.2

M.W. Kellogg Activities

Table 5-15 B – SLIGHTLY HYDROTREATED FEED

Run Number	800	793	818	821
Date (Mon-Day-Yr)	DEC-28-94	DEC-27-94	JAN-11-95	JAN-12-95
Catalyst F or AL Number	F-9804	F-9804	F-9804	F-9804
Catalyst Source	CONOCO	CONOCO	CONOCO	CONOCO
Catalyst Trade Name	Vektor 50	Vektor 50	Vektor 50	Vektor 50
Catalyst Activity	66	66	66	66
Oil Feed F# or AL#	F-9824	F-9824	F-9824	F-9824
Specific Gravity	0.914	0.914	0.914	0.914
Feed API	23.3	23.3	23.3	23.3
Feed 430 minus, wt%	0.8	0.8	0.8	0.8
Company supplying feedstock	SwRI	SwRI	SwRI	SwRI
Special Features	B-4.5	B-6	B-6	B-7.5
Catalyst Charge, grams	4.50	6.00	6.00	7.50
Feed Charge, grams	1.03	1.02	0.99	1.01
Catalyst/Oil Ratio	4.36	5.89	6.05	7.45
Initial Bed Temperature, deg F	998	998	999	999
Average Bed Temperature, deg F	972	976	977	987
Oil Inject Time, seconds	30	30	30	30
Conversion, Wt %	67.2	69.2	69.4	68.8
Kinetic Conversion	2.05	2.25	2.27	2.21
Weight % Yields, normalized: H2S	0.00	0.01	0.00	0.01
H2	0.27	0.31	0.25	0.26
CH4	0.45	0.67	0.71	0.79
C2H2	0.00	0.00	0.00	0.00
C2H4	0.49	0.62	0.67	0.68
C2H6	0.36	0.51	0.57	0.63
C3H4	0.00	0.00	0.00	0.00
C3H6	3.69	3.82	4.03	3.71
C3H8	0.82	1.07	1.26	1.39
C4H6	0.00	0.00	0.00	0.00
1-C4H8	0.68	0.67	0.68	0.51
I-C4H8	0.40	0.40	0.40	0.28
c-2-C4H8	0.52	0.51	0.52	0.40
t-2-C4H8	0.72	0.70	0.72	0.55
I-C4H10	2.93	3.37	3.51	3.29
N-C4H10	0.96	1.10	1.16	1.01
C5-430 deg F	52.86	52.31	51.80	51.18
430-680 deg F	29.02	26.84	26.75	27.11
680-800 deg F	3.10	3.16	3.04	3.19
800 deg F+	0.71	0.79	0.78	0.86
COKE	2.02	3.14	3.15	4.13
Weight Balance, %	94.8	97.1	97.4	97.1
True Conversion, wt	66.9	69.0	69.2	68.6

Table 5-16 C – VERY SEVERE HYDROTREATED FEED

Run Number	803	794	788	811	807	815
Date (Mon-Day-Yr)	JAN-05-95	DEC-27-94	DEC-21-94	JAN-09-95	JAN-06-95	JAN-10-95
Catalyst F or AL Number	F-9804	F-9804	F-9804	F-9804	F-9804	F-9804
Catalyst Source	CONOCO	CONOCO	CONOCO	CONOCO	CONOCO	CONOCO
Catalyst Trade Name	Vektor 50	Vektor 50	Vektor 50	Vektor 50	Vektor 50	Vektor 50
Catalyst Activity	66	66	66	66	66	66
Oil Feed F# or AL#	F-9826	F-9826	F-9826	F-9826	F-9826	F-9826
Specific Gravity	0.867	0.867	0.867	0.867	0.867	0.867
Feed API	31.7	31.7	31.7	31.7	31.7	31.7
Feed 430 minus, wt%	7.6	7.6	7.6	7.6	7.6	7.6
Company supplying feedstock	SwRI	SwRI	SwRI	SwRI	SwRI	SwRI
Special Features	C-3	C-4.5	C-6	C-3	C-4.5	C4.5
Catalyst Charge, grams	3.01	4.51	6.01	3.00	4.51	4.51
Feed Charge, grams	0.98	1.01	0.97	1.00	1.00	1.01
Catalyst/Oil Ratio	3.06	4.48	6.17	3.01	4.51	4.46
Initial Bed Temperature, deg F	1005	998	995	999	999	999
Average Bed Temperature, deg F	975	973	974	980	978	981
Oil Inject Time, seconds	30	30	30	30	30	30
Conversion, Wt %	73.9	76.9	78.9	74.5	77.3	77.9
Kinetic Conversion	2.83	3.32	3.75	2.92	3.41	3.53
Weight % Yields, normalized: H2S	0.00	0.01	0.01	0.00	0.01	0.01
H2	0.11	0.18	0.21	0.11	0.13	0.15
CH4	0.29	0.43	0.50	0.29	0.41	0.46
C2H2	0.00	0.00	0.00	0.00	0.00	0.00
C2H4	0.42	0.56	0.59	0.44	0.54	0.58
C2H6	0.23	0.34	0.39	0.24	0.31	0.36
C3H4	0.00	0.00	0.00	0.00	0.00	0.00
C3H6	3.49	4.13	3.89	3.53	4.06	4.05
C3H8	0.66	1.03	1.22	0.67	1.07	1.06
C4H6	0.00	0.00	0.00	0.00	0.00	0.00
1-C4H8	0.77	0.69	0.78	0.76	0.73	0.79
I-C4H8	0.57	0.43	0.46	0.55	0.45	0.48
c-2-C4H8	0.60	0.53	0.60	0.57	0.59	0.57
t-2-C4H8	0.82	0.73	0.82	0.79	0.81	0.81
I-C4H10	3.06	3.63	4.00	2.87	4.29	3.83
N-C4H10	1.13	1.10	1.41	1.12	1.23	1.27
C5-430 deg F	60.87	61.38	61.92	61.58	60.94	61.91
430-680 deg F	23.84	20.59	18.73	23.31	20.40	19.66
680-800 deg F	2.27	2.00	2.33	2.21	2.29	2.39
800 deg F+	0.00	0.55	0.00	0.00	0.00	0.00
COKE	0.88	1.71	2.13	0.96	1.76	1.60
Weight Balance, %	95.9	95.3	95.7	96.1	96.1	95.1
True Conversion, wt	71.7	75.0	77.2	72.4	75.4	76.1

Table 5-17 D – SEVERELY HYDROTREATED FEED

Run Number	789	797	819	822
Date (Mon-Day-Yr)	DEC-21-94	DEC-27-94	JAN-11-95	JAN-12-95
Catalyst F or AL Number	F-9804	F-9804	F-9804	F-9804
Catalyst Source	CONOCO	CONOCO	CONOCO	CONOCO
Catalyst Trade Name	Vektor 50	Vektor 50	Vektor 50	Vektor 50
Catalyst Activity	66	66	66	66
Oil Feed F# or AL#	F-9823	F-9823	F-9823	F-9823
Specific Gravity	0.909	0.909	0.909	0.909
Feed API	24.2	24.2	24.2	24.2
Feed 430 minus, wt%	1.8	1.8	1.8	1.8
Company supplying feedstock	SwRI	SwRI	SwRI	SwRI
Special Features	D-3	D-4.5	D-4.5	D-6
Catalyst Charge, grams	3.00	4.50	4.50	6.00
Feed Charge, grams	1.03	1.01	1.02	0.99
Catalyst/Oil Ratio	2.92	4.47	4.43	6.04
Initial Bed Temperature, deg F	995	998	999	999
Average Bed Temperature, deg F	975	978	978	978
Oil Inject Time, seconds	30	30	30	30
Conversion, Wt %	68.5	70.0	71.2	71.5
Kinetic Conversion	2.17	2.33	2.47	2.51
Weight % Yields, normalized: H2S	0.00	0.01	0.01	0.01
H2	0.12	0.25	0.20	0.26
CH4	0.28	0.48	0.53	0.70
C2H2	0.00	0.00	0.00	0.00
C2H4	0.39	0.55	0.58	0.66
C2H6	0.24	0.38	0.41	0.53
C3H4	0.00	0.00	0.00	0.00
C3H6	3.54	3.77	3.82	3.64
C3H8	0.63	0.85	0.96	1.22
C4H6	0.00	0.00	0.00	0.00
1-C4H8	0.65	0.67	0.78	0.60
I-C4H8	0.42	0.41	0.50	0.35
c-2-C4H8	0.52	0.52	0.57	0.45
t-2-C4H8	0.70	0.71	0.80	0.63
I-C4H10	2.82	2.88	3.12	3.19
N-C4H10	0.82	1.00	1.21	1.10
C5-430 deg F	56.20	55.19	55.48	54.89
430-680 deg F	28.42	26.36	25.33	24.72
680-800 deg F	3.10	2.92	2.77	2.89
800 deg F+	0.00	0.75	0.72	0.90
COKE	1.15	2.28	2.23	3.26
Weight Balance, %	94.6	94.8	98.4	95.9
True Conversion, wt	67.9	69.4	70.7	71.0

Table 5-18 E – AMOCO TYPICAL REFINERY GAS OIL

Run Number	787	792	804	812	808	816
Date (Mon-Day-Yr)	DEC-21-94	DEC-27-94	JAN-05-95	JAN-09-95	JAN-09-95	JAN-10-95
Catalyst F or AL Number	F-9804	F-9804	F-9804	F-9804	F-9804	F-9804
Catalyst Source	CONOCO	CONOCO	CONOCO	CONOCO	CONOCO	CONOCO
Catalyst Trade Name	Vektor 50	Vektor 50	Vektor 50	Vektor 50	Vektor 50	Vektor 50
Catalyst Activity	66	66	66	66	66	66
Oil Feed F# or AL#	F-9821	F-9821	F-9821	F-9821	F-9821	F-9821
Specific Gravity	0.896	0.896	0.896	0.896	0.896	0.896
Feed API	26.4	26.4	26.4	26.4	26.4	26.4
Feed 430 minus, wt%	3.1	3.1	3.1	3.1	3.1	3.1
Company supplying feedstock	AMOCO	AMOCO	AMOCO	AMOCO	AMOCO	AMOCO
Special Features	E-3	E-4.5	E-4.5	E-4.5	E-6	E-6
Catalyst Charge, grams	3.01	4.50	4.50	4.50	6.00	6.00
Feed Charge, grams	0.99	1.00	1.00	1.00	1.00	0.99
Catalyst/Oil Ratio	3.04	4.51	4.51	4.52	5.98	6.07
Initial Bed Temperature, deg F	995	998	999	999	999	999
Average Bed Temperature, deg F	980	982	982	989	982	983
Oil Inject Time, seconds	30	30	30	30	30	30
Conversion, Wt %	64.5	69.7	70.4	67.6	72.5	73.8
Kinetic Conversion	1.82	2.30	2.37	2.08	2.64	2.82
Weight % Yields, normalized: H2S	0.37	0.49	0.43	0.50	0.49	0.54
H2	0.12	0.15	0.15	0.14	0.17	0.20
CH4	0.53	0.72	0.88	0.79	0.90	1.11
C2H2	0.00	0.00	0.00	0.00	0.00	0.00
C2H4	0.52	0.68	0.76	0.70	0.76	0.90
C2H6	0.45	0.59	0.68	0.63	0.71	0.87
C3H4	0.00	0.00	0.00	0.00	0.00	0.00
C3H6	4.08	4.94	5.16	4.67	4.79	5.60
C3H8	0.52	0.83	0.92	0.83	1.05	1.26
C4H6	0.00	0.00	0.00	0.00	0.00	0.00
1-C4H8	0.78	0.88	0.95	0.82	0.81	0.95
I-C4H8	1.29	1.16	1.26	1.14	0.90	1.05
c-2-C4H8	0.63	0.72	0.77	0.65	0.64	0.81
t-2-C4H8	0.86	0.99	1.05	0.89	0.89	1.10
I-C4H10	2.52	3.67	3.81	3.21	3.68	4.75
N-C4H10	0.83	1.02	1.09	1.01	1.13	1.15
C5-430 deg F	49.07	50.02	49.43	48.52	51.04	49.08
430-680 deg F	28.62	24.72	23.73	25.80	22.61	21.13
680-800 deg F	5.03	4.08	4.19	4.81	3.57	3.53
800 deg F+	1.82	1.50	1.72	1.82	1.30	1.50
COKE	1.97	2.85	3.02	3.05	4.57	4.45
Weight Balance, %	95.4	97.5	95.3	96.3	96.3	96.0
True Conversion, wt	63.4	68.7	69.4	66.5	71.6	73.0

Table 5-19 F – BLEND OF D AND E

Run Number	796	798	820	824
Date (Mon-Day-Yr)	DEC-27-94	DEC-27-94	JAN-12-95	JAN-13-95
Catalyst F or AL Number	F-9804	F-9804	F-9804	F-9804
Catalyst Source	CONOCO	CONOCO	CONOCO	CONOCO
Catalyst Trade Name	Vektor 50	Vektor 50	Vektor 50	Vektor 50
Catalyst Activity	66	66	66	66
Oil Feed F# or AL#	F-9823/F-9821	F-9821/F-9823	F-9821/F-9823	F-9821/F-9823
Specific Gravity	0.902	0.902	0.902	0.902
Feed API	25.4	25.4	25.4	25.4
Feed 430 minus, wt%	2.5	2.5	2.5	2.5
Company supplying feedstock	NA	NA	NA	NA
Special Features	F-3	F-4.5	F-4.5	F-6
Catalyst Charge, grams	3.01	4.50	4.50	6.00
Feed Charge, grams	1.01	0.99	1.00	1.01
Catalyst/Oil Ratio	2.97	4.53	4.49	5.93
Initial Bed Temperature, deg F	998	998	999	999
Average Bed Temperature, deg F	977	975	986	975
Oil Inject Time, seconds	30	30	30	30
Conversion, Wt %	67.1	70.0	70.3	73.6
Kinetic Conversion	2.04	2.33	2.37	2.79
Weight % Yields, normalized: H2S	0.24	0.29	0.26	0.27
H2	0.11	0.16	0.19	0.22
CH4	0.42	0.58	0.81	0.88
C2H2	0.00	0.00	0.00	0.00
C2H4	0.48	0.61	0.74	0.75
C2H6	0.36	0.48	0.64	0.70
C3H4	0.00	0.00	0.00	0.00
C3H6	3.89	4.35	4.87	4.57
C3H8	0.57	0.86	1.09	1.24
C4H6	0.00	0.00	0.00	0.00
1-C4H8	0.77	0.74	0.88	0.84
I-C4H8	0.74	0.61	0.73	0.63
c-2-C4H8	0.59	0.56	0.73	0.65
t-2-C4H8	0.81	0.78	0.98	0.89
I-C4H10	2.71	3.28	4.27	3.97
N-C4H10	0.95	0.97	1.12	1.31
C5-430 deg F	52.66	53.55	50.47	52.83
430-680 deg F	28.63	25.64	25.06	22.46
680-800 deg F	3.29	3.33	3.43	3.08
800 deg F+	1.01	1.05	1.17	0.83
COKE	1.77	2.17	2.56	3.88
Weight Balance, %	96.0	96.3	96.4	95.8
True Conversion, wt	66.2	69.2	69.6	73.0

Table 5-20 ASTM REFERENCE FEED

Run Number	806	813	809	817
Date (Mon-Day-Yr)	JAN-06-95	JAN-10-95	JAN-09-95	JAN-10-95
Catalyst F or AL Number	F-9804	F-9804	F-9804	F-9804
Catalyst Source	CONOCO	CONOCO	CONOCO	NA
Catalyst Trade Name	Vektor 50	Vektor 50	Vektor 50	NA
Catalyst Activity	66	66	66	NA
Oil Feed F# or AL#	F-9603	F-9603	F-9603	F-9603
Specific Gravity	0.889	0.889	0.889	0.889
Feed API	27.6	27.6	27.6	27.6
Feed 430 minus, wt%	2.0	2.0	2.0	2.0
Company supplying feedstock	ASTM	ASTM	ASTM	ASTM
Special Features	ASTMGO-3	ASTMGO-3	ASTMGO-6	ASTMGO-6
Catalyst Charge, grams	3.00	3.00	6.00	6.00
Feed Charge, grams	0.98	1.00	0.97	1.01
Catalyst/Oil Ratio	3.05	2.99	6.19	5.94
Initial Bed Temperature, deg F	999	999	999	999
Average Bed Temperature, deg F	980	985	980	985
Oil Inject Time, seconds	30	30	30	30
Conversion, Wt %	62.6	64.9	75.6	75.7
Kinetic Conversion	1.68	1.85	3.10	3.12
Weight % Yields, normalized: H2S	0.19	0.19	0.26	0.27
H2	0.10	0.11	0.19	0.19
CH4	0.55	0.66	1.17	1.25
C2H2	0.00	0.00	0.00	0.00
C2H4	0.51	0.62	0.93	1.00
C2H6	0.45	0.55	0.89	0.94
C3H4	0.00	0.00	0.00	0.00
C3H6	4.08	4.33	5.85	6.43
C3H8	0.55	0.59	1.25	1.35
C4H6	0.00	0.00	0.00	0.00
1-C4H8	0.77	0.80	0.89	0.98
I-C4H8	1.33	1.40	1.12	1.26
c-2-C4H8	0.64	0.65	0.70	0.76
t-2-C4H8	0.87	0.89	0.97	1.05
I-C4H10	2.58	2.59	4.26	4.63
N-C4H10	0.85	0.90	1.10	1.14
C5-430 deg F	47.21	48.43	51.73	49.73
430-680 deg F	26.75	26.09	19.25	18.98
680-800 deg F	7.39	6.26	3.52	3.49
800 deg F+	3.23	2.75	1.64	1.79
COKE	1.97	2.17	4.28	4.75
Weight Balance, %	95.6	97.2	95.4	94.8
True Conversion, wt	61.9	64.2	75.1	75.2

Table 5-21 HEAT BALANCE CALCULATIONS FOR PETROLEUM FEED

AMOCO "E" PETROL. FD. / CONOCO CATALYST		
ITEM	UNITS	VALUE
TOTAL COKE YIELD	WT %	5.2
(COKE=0.88*CAT/OIL-0.87)		
CONVERSION	WT %	74.3
(CONV=100-56.5/(CAT/OIL)^0.41)		
CATALYST TO OIL RATIO		6.8
COKE ON CATALYST	WT %	0.75
RISER OUTLET TEMPERATURE	F	980.0
HEAT OF CRACKING	BTU/#FEED	183
FEED API	API DEG.	26.4
FEED RATE	BBL/DAY	100000.0
FEED RATE	#/HR	1,308,727
FEED PREHEAT TEMPERATURE	F	500.0
WATER IN WET AIR	MOL %	3.0
FLUE GAS CO_2/CO RATIO	MOL/MOL	1000.0
DELTA T DUE TO AFTERBURN	F	0.0
CATALYST CIRCULATION RATE	10^6#/HR	8.95
REACTOR HEAT LOSS	10^6 BTU/HR	15.94
CHANGE IN FEED ENTHALPY	BTU/#FEED	424
REGENERATED CAT TEMP.	F	1,263
TOTAL COKE BURNED	#/HR	67,499
C TO CO	#/HR	63
C TO CO_2	#/HR	63,116
H TO H_2O	#/HR	4,050
S TO SO_2	#/HR	270
MOLE % O_2 IN DRY FLUE GAS	%	1.0
BLOWER DISCHARGE TEMP	F	355
EXCESS AIR FACTOR		0.0105
WET AIR USED	#/HR	929,687
FLUE GAS	#/HR	997,186
HEAT OF COMBUSTION	10^6 BTU/HR	1034.8
HEAT LOSS	10^6 BTU/HR	41.4
NET HEAT TO CATALYST	10^6 BTU/HR	720.5
NET HEAT TO FLUE GAS	10^6 BTU/HR	272.9
HEAT REMOVED AS STEAM	10^6 BTU/HR	0.0

Table 5-22 HEAT BALANCE CALCULATIONS FOR BLEND

F" = BLEND OF "D" AND "E" / CONOCO CAT		
ITEM	UNITS	VALUE
TOTAL COKE YIELD	WT %	5.1
(COKE=0.71*CAT/OIL-0.56)		
CONVERSION	WT %	75.5
CONV=100-46.8/(CAT/OIL)^0.31		
CATALYST TO OIL RATIO		8.0
COKE ON CATALYST	WT %	0.64
RISER OUTLET TEMPERATURE	F	980.0
HEAT OF CRACKING	BTU/#FEED	184
FEED API	API DEG.	25.4
FEED RATE	BBL/DAY	100000.0
FEED RATE	#/HR	1,317,068
FEED PREHEAT TEMPERATURE	F	500.0
WATER IN WET AIR	MOL %	3.0
FLUE GAS CO_2/CO RATIO	MOL/MOL	1000.0
DELTA T DUE TO AFTERBURN	F	0.0
CATALYST CIRCULATION RATE	10^6#/HR	10.57
REACTOR HEAT LOSS	10^6 BTU/HR	18.83
CHANGE IN FEED ENTHALPY	BTU/#FEED	423
REGENERATED CAT TEMP.	F	1,222
TOTAL COKE BURNED	#/HR	67,194
C TO CO	#/HR	63
C TO CO_2	#/HR	62,830
H TO H_2O	#/HR	4,032
S TO SO_2	#/HR	269
MOLE % O_2 IN DRY FLUE GAS	%	1.0
BLOWER DISCHARGE TEMP	F	355
EXCESS AIR FACTOR		0.0105
WET AIR USED	#/HR	925,480
FLUE GAS	#/HR	992,673
HEAT OF COMBUSTION	10^6 BTU/HR	1030.1
HEAT LOSS	10^6 BTU/HR	41.2
NET HEAT TO CATALYST	10^6 BTU/HR	728.7
NET HEAT TO FLUE GAS	10^6 BTU/HR	260.2
HEAT REMOVED AS STEAM	10^6 BTU/HR	0.0

Table 5-23 HEAT BALANCE CALCULATIONS FOR BLEND AND TORCH OIL

F" = BLEND OF "D" AND "E" / CONOCO CAT		
ITEM	UNITS	VALUE
TOTAL COKE YIELD	WT %	4.2
(COKE=0.7O6*CAT/OIL-0.564)		
CONVERSION	WT %	74.2
CONV=100-46.8/(CAT/OIL)^0.31		
CATALYST TO OIL RATIO		6.8
COKE ON CATALYST	WT %	0.62
RISER OUTLET TEMPERATURE	F	980.0
HEAT OF CRACKING	BTU/#FEED	183
FEED API	API DEG.	25.4
FEED RATE	BBL/DAY	100000.0
FEED RATE	#/HR	1,317,068
FEED PREHEAT TEMPERATURE	F	500.0
WATER IN WET AIR	MOL %	3.0
FLUE GAS CO_2/CO RATIO	MOL/MOL	1000.0
DELTA T DUE TO AFTERBURN	F	0.0
CATALYST CIRCULATION RATE	10^6#/HR	8.96
REACTOR HEAT LOSS	10^6 BTU/HR	15.95
CHANGE IN FEED ENTHALPY	BTU/#FEED	423
REGENERATED CAT TEMP.	F	1,270
TOTAL COKE BURNED	#/HR	55,802
C TO CO	#/HR	52
C TO CO_2	#/HR	52,178
H TO H_2O	#/HR	3,348
S TO SO_2	#/HR	223
MOLE % O_2 IN DRY FLUE GAS	%	1.0
BLOWER DISCHARGE TEMP	F	355
EXCESS AIR FACTOR		0.0105
WET AIR USED	#/HR	768,574
FLUE GAS	#/HR	824,376
HEAT OF COMBUSTION	10^6 BTU/HR	855.4
HEAT LOSS	10^6 BTU/HR	34.2
NET HEAT TO CATALYST	10^6 BTU/HR	739.7
NET HEAT TO FLUE GAS	10^6 BTU/HR	227.3
HEAT REMOVED AS STEAM	10^6 BTU/HR	0.0
HEAT ADDED TO REGENERATOR	10^6 BTU/HR	145.7
HEAT ADDED	BTU/# FEED	111

Table 5-24 PILOT PLANT OPERATING CONDITIONS

FEEDSTOCK: F-	**9819**	**9820**	**9819/9820**
CATALYST: F-9804			
RUN NUMBER: F-2006-	**1**	**2**	**3**
OIL FEED RATE , GRAM/HR	1794	1808	1814
CATALYST RATE , LB/HR	48.1	48.6	48.0
CATALYST/OIL RATIO	12.2	12.2	12.0
MATERIAL BALANCE:			
CLOSURE, WT%	98.50	98.49	98.46
GASOLINE, WT%	50.52	55.17	51.01
CONVERSION, WT%	74.13	74.20	73.18
COKE YIELD, WT%	4.90	3.27	4.32
SELECTIVITY, W/W	0.68	0.74	0.70
C/(1-C), W/W	2.87	2.88	2.73
RISER OUTLET PRESSURE , PSIG	35.0	35.0	35.0
TEMPERATURES, DEG F:			
OIL PREHEAT	212	212	214
CATALYST INLET	1265	1253	1252
RISER PROFILE, FT			
0.58 (MIXING ZONE)	983	985	982
5.47	983	986	982
9.22	978	982	978
17.1	988	992	988
19.18	981	985	981
22.87	989	993	989
26.12	991	995	990
28.13	976	981	977
RISER AVERAGE	984	987	983

Table 5-25 PILOT PLANT YIELDS

PRODUCT YIELD SPECTRUM NORMALIZED, BASIS FRESH FEED, WT %				
FEEDSTOCK: F-	**9819**	**9820**	**9819/9820**	**WEIGHTED AVERAGE (CALC'D)**
CATALYST: F-9804				
RUN NUMBER: H-2006-	**1**	**2**	**3**	
H2S	0.00	0.00	0.00	0.00
H2	0.14	0.16	0.16	0.15
CH4	1.29	0.73	1.07	1.10
C2H4	0.76	0.51	0.65	0.68
C2H6	1.15	0.63	0.95	0.98
C3H6	5.04	4.10	4.71	4.73
C3H8	0.95	1.08	0.98	0.99
C4H6	0.02	0.02	0.02	0.02
1-C4H8	0.72	0.62	0.70	0.69
I-C4H8	1.82	0.64	1.36	1.43
T-2-C4H8	1.43	1.08	1.35	1.31
C-2-C4H8	1.06	0.82	0.98	0.98
IC4H10	2.86	3.32	3.24	3.01
NC4H10	1.47	2.05	1.68	1.66
C5+ IN GAS	4.79	4.12	4.49	4.57
IBP-430 F	45.73	51.05	46.52	47.50
430-650 F	19.75	22.65	21.77	20.72
650+ F	6.12	3.15	5.05	5.13
COKE	4.90	3.27	4.32	4.36
TOTAL	100.00	100.00	100.00	100.00
SUMMARY				
TOTAL C2 & LIGHTER	3.34	2.03	2.83	2.90
TOTAL C3'S	5.99	5.18	5.69	5.72
TOTAL C4'S	9.38	8.55	9.33	9.10
TOTAL GASOLINE	50.52	55.17	51.01	52.07
TOTAL CYCLE OIL	25.87	25.80	26.82	25.85
COKE	4.90	3.27	4.32	4.36
CONVERSION	74.13	74.20	73.18	74.15

TABLE 5-26 PIANO ANALYSIS

FEED	A	B	C	D	E	F	ASTM
Paraffins	4.23	3.91	4.72	3.92	5.67	5.50	4.11
Iso-paraffins	37.50	36.22	38.78	37.95	41.34	42.18	34.79
Naphthenes	19.76	19.09	21.60	19.59	9.08	13.06	10.45
Aromatics	30.71	32.62	27.24	31.76	27.88	26.78	43.32
Olefins	6.89	6.79	6.20	5.41	12.74	10.19	3.73
Unknowns	0.91	1.37	1.46	1.37	3.29	2.29	3.60

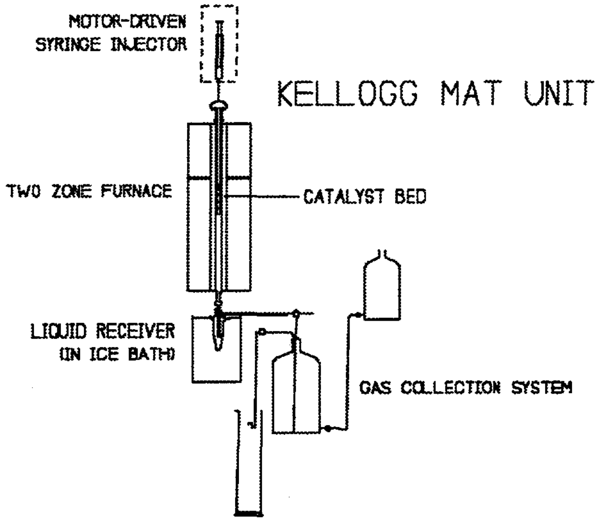


Figure 5-1 MAT Unit Schematic

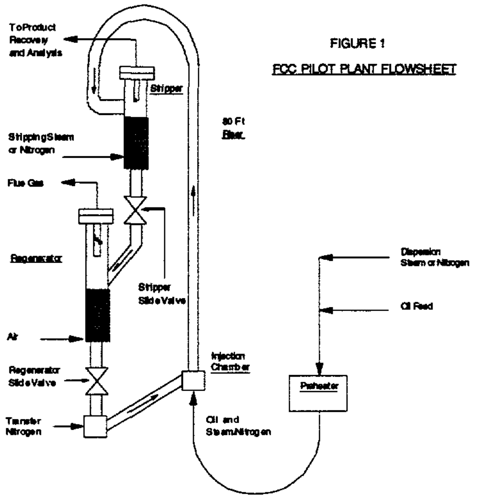


Figure 5-2 Pilot Plant Schematic

M.W. Kellogg Activities

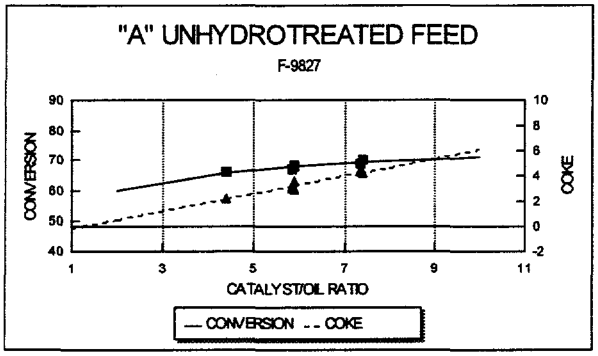


Figure 5-3 Unhydrotreated Feed

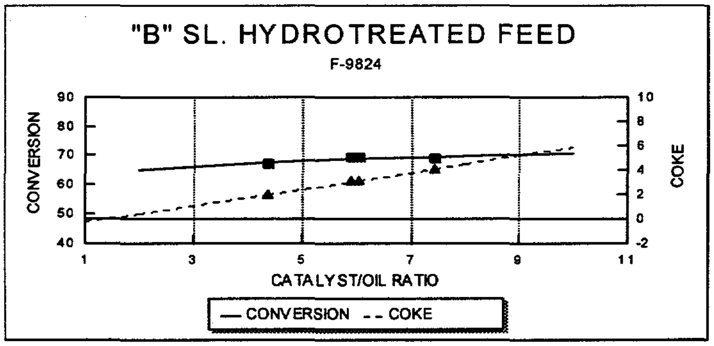


Figure 5-4 Slightly Hydrotreated Feed

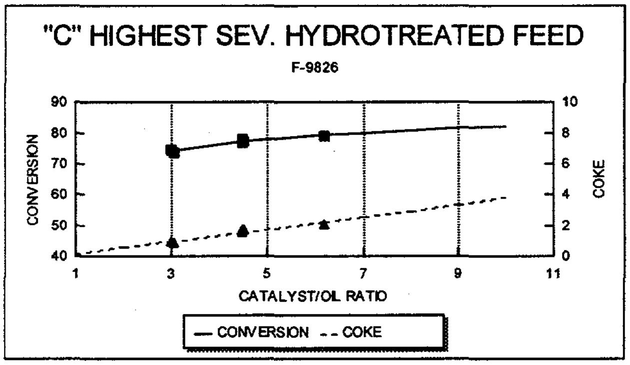


Figure 5-5 Highest Severity Hydrotreating

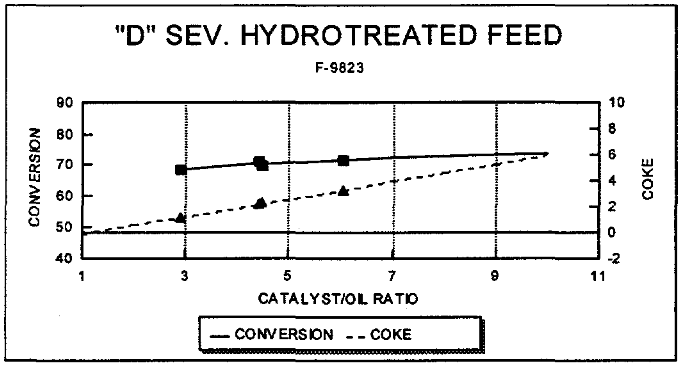


Figure 5-6 Work Plan High Severity

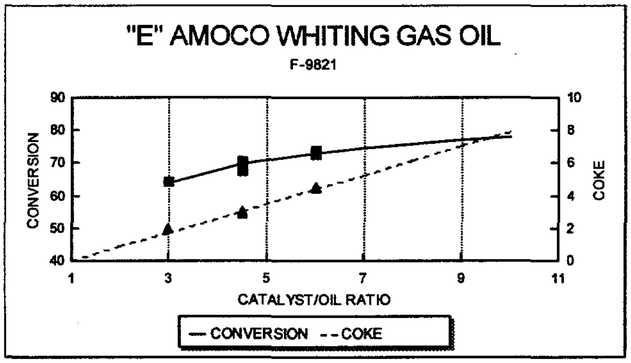


Figure 5-7 Petroleum Base Gas Oil

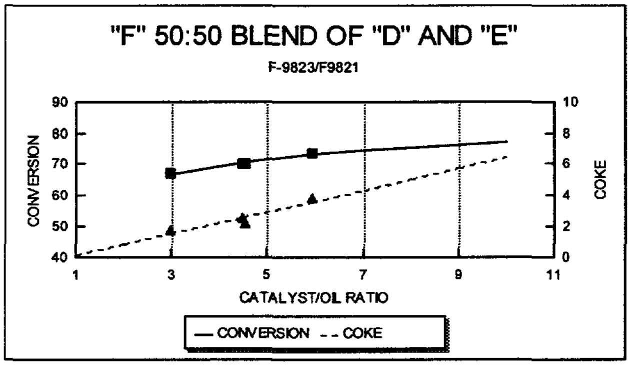


Figure 5-8 Petroleum + HT Coal Liquid Blend

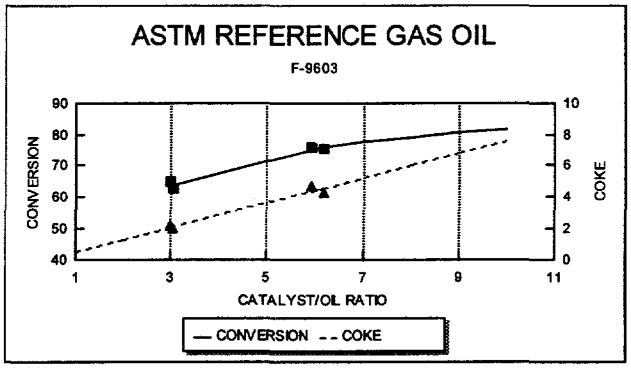


Figure 5-9 Reference Petroleum Feed

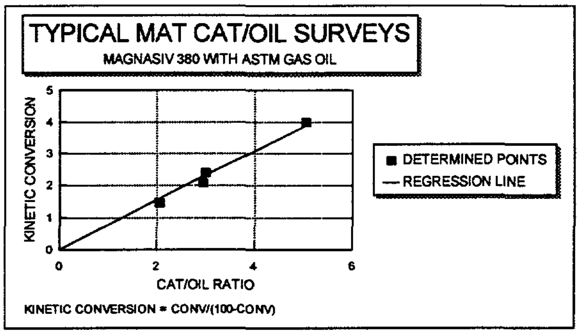


Figure 5-10 Reference Feed with Catalyst "A"

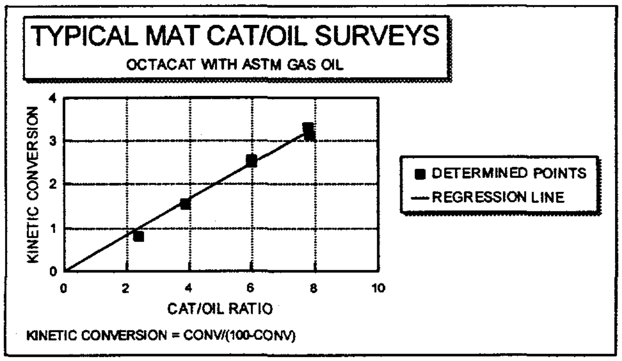


Figure 5-11 Reference Feed with Catalyst "B"

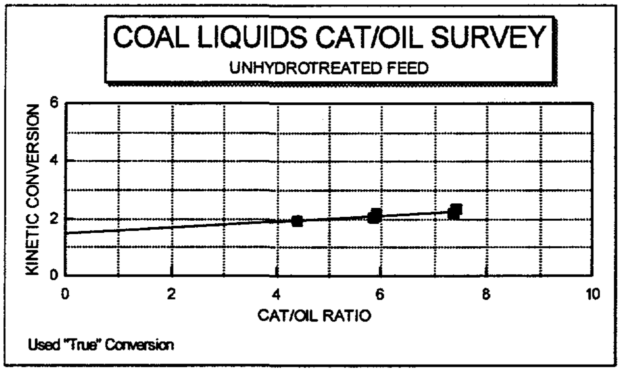


Figure 5-12 Coal Feed Before Hydrotreating

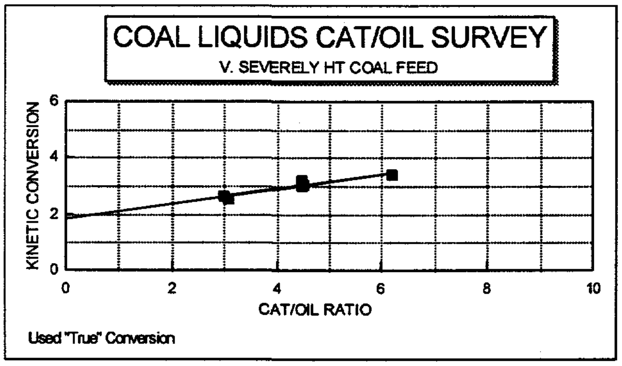


Figure 5-13 Coal Feed After Hydrotreating

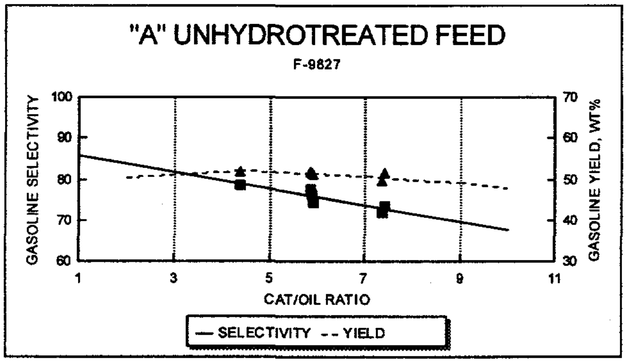


Figure 5-14 Feed “A” Gasoline

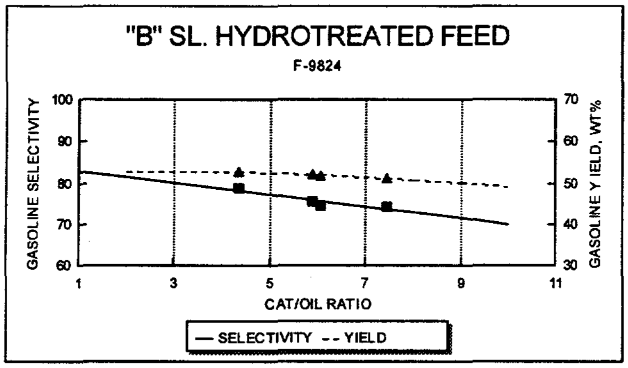


Figure 5-15 Feed "B" Gasoline

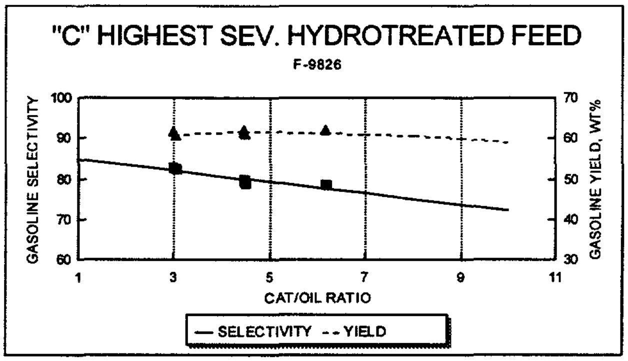


Figure 5-16 Feed "C" Gasoline

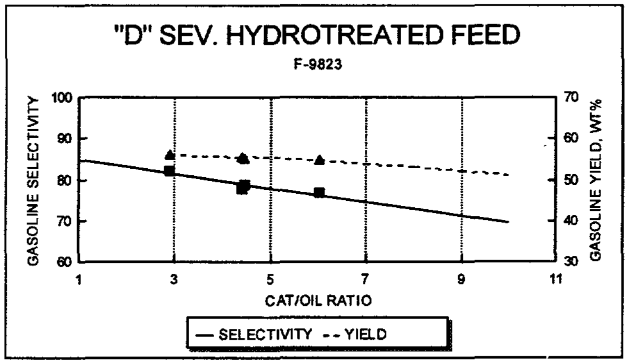


Figure 5-17 Feed "D" Gasoline

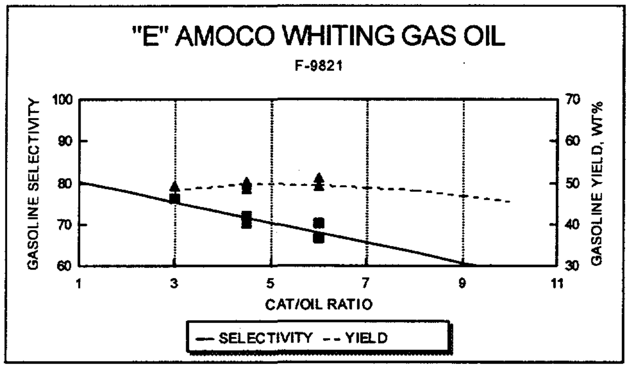


Figure 5-18 Feed "E" Gasoline

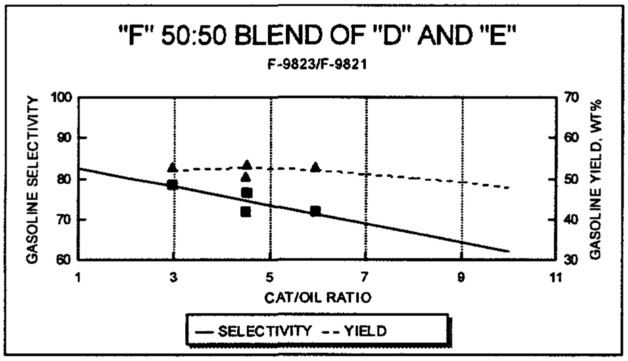


Figure 5-19 Feed "F" Gasoline

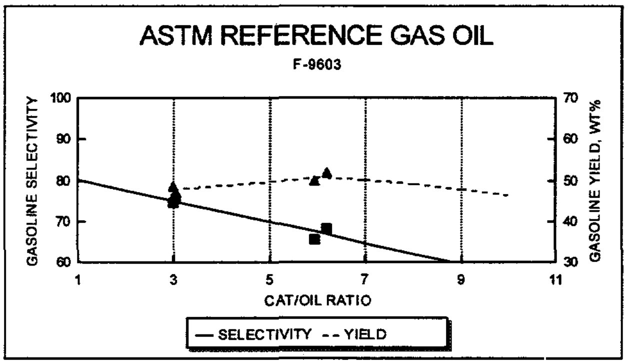


Figure 5-20 ASTM Feed Gasoline

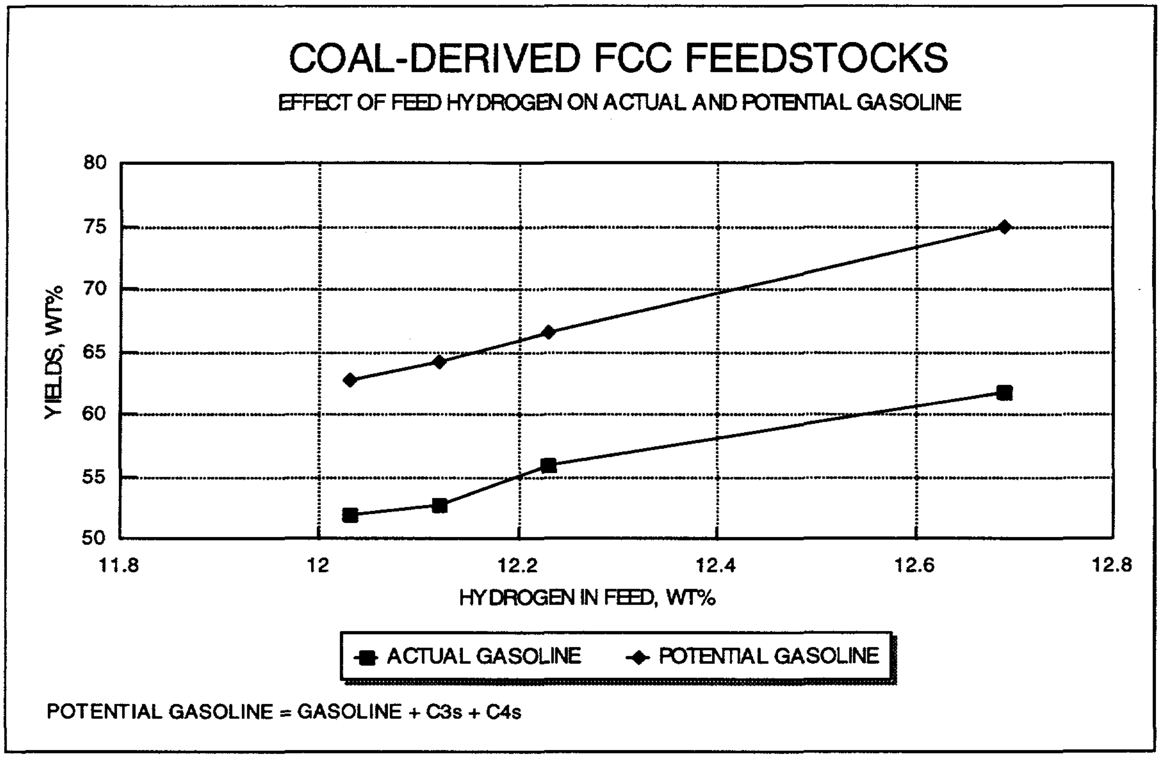


Figure 5-21 Actual and Potential Gasoline versus Feed Hydrogen

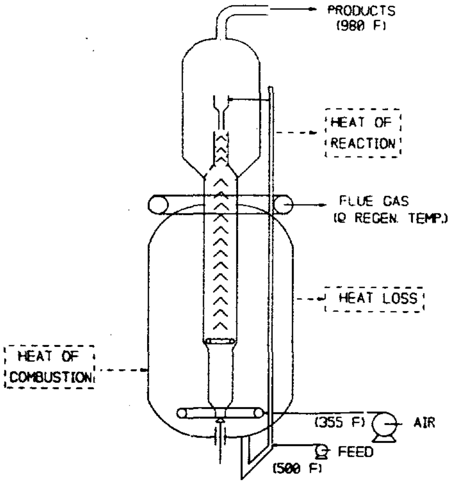


Figure 5-22 FCCU Heat Balance

Section 6

Project Management

6.1 Plans

6.2 Reports and Schedules

The milestone schedule and status for the Basic Program and Option 1 is shown in Figure 6-1.

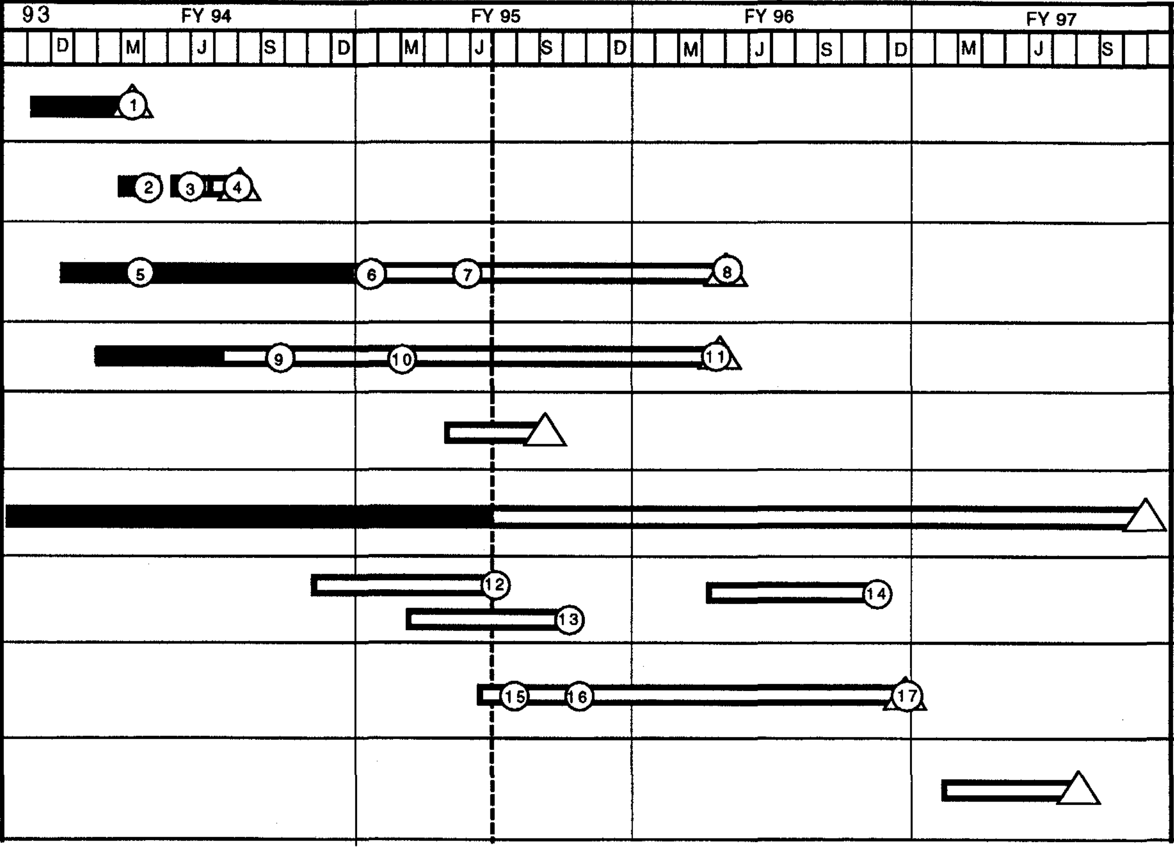
DOE F1332.3
(11.84)

Figure 6-1
Milestone Schedule for Basic Program & Option 1

☐ PLAN ■ STATUS REPORT

FORM APPROVED
OMB NO 1901.1400

1. TITLE Refining and End Use Study of Coal Liquids	2. REPORTING PERIOD 3/26/95 to 6/30/95	3. IDENTIFICATION NUMBER DE-RP22-93PC91029
4. PARTICIPANT NAME AND ADDRESS Bechtel Corporation 50 Beale Street San Francisco, CA 94105		5. START DATE 11/1/93 6. COMPLETION DATE 9/30/97



7. ELEMENT CODE	8. REPORTING ELEMENT	10. PERCENT COMPLETE a. Plan	10. PERCENT COMPLETE b. Actual
Task 1	Project Work Plan	100	100
Task 2	Feed Characterization	100	39
Task 3	Linear Programming (LP) Analysis	84	70
Task 4	Pilot Plant Analysis	72	23
Task 5	Option 1 Work Plan	0	0
Task 6	Administration Task	42	42
Option I Task 1	Pilot Plant Analysis (Produce Fuels)	31	0
Option 1 Task 2	Characterization, Blending, and Testing	0	0
Option 1 Task 3	Economic Study	0	0

1 Submit final Project Work Plan
2 Characterize DL1 liquid
3 Characterize IL liquid
4 Characterize DL2 liquid
5 Develop LP model
6 Conduct final DL1 LP runs
7 Conduct final IL LP runs
8 Conduct final DL2 runs
9 Conduct DL1 pilot plant tests
10 Conduct IL pilot plant tests
11 Conduct DL2 pilot plant tests
12 Production runs for DL1
13 Production runs for IL
14 Production runs for DL2
15 ASTM tests for DL1
16 ASTM tests for IL
17 ASTM tests for DL2

11. SIGNATURE OF PARTICIPANT'S PROJECT MANAGER AND DATE

7/25/95